Solid Spectroscopy Data Model (SSDM) of the SSHADE database infrastructure

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Abstract: The "Solid Spectroscopy Data Model" (SSDM) is a relational data model allowing a complete description of spectral data of solid materials. It includes a detailed description of the solid samples through their layers, materials, constituents and species. Natural matters have their specific description. The instruments and techniques used for the measurements are also described. The spectral data are of two types: spectra and their various higher levels products (instrument specific) and band lists (band parameters and transition attributions). Publications associated with the spectral data are also included in this data model. SSDM is the base of the SSHADE database infrastructure of spectroscopy of solids.

Version History

Version	Date	Modified By	Description of Change
v0.1	25/02/09	Bernard Schmitt	Initial draft version of Ghosst DataModel
v0.2	26/06/09	Bernard Schmitt	Initial version of SSDM DataModel
v0.3.0	16/02/10	Bernard Schmitt	Draft implementation of SSDM expert working group recommendations
v0.3.1	26/06/10	Bernard Schmitt	Many changes ... Reorganisation and renaming of keywords.
v0.3.2a	06/09/10	Bernard Schmitt	Many changes. Large reorganisation of tables and keywords.
v0.3.2b	09/09/10	Bernard Schmitt	Several fundamental changes
v0.3.2c	05/10/10	Bernard Schmitt	Many changes ... Reorganisation of tables during implementation.
v0.3.2d	17/11/10	Bernard Schmitt	Many changes ... Reorganisation of tables during implementation.
v0.3.2e	04/03/11	Bernard Schmitt	Changes in Band list, molecules, atoms.
v0.3.3	27/03/11	Bernard Schmitt	Changes in general description, molecules, atoms, sample/layers/materials/constituents: stable version for these parts
v0.3.3a	03/04/11	Bernard Schmitt	Few small changes
v0.3.3b	06/04/11	Bernard Schmitt	Few small changes in layer and spectra tables
v0.3.3c	12/04/11	Bernard Schmitt	Few small changes in sample tables
v0.3.3d	19/04/11	Bernard Schmitt	Major changes in Instruments, + some minors
v0.3.3e	25/04/11	Bernard Schmitt	Major changes in Instruments and experiment.
v0.3.3f	29/04/11	Bernard Schmitt	Splitting Instruments table in two.
v0.3.3g	01/05/11	Bernard Schmitt	DM meteorite object and extraterrestrial matter (draft)
v0.3.3h	23/05/11	Bernard Schmitt	Major changes in spectra, spectra files and spectrum bands
v0.3.3i	30/05/11	Bernard Schmitt	Minor changes in Instruments
v0.3.4	15/06/11	Bernard Schmitt	Major changes in meteorites and in general and detailed documentation
v0.3.4a	23/06/11	Bernard Schmitt	Major changes in enumeration lists
v0.3.4b	11/07/11	Bernard Schmitt	Medium addition and change of keywords and enumerations in Sample (+ a few others)
v0.3.4c	28/11/11	Bernard Schmitt	Major changes in Mineral species and mineral matters. Other minor changes everywhere
v0.3.4d	02/02/12	Bernard Schmitt	Major changes in Mineral species, mineral matters and Publications
v0.3.5b	06/03/12	Bernard Schmitt	Changes in molecules, atoms, minerals and mineral matters. Major changes in Band list. Creation of Band and States tables
v0.3.6a	26/03/12	Bernard Schmitt	Creation of ‘chemical functions table’ + minor changes. Finalisation of Atoms, Molecules species
v0.3.6b	26/03/12	Bernard Schmitt	Finalisation of Laboratory and

			Instruments
v0.3.6c	04/04/12	Bernard Schmitt	Various improvements and homogenizations
v0.4.0 (=0.3.6d)	11/04/12	Bernard Schmitt	Various documentation - version of the 3rd SSDM meeting
v0.4.1	23/04/12	Bernard Schmitt	Various small changes from 3rd SSDM meeting
v0.4.2	03/05/12	Bernard Schmitt	New Experimentalist table. Various small changes.
v0.4.3	12/05/12	Bernard Schmitt	Fusion spectra and advanced spectra + small changes in spectra, experiment
v0.4.4	20/05/12	Bernard Schmitt	Various changes in instrument parameters, spectra and experiment => stable version Start of sample reorganization
v0.4.5	05/06/12	Bernard Schmitt	Major changes in Sample (units, processing, adsorption, matter call). Add “solution” species, "Matter_fluid". Few changes in molecule, experiment, ….
v0.4.5a	11/06/12	Bernard Schmitt	Major changes in Sample (errors, adsorption, …). Stable version !
v0.4.6	18/06/12	Bernard Schmitt	Small changes in instrument parameters
v0.4.6a	01/07/12	Bernard Schmitt	Small additions in instrument, minerals, solution, and expanded enumerations.
v0.4.6b	05/07/12	Bernard Schmitt	Various small adding/corrections
v0.4.6c	13/07/12	Bernard Schmitt	Various small adding/corrections: import mode, …
v0.4.6d	16/07/12	Bernard Schmitt	Changes in mineral species (add hydration KW) and in Sample (irradiation) + various Enum
v0.4.6e	??/07/12	Bernard Schmitt	Major changes in Enum of material / constituent / species, some changes in matters. Fixing Enum/OpenEnum
v0.4.6f	30/07/12	Bernard Schmitt	Enum of mineral species, adding KW to mineral matters, moving unit KW from parameters to experiment.
v0.4.6g	03/08/12	Bernard Schmitt	Storage units of float values, completion/correction of some Enum, some changes in mineral and molecule
v0.4.6h	01/10/12	Bernard Schmitt	Some addition & changes in species and other minor addition in various parts
v0.5.0a	07/10/12	Bernard Schmitt	Important changes and adding to Band list and bands. Few name changes in spectrum
v0.5.1 (=0.5.0b)	23/10/12	Bernard Schmitt	Final changes to Band list, bands, states. Develoment of molecular modes parameters. Small changes to spectrum and mineral species.
v0.5.1a	05/11/12	Bernard Schmitt	Few addition and changes in Mineral, spectrum, bandlist, band, …
v0.5.1b	05/12/12	Bernard Schmitt	Few addition and changes in ???
v0.5.1c	15/03/13	Bernard Schmitt	Addition of enum attributes in sample. Few additions in chemical function and changes in spectrum.
v0.5.2 (=0.5.1c)	15/03/13	Bernard Schmitt	Cleaned version. Some additional or revised general description
v0.5.2a	30/03/13	Bernard Schmitt	Addition of extraterrestrial matters and organic matters + small additions in

			atoms, molecule, mineral matter, fluid matter and instrument parameters
v0.5.2b	10/04/13	Bernard Schmitt	Major changes in layer/materials and in all matters: precursors materials and processings
v0.5.2c	11/04/13	Bernard Schmitt	Small change in material, atoms, … Major changes in object_meteorite, small change in matter_meteorite.
v0.5.3a	17/05/13	Bernard Schmitt	Changed structure of processings in sample. Some changes in processings for all matters
v0.5.3b	23/05/13	Bernard Schmitt	Many changes in meteorite_object, minor ones in all matters.
v0.5.4a	05/06/13	Bernard Schmitt	Changes in matter_organic
v0.5.4b	25/06/13	Bernard Schmitt	Changes in all matters (homogeneisation KW)
v0.5.4c	11/07/13	Bernard Schmitt	Small Enum change in Layer and Mineral
v0.5.4d	23/07/13	Bernard Schmitt	Some changes in all matters (2 KW)
v0.5.5a	09/08/13	Bernard Schmitt	Some changes in sample/matter processings, molecule and all matters
v0.5.5b	10/10/13	Bernard Schmitt	One keyword added in publications and mineral species. 2 changed Enum in Matters and sample
v0.5.5c	26/11/13	Bernard Schmitt	Added KW in chemical functions + changed a few enum in mineral, matters, object, instrument, experiment, bandlist
v0.5.5d	12/12/13	Bernard Schmitt	Added a few enum + 1 KW in Sample, changed KW + Enum in organic matter
v0.5.6a	06/04/14	Bernard Schmitt	Reorganization of Mandatory. Definition of some calculated KW. Some Kw changes in minerals. Some changes in Enum. Added Enum and KW for X spectroscopy extension.
v0.5.6b	29/08/14	Bernard Schmitt	Two KW added in fluid_matter & experiment. Several arguments added in various Enums.
v0.5.6c	29/07/15	Bernard Schmitt	Small modification of absolute mandatory KW
v0.5.7a	29/03/16	Bernard Schmitt	Changes in “Experimentalists” (copyrights), “Instruments”, Exp-spectra” (copyrights), “Minerals” (crystal_sites)
v0.5.7b	11/05/16	Bernard Schmitt	Added table ‘database’ and links DB_uid, changes Enum Minerals, laboratory_date
v0.6.0a	17/06/16	Bernard Schmitt	Numerous and major changes in KW and conditions, especially in Sample, Mineral species, Instrument, Experimentalist, Spectra and bandlists. Fewer in other tables
v0.6.0b	04/07/16	Bernard Schmitt	Major changes in “processings”. Add and changes KW in “atom” and “molecule” (+ add ‘variables’). Remove KW in “solution” and “mineral”. Small add in all “matters”. Small changes in “instrument parameters” and “spectrum”.
v0.6.0c	09/07/16	Bernard Schmitt	Change of conditions in Sample + few Enum. Changes in matter meteorite=>extraterrestrial), spectrum

			and database. + little in experimentalists
v0.6.0d	25/07/16	Bernard Schmitt	Changes in Enum in Sample, change in KW/Enumin all species, few Enum/KW changes in all matters. Add Object micrometeorites table. Several changes in Spectrum + few in other tables.
v0.6.0e	26/07/16	Bernard Schmitt	Various Enum and Conditions changes everywhere. Split of the “Chemical function” table => “chemical bonds”. Finalization of Object micrometeorites table. Minor changes in Publications.
v0.7.0 (=0.6.0e)	26/07/16	Bernard Schmitt	Same as v0.6.0e but with all v0.6.0 changes marks cleaned + minor changes
v0.7.0a	25/08/16	Bernard Schmitt	Adding a table ‘Journal’ + link from “Publi”. Sample+Matters: Modification of Matter-material choice. Changes in isotopic species. Add bonds in minerals. Various small KW, attribute and conditions changes
v0.7.0b	02/09/16	Bernard Schmitt	Small changes in KW in sample, chemical bonds, molecules and minerals. A few other minor changes
v0.7.0c	08/09/16	Bernard Schmitt	Several sddition in Experiment. A few small changes in Laboratory, spectrum, Bandlist and Publication
v0.7.1 (=0.7.0c)	08/09/16	Bernard Schmitt	Same as v0.7.0c but with all v0.7.0 changes marks cleaned + minor changes
v0.7.1a	18/09/16	Bernard Schmitt	Few addition of KW in Chemical bonds and molecules, and change of Enum (mostly in vibration_mode)
v0.7.1b	03/11/16	Bernard Schmitt	Added DB management, data validation and access right, user rights. Add table “access_group”. Change KW in Publications. Changed conditions in sample (mass, errors, …) and in variables (mineral, solutions)
v0.7.2 (=0.7.1b)	03/11/16	Bernard Schmitt	Same as v0.7.1b but with all v0.7.1 changes marks cleaned + minor changes
v0.7.2a	10/11/16	Bernard Schmitt	Large KW addition or changes in tables Experimentalist, laboratory and Database. Some KW changes in Experiment/spectra. Small changes in Publication and User.
v0.7.2b	23/11/16	Bernard Schmitt	Large additions and changes of KW in Laboratory Database and Experimentalists tables (for Doi). Large changes in Experiment and Spectra, Small addition in Sample.
v0.7.2c	30/11/16	Bernard Schmitt	Adding of a bloc “structure” in “experiment”. Addition and changes in “laboratory”, “database”, “instrument parameters” and “experiment”. Changes in “mineral variables”, “experimentlists”.
v0.7.2d	03/12/16	Bernard Schmitt	Addition in Spectrum. Small changes in Experiment, Structure, Experimentalist, Database, Publication and User
v0.8.0 (=0.7.2d)	03/11/16	Bernard Schmitt	Same as v0.7.2d but with all v0.7.2 changes marks cleaned + minor changes

v0.8.0a	12/12/16	Bernard Schmitt	Large reorganization of “Sample parameters”. XAS option added in Instrument parameters and Atom. Small changes in spectra, experiment, structure, …
v0.8.0b	21/12/16	Bernard Schmitt	Small changes in enums of Sample, Instruments, and Spectra. Added conditions in Parameters_instrument (variables) and Publication. Small name changes in Spectra and Journal.
v0.8.1	09/01/17	Bernard Schmitt	Same as v0.8.0b but with all v0.8.0 changes marks cleaned
v0.8.1a	18/01/17	Bernard Schmitt	Add Basic constituent table. Modif/add KW Constituents and Species. Small changes in Atom, Chemical bonds, and Molecules. Changes in Mineral. Add Molecular solids constituent table.
v0.8.1b	14/02/17	Bernard Schmitt	Extend Molecular solids to all Solids. Large Large addition to Minerals. Add Basic constituents option in Sample. Homogeneize Constituent KW and attributes between Constituents, Solids and Minerals. Small changes in chemical bonds and functions.
v0.8.1c	16/02/17	Bernard Schmitt	Small KW addition in Sample and Spectra + small attribute changes in spectra
v0.8.1d	22/03/17	Bernard Schmitt	Large KW changes in Basic constituent table. Several Enum changes in Constituents, Solids and Mineral. Small change in Spectra.
v0.8.1e	24/04/17	Bernard Schmitt	Change of Fundamental constituent to Basic constituent & Fundamental phases + small change. Changes in Material and Constituents, Small change in Minerals, Solids and Matters. Large change in Liquid.
v0.8.1f	05/05/17	Bernard Schmitt	Add bloc “stereo-isomers’in Molecule. Add BRDF data in Experiment/ Spectrum/ Parameters spectrum. Add ROI in imaging in Spectrum. Add preview control in Exp/spectra
v0.8.1g	03/06/17	Bernard Schmitt	Changes in KW names in Parameters intruments. Changes in KW name, Enum and conditions in Experiment and Spectrum. Modification conditions in molecule. Small changes in Liquid.
v0.8.2	03/06/17	Bernard Schmitt	Same as v0.8.1g but with all v0.8.1 changes marks cleaned
v0.8.2a	11/06/17	Bernard Schmitt	Small changes in conditions in Experimentalist, Molecules, Liquids, Matters, Instrument parameters, Experiment, spectra. Few change of KW/Enum in Liquid. Calcul in Solid.
v0.8.2b	02/07/17	Bernard Schmitt	Changes in condition in Species. Small changes in condition and Enum in Mineral and Solids and Matters. Changes in Enum in Object_idp and

			sample_fluid. Various small changes in instrument, experiment, spectra.
v0.8.3	03/07/17	Bernard Schmitt	Same as v0.8.2b but with all v0.8.2 changes marks and draft parts cleaned
v0.8.3a	29/09/17	Bernard Schmitt	Changes of KW/enum/conditions in Mineral ans Solid (+some in Liquid). Small changes in Object. Major changes and additions in Constituent. Small changes and additions in sample, experiment and spectra.
v0.8.4	29/09/17	Bernard Schmitt	Same as v0.8.3a but with all v0.8.3 changes marks and draft parts cleaned
v0.8.4a	13/01/18	Bernard Schmitt	Few additions in Users, some condition changes in Publications. Small Enum change in Liquid, solid, Mineral.
v0.8.5	13/01/18	Bernard Schmitt	Same as v0.8.4a but with all v0.8.4 changes marks and draft parts cleaned
v0.8.5a	11/02/19	Bernard Schmitt	Major SSDM upgrade: Addition of a Body table. Synchronisation of Users and Groups. Sel changes/additions in Database, Publication, Molecule, Solid, all Matters, Object meteorite, Object micromet, Sample, Material, Constituent, Instrument parameters, Experiment, Spectrum. Small changes/additions in journal, Liquid, Mineral, Object IDP, Layer, Instrument. Various changes of Enum, mandatory, conditions… in many tables.
v0.8.5b	11/04/19 to 20/05/20	Bernard Schmitt	Modification of a few Mandatory conditions
v0.9.0	22/05/20	Bernard Schmitt	Same as v0.8.5b but with all v0.8.5 changes marks and draft parts cleaned

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1. INTRODUCTION

This project of "Solid Spectroscopy Data Model" (SSDM) started to be developed at LPG in the frame of the Observatoire des Sciences de l'Univers de Grenoble (OSUG) in 2006 for a first prototype database called STSP, then get large developments for the GhoSST database in the frame of the contribution of IPAG to the VAMDC FP7 European program and Europlanet RI FP7 European programs (2009-2012). Its development continued at low pace until the start of the current Europlanet2020-RI program (2015-2019) in which SSDM is strongly evolving to meet the SSHADE database infrastructure requirements.

Since the first basic version developed for the GhoSST database, the SSDM has been subjected to large extensions and modifications as partly defined at a series of meetings of the "Expert Working Group on Solid Spectroscopy Data Model" and then of the "SSHADE consortium partners team" who gathered representatives of the different European solid spectroscopy data producers and a few laboratory data users of the astrophysical-planetary sciences communities. Improvements and extensions of the core of SSDM (fundamental species, samples, instruments, experiments, spectra) have been done in several steps. One major addition, band list, occurred in 2011. Several important extensions (various types of fundamental phases, matters, and objects, publications) have been developed since 2011.

The current version of SSDM has evolved in the frame of the Europlanet2020-RI program to be now the common data model of all the Solid Spectroscopy Data Bases that are, or will be, included in the SSHADE database infrastructure, including the first one, the GhoSST database of IPAG.

The structure of SSDM is presented in some details in this document and all its key-words are organized and listed in tables below with full description, notes and exemples as well as units, data type and conditions and constraints information.
The global graphical relational structure of SSDM used to build the relational database is presented in Figure 1. It shows schematically how the main parts of SSDM are interconnected

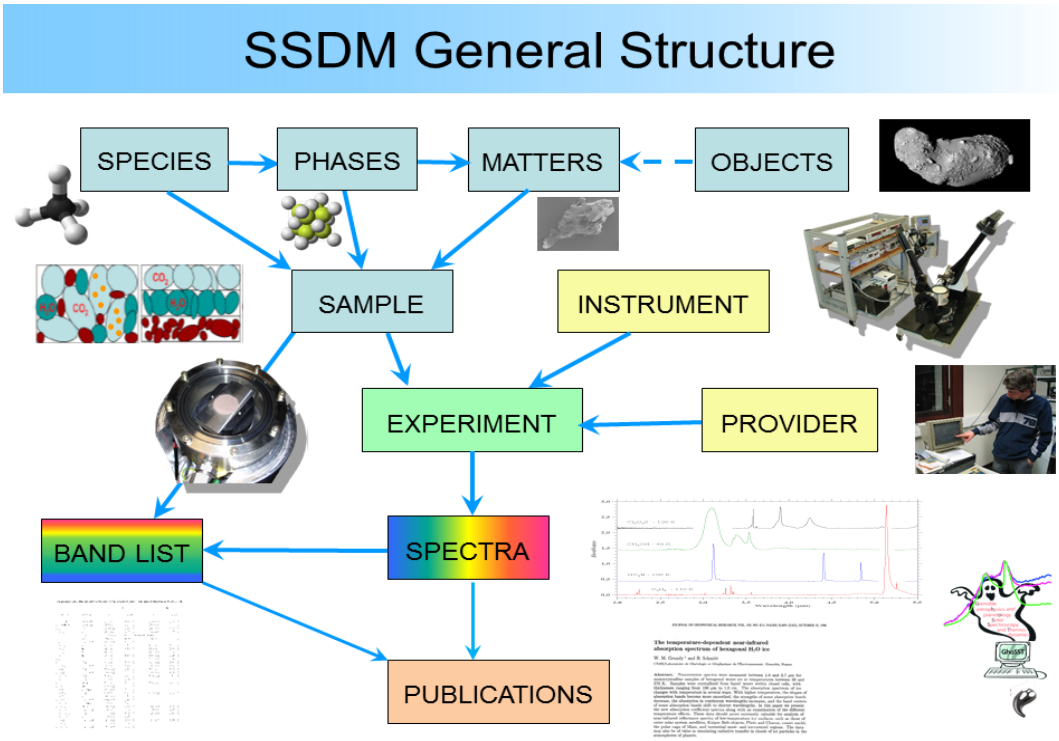

Figure 1: graphical relational structure of SSDM

2. GENERAL DESCRIPTION

2.1 Data Model Structure

The current data model is split in 13 main parts which contain the relevant keywords to describe them and that are linked with relevant relations. Figure 2 presents the global SSDM structure in more details including the sub-tables and some of the main types they contain. Figure 3 provide the detailed map of the links between tables.

- The **"Sample"** table which describes the sample, its *"layers"* of *"materials"*, and then the *"constituents"* (minerals, synthetic solids, liquids, …) of each material down to their basic constitutive *"fundamental species"* (molecules, atoms, …).

- The **"Matters"**, made of "*materials*" (or mixtures of materials), are used to describe the natural or synthetic matters (minerals/rocks & synthetic solids, carbonaceous, extraterrestrial, fluid, …) collected on the field or synthesized, from which some samples are made.

- The **"Fundamental Phases"**, which can be the *"constituents"* of the samples and matters, are either the different families of synthetic solids or liquids or the natural mineral phases.

- The **"Fundamental Species"** (atoms, molecules, ions, …), which are the building blocs of the *"contituents"* of the samples and of the *"fundamental phases"*. We added the "**Chemical functions and bonds**" that describe the bonds and functional groups of the *"molecules"* in molecular solids or liquids and of the *"anionic radicals"* in minerals.

- The **Objects** are the geologic objects from which some *"natural matters"* (terrestrials or extraterrestrials) come from (e.g. meteorites, micrometeorites, IDPs, …).

- The **"Instrument"** table which describes the laboratory instruments and techniques used and their measurement parameters (instrument specific).

- The **"Experiment"** table which describes the structure of the set of **"***spectroscopic data***"** and provide the common instrument parameters.

- The **"Spectroscopic data"** (called "**Spectra**") table which describes the spectral data or products recorded on a *"sample"* with an *"instrument"* and their specific sample environment and measurement parameters.

- There is also a set of **"Provider"** tables that store the information on each partner "**Database**" of SSHADE, "**Laboratory**" and "**Experimentalist**"

- The **"User"** and **"Group"** tables store the information necessary for the management of the user accounts.

- The **"Publication"** table (and its associated **"Journal"** table) which provides all information on publications linked with the spectral data (*"spectra"* and *"band list"*), but also with *"sample", "instrument", "matters", "objects"*, but also on any related subject.

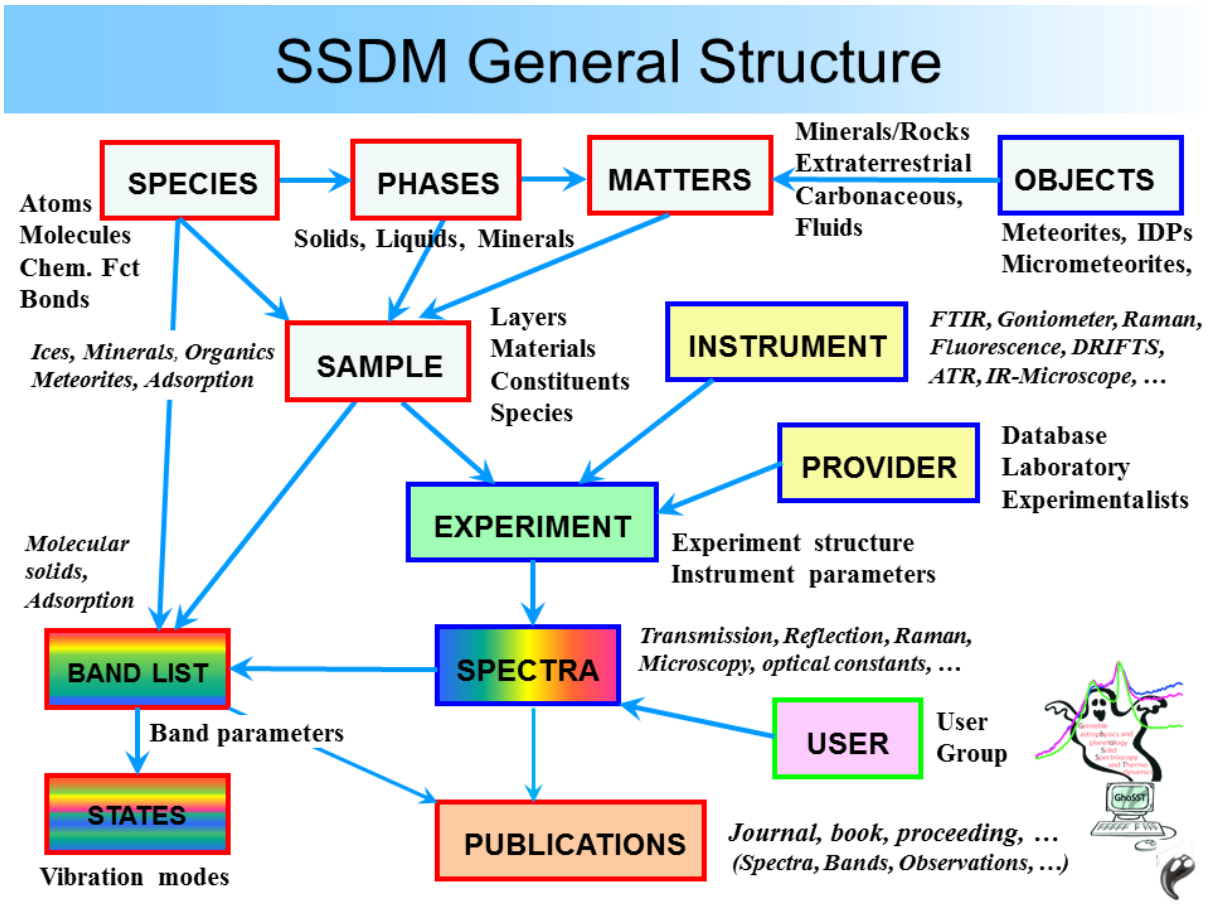

Figure 2: SSDM general structure with list of sub-tables (bold) or main types (italic)

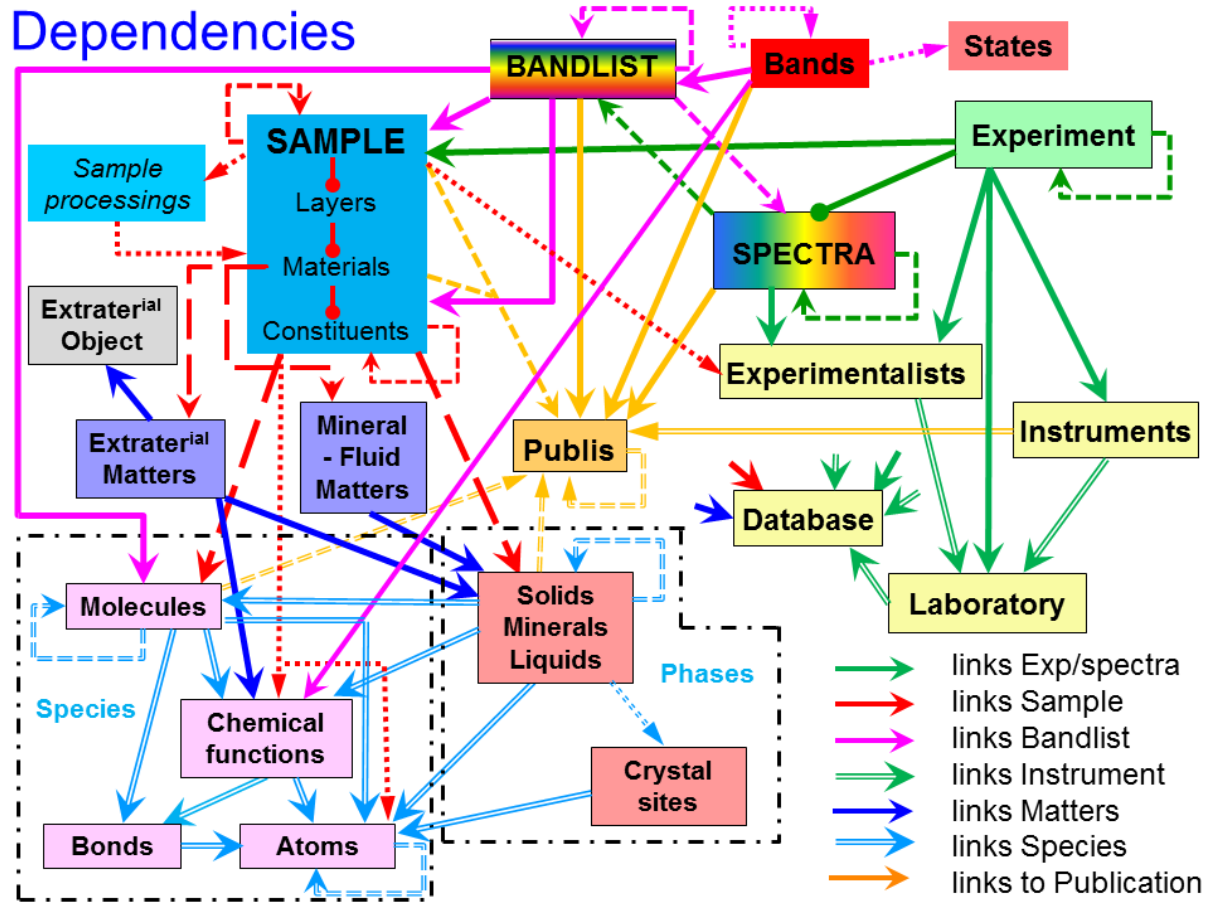

Figure 3: SSDM detailled structure (except user) with almost all existing links between tables

2.2 Data Model Content

Each table contain a set of key-words that allow to describe their object (sample, spectra, …)

As seen from their use side there are typically four types of key-words:

1) those who will be mostly used by "users" to Search spectral data (tagged 'S'). They constitute the main information. They are generally absolute mandatory or mandatory.
2) those who contain additional information useful for the *"user"* (also searchable by expert user, and to be delivered) (U). They are generally optional.
3) those who contain additional information useful for the *"data provider"* (import mode, data history, …) and not intended to be delivered to the "user" (P)
4) those who are generated automatically by the database software during data ingestion (mainly "xxx_index") and that sometimes may be also useful to expert users or data providers to access directly to some information (unique identification number of sample, spectrum, molecule, matter, …) (B)

The following chapters list the key-words of each table after a definition and a general description of their content and structure. For each key-word a definition and its properties (data type, links, mandatory type, units, keyword level, conditions, constraints, …) are given. Notes, exemples and possibly web links complement this information.

2.3 Tables Content Description

- The **"Key-Word"** column gives its effective name starting with its common table root, in italic. They are always noted within double quotes: "key_word".
  - A value or an attribute (for Enum) of a KW will be noted within simple quotes: 'value', 'attribute'.
  - A list of multiple values or attributes of a KW may be also listed between parentheses: {'value_1', 'value_2', ...}, {'attribute_1', 'attribute_2', …}

Special key-words (KWs):

- KWs ending with "_index" refer to automatically attributed (randomly but uniquely) internal database indexes.
- KWs ending with "_uid" refer to manually CREATED database "*unique identifiers*", or to LINKS to an "*unique identifier*" key-word (in another table or in the same table). Some of them are virtuals but are noted for completeness to provide the logical links which are directly implemented in the database schema.
  Note: there is here a possible small confusion (same ending '_uid') between the created UID of a table and a KW providing a link to an existing UID. In the xml they are differenciated by the comments:
  - '**ABS MANDATORY to CREATE** Unique identifier code given to …' for the first (generally following an "_import_mode" KW)
  - 'LINK to the existing UID of …' for the second.
  - In a few cases either types can occur in the same KW (but when "import_mode" = 'use existing' => LINK, and => CREATE in all other cases)
  - UID names should strictly use the very basic ascii characters: only alphanumeric and '_'
- For a list of keywords (called a 'bloc') that can have multiple instances, the generic root of this list is given in italic in this column. The limit of the bloc is materialized

with an horizontal dashed line

Signs after KW:

- [**]: KW of type ID (ending with '_index') or UID (ending with '_uid') which define the table (to be created)
- [*]: KW of type UID (ending with '_uid') creating a link with another table through an existing UID (ending with '_uid') (link to the previous)
- [*§]: means direct internal link to another table (KW did not really exist).
- [-xml]: the KW did not appear in the corresponding xml file. i.e. not to be filled because it is determined automatically, calculated from others KW, virtual, or defined through an interface (SSHADE manager, …), … (see 'Level')
- [-xml except in variables]: the KW appears in some other xml files only in its variable blocs (associated with V*: VM, VS, VL, …in the 'Exp' column)
- [ui]: keyword only accessed through the 'user management interface'
- [pi]: keyword only accessed through the 'provider management interface'
- [si]: keyword only accessed through the 'sshade management interface'
- [+]: this KW defines info related to the next table (mostly in "Sample")

Key-word equivalance:

- [key-word names] in fushia in second line are generic key-word names allowing to identify equivalent keywords in several parallel tables (species, phases, matters, objects, …).
- [key-word names] in violet are equivalent XSAMS keywords for SSDM-XSAMS mapping.

Key-word history:

- Key-words in light blue are new or modified key-words relative to previous version
- key-word names in green below actual key-words are previous names, when changed
- Key-words in grey are suppressed key-words relative to the previous version. Reason for this is in dark orange.

- The **"Type"** column describes the data format type:

- *Numerical* (int(n), float, …): need to define the unit, if any. For 'float' 2 formats are possible: decimal (123.456) or scientific (1.234e-56)
- *Text* (varchar255(text), blob): free text (character string). This text can contain LaTeX expressions (they should be written as xxx).
  - 'blob' has no size limit.
  - 'varchar255' is limited to 256 characters.
  - 'CS-varchar255': limited to simple ASCII (mostly for Enum of symbols)
- *Enumeration* (enum[type]): exhaustive list of fixed values {xxx, yyy}, called 'attributes', useful for search efficiency (list of choices) but directly implemented inside the database software and data ingestion parser and thus difficult to extend.
- *Enumeration* (CS-enum(text)): limited to simple ASCII; used for the list of symbols
- *Open enumeration* (openum[type]): open list of homogeneous set of fixed attribute values {xxx}, useful for data ingestion and search efficiency (values). Implemented only in the database. Easy to extend.
- *Boolean:* same as Enum but only with attributes {yes, no} or {true, false}

Also when

- List [Ln]: list of potentially multiple values of a single keyword. They may group several keywords which are linked in a same list. They are marked with 'Ln' in the "Table" column.

Special values in xml

- Any mandatory value may be set to 'void' by putting the 'NULL' value, whatever is the format of the data.
- In 'variable parameters' any original value can be set back to 'void' by using 'NULL'. A new value will replace the original one; and a void field will keep the original value.
- (to be completed)

- The **"Level"** column gives the level of keywords in term of use and its "mandatory" level and mode of filling (for database filling):

User-Provider level

- S = main Searchable by user (will be mostly 'absolute mandatory' or 'mandatory')
- U = Useful info for User
- P = only for data Provider (will not ppear on user interface)
- M = only for SSHADE manager (will not ppear on provider interface)
- B = automatically created by data Base.

  Note: the Search level 'S' is postfixed with a integer (0 to 5) depending on the level of priority attributed to this KW in the search algorithm.

Filing mode and mandatory level

- The first signs define the mandatory keywords ([!!] and [!]: need to be filled at data ingestion, and will be checked by import parser), or the compulsory ones [£] or the recommendend ones [$] (last 2 cannot be checked by import parser).
- 'd' and 'o' modulate these mandatory options.
- The second sign after '_' ([m], [g], [c] and [v]) tell the way they are filled.
- When a second set of signs appear after a [V:] it indicates that the mandatory level that follows is defined for the keyword when used as a variable parameter.

  [!!_]: absolute mandatory (needed to make working the database). No way to avoid to fill them. Will be checked by the import parser.

  [!!o_]: absolute mandatory in option (needed to make working the database in some specific cases): only if a specific condition is satisfied (precised in *'Condition:'*). This KW has generally no meaning when the condition is not satisfied. Will be checked by the import parser.

  [!_]: mandatory (needed for search or major information). 'NULL' is used to ignore this mandatory keyword. Will be checked by the import parser.

  [£_]: compulsory: as 'mandatory' but it cannot be checked by the import parser.

  [$_]: strongly recommended when exist: non-mandatory but strongly recommended to fill because used in some search or other important info (link, …).

  [!d_]: mandatory but with a default value (needed for search or major info). It will be automatically filled with a default value if not filled manually.

  [!o_]: mandatory in option (needed for search or major info): either under a specific condition (given in *'Condition:'*) or inside an optional block (marqued [o] with option described in *'Condition:'*), i.e. mandatory only if the block need to be filled.

  [_m]: to be filled manually in the import xml file

  [_g]: internally generated value of KW (ex: _index). Automatically generated during import (did not appear in xml)

  [_c]: calculated during import from other(s) keywords (calculation given in 'description' column) or pre-determined Enum attribute. Did not appear in xml if not associated with 'm': [_mc]. In this case it is calculated if not filled.

  [_v]: virtual keyword representing an implicit internal link. Did not have to be filled (and did not appear in xml).

- The **"Table"** column refers to the name (abbreviation) of the current table. When there is a logical link with another table(s), this table name(s) is added below.
    - Ln (with 'n' an integer, such as 'L3'), sometimes noted below in a series of KW, allows us to indicate the bloc of keywords belonging to a common 'list Ln'.

- The **"Exp"** column defines if the value of this KW (limited to "sample" ("_parameters_environment"), "parameters_instrument" and "Liquid", "Solid", "Minerals" tables) is allowed to vary within an "experiment": (à revoir)
    - F = 'fixed'
    - V = 'variable'
    - V+ = 'main variable' (quite subjectif)
    - Vc = 'variable by consequence' (such as "errors" of a 'variable')
    - (V) = 'variable' to be used only when it implies no significant change in "sample"

Other cases are the KW in the "mineral phase", "solid phase" and "liquid phase" tables that can have modified values when used in a "sample" or a "matter"

- VM = 'variable mineral'
- VS = 'variable solid'
- VL = 'variable liquid'

For multiple versions of "Spectra" and "Bandlist" the KW for which the values are kept in memory for the old versions are also taged in this column.

- [Ver] tell that the value of this KW is permanently stored with each older version of the spectrum or bandlist. Only the major KWs of the previous version are archived when a new version is uploaded. The values of the other KWs are kept only for the current version.

- The **"Unit"** column gives the unit of the value of the KW when it is a numerical. But:
    - 'no' means "number without unit" (e.g. mass fraction, ...).
    - '--' means "not relevant" (text, conditional, ...)
    - 'var' when several alternative units are listed in another keyword that defines the unit to be used. Or it can be free unit to be specified with the value (in varchar)

- The **"Description"** column gives first a detailed definition and/or physical description of the Keyword.
    - *Enumerations:* If the KW is an *enumeration* or an *open enumeration* the description will list all possible values of the attribute (Enum: {xxx, yyy, zzz}, or OpenEnum: {aaa, bbb, ccc, …}).
    - *Note:* For some OpenEnum a few attributes needs to be fixed (not allowed to change them) because they are used in some 'Conditions': they are underlined
    - FreeList: Not an enumeration but only a list of exemples in order to keep some homogeneity of style and description.
    - *Definition(s):* provide the detailed definition(s) either of the KW itself, or of the different attribute values of its enumeration.
    - "➔ calculated ...": the values of these KWs are calculated (only if not filled directly) from other(s) specified KW(s) if all these keywords have valid values.
    - *Condition(s):* Condtion(s) on the mandatory level of these keywords ([!!o_] or [!o_] in 'level' column) are defined here in terms of value of (an)other keyword(s).
    - *Constraint(s):* Constraint(s) on the value of a KW. Its can be a numerical constraint, or a constraint to have no value in some specific cases (because not relevant). It will be verified by the import parser.
    - *Note:* various types of notes may be added under *"Note"* to give more precise information.
    - *Note xml:* specific note for the representation of this KW or the filling of the KW in

the corresponding xml file.

- *Ex:* various examples of keyword values may be given here. Useful when a specific format needs to be followed.
- **Variable:** this part, present only for variable parameters (V), provides the same type of specific information when the keyword is used as a variable.
- In this column keywords names are always noted as: "*table*_keyword_name" (ex: "*molecule*_index", "*sample*_mass_error", …)
- And values of keywords are always noted: 'keyword-value' (ex: 'amorphous', 'true', 'MgF2', …)
- in red:
    - some future changes, addition or comments (or questions) that should be introduced in next version:
        - (TBD): To Be Done
        - (TBC): To Be Conpleted or Confirmed
        - (TBDef): To Be Defined

- In all columns: in red such as the changes, addition or suppression in the relevant part of the KW.

Key-word types common to all tables

Almost all tables have a few generic but specific KW that are described below and not repeated in the general description of each table.

At the beginning of (almost) all tables:

- "*root*_import_mode": Mode of import of the "root" data
- "*root*_xml_filename" [-xml]: Name of the storage copy of the xml import file of the "root" metadata
- "*root*_index"[**][-xml]: Automatic random but unique number (internal ID) given to new "root" table.
- "*root*_uid" [**]: Unique identifier code (UID) given to the "root" table (to be created). It should follow a specific nomenclature given in the 'Description' column

In several tables:

- "*root*_manager_database_uid" or "*root*_owner_database_uid": Link to the database which manages (and for 'matters', 'sample' and 'experiment' also owns) the data of this table.

At the end of (almost) all tables:

- "*root*_comments": Additional information on the "root" data
  Note: other more specific "*root*_xxx_comments" (ex: *root*_composition_comments") may occur at the end of some specific bloc or group of KW. They should be used only for their specific use and all other comments should go into "*root*_comments".

3. PROVIDER (DATABASE, LABORATORY, EXPERIMENTALIST)

3.1 Description

* The **"Database"** table defines the information related to each database of SSHADE.

Each research group of the SSHADE consortium has its own *"database"* that need to be defined. A few other specific databses will be set to deserve some specific needs (such as a 'SSHADE database", a database to store the data recorded during the Trans-National Access visits (TNA), …).

- The database is first defined by its "name and acronym" and a description of its content as well as information about when it was created and who are its creators. Then the organizations to which belong the database and the laboratory(ies) which host and is responsible of this database are listed, followed by the institution(s) that provide regular financial support to the database (the 'funders') and the organizations that provide ponctual financial support to the database content. The direct link to the front page of the database in the laboratory/institution web site is then given.

Most of this information are required for the creation of a DOI for the database and for DOIs of the experiments.

The *"laboratory", "experimentalist", "group", "matters", "sample", "instrument"* and *"experiment"* tables refer to this laboratory table in order to set the rights of management of these data.

* The **"Laboratory"** table gives basic information on the laboratory in which an experiment is performed, or in which an experimentalist works.

- The laboratory is first defined by its name & acronym, followed by a description, and by the organizations to which it belongs. Then the address and web site are given, plus some possible creation/end dates.

The *"experimentalist", "instrument"* and *"experiment"* tables refer to this laboratory table.

* The "**Experimentalist"** table gives the information on the experimentalist which perform an experiment or analyse its data.

- An experimentalist is a person that prepare sample or matters and/or perform experiments or which analyse data (will be called "validator" in such case). He belongs to one or more laboratories and may have been previously in one or more other laboratories.

- The experimentalist table record its name, identifiers, phone number, email, web site, and current satus (laboratory(ies), status, date of presence, …) as well those of his/her previous laboratory(ies).

The *"matters", "sample"*, *"experiment"*, *"spectra", "bandlist"* and *"user"* tables refer to this experimentalist table.

3.2 Database Table

Root of the table: ***database***

Data type: 'Database'

Key-word	Type	Level	Table	Exp	Unit	Description
Database import mode and indexes						
*database*_import_mode	enum(text)	P [!!_m]	DatBas	F	--	Mode of import of the "database" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*database*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	DatBas	(V)	--	Name of the storage copy of the xml import file of the database metadata ➔ determined automatically during import (from "*database*_uid"?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*database*_index [**][-xml]	int(10)	B [!!_g]	DatBas	F	--	Automatic random but unique number (internal ID) given to new database.
*database*_uid [**]	varchar(255)	S0 [!!_m]	DatBas	F	--	Unique identifier code (UID) given to the database table (to be created) *Nomenclature:* Create this code name with 'DB_' in order to be be unique. It should be of the style 'DB_DatabaseAcronym' where 'DatabaseAcronym' is the acronym of the database. *Note:* use only UPPERCASE *Ex:* 'DB_GHOSST', 'DB_FAME', 'DB_REFL_SLAB', …
*database*_sshade_doi [-xml]	varchar(255)	S0 [!!_c]	DatBas	F	--	DOI code of the database ➔ automatically calculated using the database acronym: ⇨ 10.26302/SSHADE."*database*_acronym"

Definition: http://en.wikipedia.org/wiki/Digital_object_identifier

Notes:

- the DOI is determined with "*database*_acronym"
- the prefix '10. 26302' has been attributed by INIST to SSHADE who will manage the doi creations.
- the DOI is not case sensitive.
- the url of the doi is obtained by adding 'https://doi.org/' (note: the former standard whas 'http://dx.doi.org/')
- the DOI will redirect to the SSHADE page displaying the database metadata (through a landing page)

Ex: 10. 26302/SSHADE.GHOSST

Database name and description

*database*_acronym	varchar(255)	S0 [!!_m]	DatBas	F	--	Acronym of the database *Constaint:* use alpha-numeric characters possibly with '_' or '-' but without space *Ex:* 'GhoSST', 'REFL_SLAB', … *Note DOI:* requested: - Absolute mandatory for buiding the "Identifier" (for 'database', and 'experiment'), - Absolute mandatory as "Title" (3) for 'Database' and for 'SSHADE' o *Convention*: 'SSHADE / "database_acronym": "database_name"' - Absolute mandatory as "Publisher" (4) for 'Experiment' o *Convention*: 'SSHADE / "database_acronym" (OSUG-DC)'
*database*_name	varchar(255)	S0 [!!_m]	DatBas	F	--	Full Name of the database *Ex:* 'Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics service'... *Note DOI:* - Absolute mandatory as "Title" (3) for 'Database' and for 'SSHADE'

- option as “Title/titleType” (3.1)

*database*_description	blob	U [!_m]	DatBas	F	--	Description of the database and its scientific content *Note:* describe the type(s) of data present in the database: wavelength range(s), type(s) of materials, types of data and products, … *Note DOI:* - Recommended option as “Description / descriptionType=Abstract” (17)
database_keywords	***List [L0]***	[!]				£: List of keywords describing the scientific content of the database
*database*_keyword	varchar(255)	S0 [!_m] L0	DatBas	F	--	Keyword describing the scientific content of the database *Note:* describe the type(s) of data present in the database: typical wavelength range(s), type(s) of materials, types of data and products, plus some general keywords such as ‘database’, ‘spectroscopy’… *Ex:* - ‘database’, - ‘spectroscopy’, ‘Raman’ - ‘visible’, ‘near-infrared’, - ‘molecular solids ‘, ‘ices’, ‘snow’, ‘minerals’, ‘rocks’, - ‘meteorites’, … - ‘low temperature’ - ‘planetary sciences’, ‘astrophysics’ *Note DOI:* - Recommended option as “Subject” (0-n) (6)
*database*_logo_filename	varchar(255)	P [!_m]	DatBas	F	--	File name (with extension) of the logo of the database *Image formats:* .png *Note:* should follow the following rules for the format: • Larger size L = 600 pix • L/h = 1.2 to 3 maxi

						• Format: .png, transparent background (alpha canal of png) • cropped (i.e. no margin around the logo) *Note:* this file will be imported in the database and displayed in the front page of the SSHADE web site as well as in the database page.
Database creators and managers						*Note*: the Scientific and Database managers of a database and their Providers can be determined through the KW "*user*_database_role"
database_creators	***List [L1a]***	[!!]				£: Creator(s) of the database
*database*_creator_first_name	varchar(255)	S2 [!!_m]	DatBas L1a	F	--	First name (given name) of the creator(s) of the database *Note DOI:* - Absolute mandatory as "Creator / creatorName / givenName" (2.1.2) for 'Database'
*database*_creator_family_name	varchar(255)	S1 [!!_m]	DatBas L1a	F	--	Family name (last name) of the creator(s) of the database *Note DOI:* - Absolute mandatory as "Creator / creatorName / familyName" (2.1.1) for 'Database'
*database*_creator_orcid_identifier	varchar(255)	S0 [!_m]	DatBas L1a	F	--	ORCID identifier code that uniquely identify the database creator *Definition*: see "*experimentalist*_orcid_identifier" *Ex:* '0000-0002-7285-027X' (ORCID-ID) *Note DOI:* requested in: - "Creator/nameIdentifier" (2.2) for 'database'
*database*_creator_affiliation	varchar(255)	S2 [!_m]	DatBas L1a	F	--	Affiliation (Laboratory acronym / Organization acronym) of the creator(s) of the database *Ex*: 'IPAG / CNRS', 'IPAG / UGA', … *Note DOI:* - Recommended as "Creator / creatorName / affiliation" (2.5) for

						‘Database’
*database*_date_created	date	S2 [!!_m]	DatBas	F	YYYY-MM-DD	Date of creation of the database *Note:* it is the date of the first import in SSHADE of this file that describes the database *Note DOI:* - Absolute mandatory as “PublicationYear” (5) for ‘Database’ - requested as “Date”
Database organizations and laboratories						
database_organizations	***List [L1b]***	[!!]				£: Organizations to which belong the database
*database*_organization_acronym	varchar(255)	S1 [!!_m]	DatBas L1b	F	--	Acronym of the organization to which belong the database *Ex*: ‘CNRS’ & ‘UGA’ & ‘OSUG’, … *Note DOI:* - same as “organization_name” o *Convention:* “organization_name” (“organization_acronym”)
*database*_organization_name	varchar(255)	S2 [!!_m]	DatBas L1b	F	--	Name of the organization to which belong the database *Note:* depending on the country law this organization may have the legal copyrights on the database content. However, these legal aspects are not included in SSHADE. *Ex*: ‘Centre National de la Recherche Scientifique’, ‘Université Grenoble Alpes’, ‘Observatoire des Sciences de l’Univers de Grenoble’, … *Note DOI:* - option as “Creator/affiliation” (2.3) for ‘Database’ - option as “Creator/affiliation” (2.3) for ‘Bandlist’ - mandatory as “Publisher” (4) for ‘Database’ and ‘Bandlist’ - mandatory as “Publisher” (4) for ‘Experiment’ via

						"*experiment*_owner_database_uid" - for 'SSHADE' and 'Bandlist': it is the SSHADE organizations - The right holder is requested in option "Contributor = RightHolder" but OSUG-DC did not recommend its use.
*database*_organization_region	varchar(255)	S2 [m]	DatBas L1b	F	--	Region, state, province, or county of the organization to which belong the database *Ex:* 'Hampshire', 'Rhône-Alpes', 'Arizona', …
*database*_organization_country_code	enum(text)	S1 [!!_m]	DatBas L1b	F	--	2-digit country code of the organization to which belong the database Enum: {CH, DE, DZ, ES, FR, GB, HU, IN, IT, PL, TW…} Label (code): see "*laboratory*_address_country_code" *Definitions:* see "*laboratory*_address_country_code"
*database*_organization_logo_filename	varchar(255)	P [!_m]	DatBas L1b	F	--	File name (with extension) of the logo of the organization *Image formats:* .png *Note:* should follow the following rules for the format: • Larger size L > 300 pix • Format: .png, transparent background (alpha canal of png) • cropped (i.e. no margin around the logo) *Note:* this file will be imported in the database and displayed in the database page of the SSHADE web site.
database_laboratories	***List [L2]***	[!]				£: Laboratories which host and are responsible of this database *Note:* most of the time, but not necessarily, the laboratory(ies) of the database manager and/or scientific manager of the database
*database*_laboratory_acronym	varchar(255)	S1 [!_m]	DatBas L2	F	--	Acronym of the laboratory which host and is responsible of this database *Note DOI:* - recommended option as "Contributor / contributorType=

						ResearchGroup / contributorName" (7): "*laboratory*_name" ("*laboratory*_acronym") for "Database"
*database*_laboratory_name	varchar(255)	S2 [!_m]	DatBas L2	F	--	Name of the laboratory which host and is responsible of this database *Note DOI:* - see above
*database*_laboratory_logo_filename	varchar(255)	P [!_m]	DatBas L2	F	--	File name (with extension) of the logo of the laboratory *Image formats:* .png, .jpg, (.gif) *Note:* should follow the following rules for the format: • Larger size L > 300 pix • Format: .png, transparent background (alpha canal of png) • cropped (i.e. no margin around the logo) *Note:* this file will be imported in the database and displayed in the database page of the SSHADE web site.
database_funders	***List [L3]***	[!]				£: List of institution(s) that provide regular financial support for the development of the database infrastructure and:or content *Note:* Includes organizations that provide funding via regular budget allocations, through grants or awards *Note DOI:* o recommended option as "FundingReference" (19) for "Database" o taken into account the DOI v4.0 properties "funderName" (19.1), "awardNumber" (19.3), "awardTitle" (19.4) o not taken into account the DOI v4.0 properties "funderIdentifier" (19.2), funderIdentifierType" (19.2.1), "awardURI" (19.3.1)
*database*_funder_acronym	varchar(255)	S2 [m]	DatBas L3	F	--	Acronym of the institution that provide regular financial support to the database infrastructure and/or content *Ex*: 'CNRS/INSU', 'OSUG', 'CNES', …

						Note DOI: - recommended option as “FundingReference / funderName” (19.1) for “Database”. o *Convention*: It will be combined with “database_funder_name”: ‘Institution full name (acronym)’
*database*_funder_name	varchar(255)	S2 [!_m]	DatBas L3	F	--	Name of the institution that provide regular financial support to the database infrastructure and/or content *Ex*: ‘Observatoire des Sciences de l’Univers de Grenoble’, ‘Centre National de’Etudes spatiales’, … *Note DOI:* see “*database*_funder_acronym”
*database*_funder_logo_filename	varchar(255)	P [m]	DatBas L3	F	--	File name (with extension) of the logo of the funder *Image formats:* .png *Note:* should follow the following rules for the format: • Larger size L > 300 pix • Format: .png, transparent background (alpha canal of png) • cropped (i.e. no margin around the logo) *Note:* this file will be imported in the database and displayed in the database page of the SSHADE web site.
*database*_funder_award_number	varchar(255)	S3 [m]	DatBas L3	F	--	Code assigned by the funder to a sponsored award (grant) to support the database infrastructure and/or content *Ex:* ‘GBMF3859.01’ *Note DOI:* - recommended option as “FundingReference / awardNumber” (19.3) for for “Database” and “Experiment” (from “*experiment*_owner_database”)
*database*_funder_award_title	varchar(255)	S3 [m]	DatBas L3	F	--	Acronym and title of the sponsored award (grant) to support the database infrastructure and/or content

						Format: 'ACRONYM: Title' *Ex:* 'SPRING: SPectroscopie InfraRouGe des matériaux planétaires hydratés' *Note DOI:* - recommended option as "FundingReference / awardTitle" (19.4) for "Database" and "Experiment" (from "*experiment*_owner_database")
*database*_sponsors	***List [L4]***	[O]				£: List of organizations that provide ponctual financial support for the development of part of the database content. *Note DOI:* - recommended option as "ContributorType=Sponsor" (7.1)
*database*_sponsor_acronym	varchar(255)	S2 [O!_m]	DatBas L4	F	--	Acronym of the organization that provide ponctual financial support for the development of part of the database content. *Condition*: mandatory when " *database*_sponsor_name" or "*database*_logo_filename" ≠ Ø *Notes:* - Includes organizations that issued a contract or under the auspices of which a work has been written, printed, published, developed, etc. - Includes organizations that provide in-kind support, through donation, provision of people or a facility or instrumentation necessary for the development of the database content, etc. *Note DOI:* requested in recommended option as "Contributor / contributorType=Sponsor / ContributorName" (7.2) for "Database" and "Bandlist". It will be combined with "*database*_sponsor_name": 'Institution full name (acronym)' *Ex*: 'ANR', 'Labex', …
*database*_sponsor_name	varchar(255)	S2 [m]	DatBas L4	F	--	Name of the organization that provide ponctual financial support for the development of part of the database content (+ grant #) *Notes:* see "*database*_sponsor_acronym" - a award/grant # can be added

						Note DOI: see "*database*_sponsor_acronym" *Ex*: 'Agence Nationale de la Recherche (LABEX-OSUG #123-456)', 'Laboratoires d'excellence', …
*database*_sponsor_logo_filename	varchar(255)	P [m]	DatBas L4	F	--	File name (with extension) of the logo of the sponsor *Image formats:* .png *Note:* should follow the following rules for the format: • Larger size L > 300 pix • Format: .png, transparent background (alpha canal of png) • cropped (i.e. no margin around the logo) *Note:* this file will be imported in the database and displayed in the database page of the SSHADE web site.
Database web sites						
database_links	***List [L3]***	[!]				£: web pages of the database
*database*_link_name [*xxx*_link_name]	varchar(255)	U [!_m]	DatBas L3	F	--	Name of the web site(s) of the database at its laboratory/organization *Ex:* 'GhoSST database web page', ……
*database*_link_url [*xxx*_link_url]	CS-varchar(255)	S2 [!_m]	DatBas L3	F	--	URL address(es) of the entry web page of the database at its laboratory/organization *Ex:* 'http://ghosst.osug.fr/', *Note:* this front web page of the database will redirect to the SSHADE infrastructure front & search page. It is requested but not absolute mandatory as the access can be also done directly through the SSHADE web page.
*database*_comments	blob	U [m]	DatBas	F	--	Additional information on the database.

3.3 Laboratory Table

Root of the table: ***laboratory***

Data type: 'Laboratory'

Key-word	Type	Level	Table	Exp	Unit	Description
Laboratory import mode and indexes						
*laboratory*_import_mode	enum(text)	P [!!_m]	Labo	F	--	Mode of import of the "laboratories" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*laboratory*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Labo	(V)	--	Name of the storage copy of the xml import file of the laboratory metadata ➔ determined automatically during import (from "*laboratory*_uid"?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*laboratory*_index [**][-xml]	int(10)	B [!!_g]	Labo	F	--	Automatic random but unique number (internal ID) given to new laboratory.
*laboratory*_uid [**]	varchar(255)	S0 [!!_m]	Labo	F	--	Unique identifier code (UID) given to the laboratory table (to be created) *Nomenclature:* Create this code name with 'LAB_' in order to be unique. It should be of the style 'LAB_LabAcronym A laboratory UID should be of the style 'LAB_LabAcronym(_InstAcronym)' where 'LabAcronym' is the acronym of the laboratory, possibly followed by the institute laboratory 'InstAcronym'. *Note*: use only UPPERCASES *Ex:* 'LAB_IPAG', 'LAB_WP_UNIBE', 'LAB_CML_IGSPAS'

laboratory_manager_databases	***List [L1]***	[!!]				£: databases which manage this laboratory
*laboratory*_manager_database_uid [*]	varchar(255)	S1 [!!o_m]	Labo DatBas L1	F	--	Link(s) to the existing UID(s) of the database which manages this laboratory information *Condition:* at least one database *Note:* For external laboratories, not managed by a database, it should be 'DB_SSHADE'
Laboratory name and address						
*laboratory*_acronym	varchar(255)	S0 [!!_m]	Labo	F	--	Acronym of the laboratory *Ex:* 'LPG', 'IPAG', 'ENS-Lyon', 'LGGE', …
*laboratory*_name	varchar(255)	S0 [!!_m]	Labo	F	--	Full Name of the laboratory *Ex:* 'Laboratoire de Planétologie de Grenoble', 'Institut de Planétologie et d'Astrophysique de Grenoble', 'Laboratoire de Géologie - Ecole Normale Supérieure de Lyon', 'Laboratoire de Glaciologie et Géophysique de Grenoble'...
*laboratory*_description	blob	S3 [m]	Labo	F	--	General description of the scientific/technical activity of the laboratory *Note:* you can give some details about the different geographic sites, if any
laboratory_organizations	***List [L2]***	[!]				£: Parent organizations to which belong the laboratory *Note:* the laboratory can have multiple parent organization
*laboratory*_organization_acronym	varchar(255)	S1 [!_m]	Labo L2	F	--	Acronym of the parent organization to which belong the laboratory *Ex: '*CNRS', 'UGA, 'UCBL, …
*laboratory*_organization_name	varchar(255)	S2 [!_m]	Labo L2	F	--	Name of the parent organization to which belong the laboratory *Ex: '*Centre National de la Recherche Scientifique', 'Université Grenoble

						Alpes', 'Université Claude Bernard – Lyon', … *Note DOI:* needed in: - "Creator/affiliation" (2.3) for 'experiment' (via "experiment_experimentalist_uid"+"experimentalist_laboratory(current)")
laboratory_addresses	***List [L3]***	[!!]				£: Addresses of the laboratory *Note:* the laboratory can be split in multiple geographic sites or you can put its geographic address and its postal address
*laboratory*_address_label	varchar(255)	U [m]	Labo L3	F	--	Label of the address or name of the geographic site of the laboratory *Notes:* - to discriminate between geographic and postal addresses - in case the laboratory has multiple geographic sites - you can put either the building name or any site label or name - you can shortly describe what is on this site *Ex:* 'Site Roche - Toulouse', 'Site Belin - Toulouse', 'Site - Tarbes' (for IRAP). *Ex:* 'Bâtiment A (Astrophysics groups)', ' Bâtiment PhITEM D (Planetary Sciences group)' (for IPAG)
*laboratory*_address_street	varchar(255)	U [!_m]	Labo L3	F	--	Street address and building number/name of the laboratory, and/or PO Box *Note:* can also include building name/number *Ex:* '122 rue de la Piscine', 'BP 59, Cedex 9'
*laboratory*_address_postal_code	varchar(255)	S2 [!_m]	Labo L3	F	--	Postal code of the laboratory *Ex:* '38000', '38042'
*laboratory*_address_city	varchar(255)	S1 [!_m]	Labo L3	--	--	City or locality of the laboratory *Ex:* 'Saint Martin d'Hères', 'Grenoble'

*laboratory*_address_region	varchar(255)	S2 [m]	Labo L3	--	--	Region, state, province, or county of the laboratory *Ex:* ‘Hampshire’, ‘Rhône-Alpes’, ‘Arizona’, …
*laboratory*_address_country_code	enum(text)	S1 [!!_m]	Labo L3	F	--	2-digit country code of the laboratory Enum: {CH, DE, DZ, ES, FR, GB, HU, IN, IT, PL, TW…} Label (code): Albania (AL), Algeria (DZ), Andorra (AD), Argentina (AR), Armenia (AM), Australia (AU), Austria (AT), Azerbaijan (AZ), Belarus (BY), Belgium (BE), Bolivia (BO), Bosnia and Herzegovina (BA), Brazil (BR), Bulgaria (BG), Canada (CA), Chile (CL), China (CN), Croatia (HR), Cyprus (CY), Czechia (CZ), Denmark (DK), Estonia (EE), Finland (FI), France (FR), French Guiana (GF), French Polynesia (PF), Georgia (GE), Germany (DE), Greece (GR), Guadeloupe (GP), Hoy See (Vatican city) (VA), Hungary (HU), Hong Kong (HK), Iceland (IS), India (IN), Indonesia (ID), Ireland (IE), Israel (IL), Italy (IT), Japan (JP), Kazakhstan (KZ), Korea (republic of) (KR), Kosovo (??), Latvia (LV), Lebanon (LB), Liechtenstein (LI), Lithuania (LT), Luxembourg (LU), Macedonia (MK), Malta (MT), Mexico (MX), Moldova (MD), Monaco (MC), Montenegro (ME), Morocco (MA), Netherlands (NL), New Zealand (NZ), Norway (NO), Pakistan (PK), Poland (PL), Portugal (PT), Réunion (RE), Romania (RO), Russian Federation (RU), San Marino (SM), Serbia (RS), Slovakia (SK), Slovenia (SI), South Africa (ZA), Spain (ES), Svalbard and Jan Mayen (SJ), Sweden (SE), Switzerland (CH), Taiwan (TW), Tunisia (TN), Turkey (TR), Ukraine (UA), United Kingdom (GB), United States (US), Venezuela (VE), Viet Nam (VN), …} *Definitions:* - Follow the international norm ISO 3166-1 alpha-2 two-letter country codes - list defined in https://en.wikipedia.org/wiki/ISO_3166-1_alpha-2 or - https://www.iso.org/obp/ui/#search/code/

Laboratory history

*laboratory*_date_begin	date	U [m]	Labo	F	YYYY-MM-DD	Beginning date of the laboratory *Ex:* '1995-10-01'
*laboratory*_date_end	date	U [£o_m]	Labo	F	YYYY-MM-DD	Ending date of the laboratory *Condition:* Compulsory when the laboratory stop its activity (under this name) *Note:* for currently active laboratory, keep it void. *Ex:* '1999-10-05', ''
Laboratory web sites						
laboratory_links	***List [L3]***	[!]				£: web pages of the laboratory and organization(s)
*laboratory*_link_name [*xxx*_link_name]	varchar(255)	U [!_m]	Labo L3	F	--	Name of the web site(s) of the laboratory *Ex:* 'IPAG web site', …
*laboratory*_link_url [*xxx*_link_url]	CS-varchar(255)	U [!_m]	Labo L3	F	--	URL address of the web pages of the laboratory or organization *Ex:* 'http://ipag.osug.fr/', …
*laboratory*_comments	blob	U [m]	Labo	F	--	Additional information on the laboratory (Tel, …).

3.4 Experimentalist Table

Root of the table: ***experimentalist***

Data type: 'Experimentalist'

Key-word	Type	Level	Table	Exp	Unit	Description
User + Experimentalist import mode and indexes						
*experimentalist*_import_mode	enum(text)	P [!!_m]	Exper	F	--	Mode of import of the "experimentalists" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*experimentalist*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Exper	(V)	--	Name of the storage copy of the xml import file of the experimentalist metadata ➔ determined automatically during import (from "*experimentalist*_uid"?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*experimentalist*_index [**][-xml]	int(10)	B [!!_g]	Exper	F	--	Automatic random but unique number (internal) given to new experimentalist
*experimentalist*_uid [**]	varchar(255)	S0 [!!_m]	Exper	F	--	Unique identifier code given to the experimentalist table (to be created) *Nomenclature:* Create this code name with 'EXPER_' in order to be unique. It should be of the style 'EXPER_FirstName_FamilyName(_n) where 'n' is an optional integer when there are 2 or more homonyms. *Note:* use UPPERCASES for the first letters of FirstName and FamilyName and lowercase for the other *Ex:* 'EXPER_Bernard_Schmitt'

experimentalist_manager_databases	***List [L0]***	[!!]				£: databases which manage this experimentalist
*experimentalist*_manager_database_uid [*]	varchar(255)	S1 [!!o_m]	Exper DatBas L0	F	--	Link(s) to the existing UID(s) of the database which manages this experimentalist information *Condition:* at least one database *Note:* For external experimentalists, not managed by a database, it should be 'DB_SSHADE'

Experimentalist name and identifiers

*experimentalist*_first_name	varchar(255)	S1 [!!_m]	Exper	F	--	First Name (given name) of the user/experimentalist *Note DOI:* requested in: - "creatorName" and "givenName" for 'experiment' (via "experiment_experimentalist_uid") *Ex:* 'Bernard'
*experimentalist*_family_name	varchar(255)	S1 [!!_m]	Exper	F	--	Family Name (last name) of the user/experimentalist *Note DOI:* requested in: - "creatorName" and "familyName" for 'experiment' (via "experiment_experimentalist_uid") *Ex:* 'Schmitt'
*experimentalist*_acronym	CS-varchar(255)	S0 [!_m]	Exper	F	--	Acronym of the experimentalist: initials of first and last names *Ex:* 'BS', 'EQ', 'FROD'
*experimentalist*_orcid_identifier	varchar(255)	S0 [!_m]	Exper	F	--	ORCID identifier code that uniquely identify the experimentalist *Definition*: - ORCID': http://orcid.org. ORCID (Open Researcher and Contributor ID) is a nonproprietary alphanumeric code to uniquely identify scientific and other academic

						authors and contributors. These identifiers consist of a reserved block of ISNI identifiers for scholarly researchers and administered by a separate organization (https://en.wikipedia.org/wiki/ORCID) *Note:* by default, the identifier scheme is 'ORCID' *Ex:* '0000-0002-7285-027X' (ORCID-ID) *Note DOI:* requested in: - "Creator/nameIdentifier" (2.2) for 'experiment' (via "experiment_experimentalist_uid")
experimentalist_alternate_identifiers	***List [L0]***	[O]				£: other alternate unique identifiers(s) of the experimentalist
*experimentalist*_alternate_identifier_scheme	enum(text)	U [O!!_m]	Exper L0	F	--	Scheme(s) that provideds the unique identifiers(s) of the experimentalist Enum: {ISNI, ResearcherID, ScopusAuthorID} *Definitions*: - '*ISNI*': http://www.isni.org The International Standard Name Identifier (ISNI) is an identifier for uniquely identifying the public identities of contributors to media content such as books, TV programmes, and newspaper articles. Such an identifier consists of 16 digits. It can optionally be displayed as divided into four blocks (https://en.wikipedia.org/wiki/International_Standard_Name_Identifier) - '*ResearcherID*': http://www.researcherid.com/rid. ResearcherID is an identifying system for scientific authors. The system was introduced in January 2008 by Thomson Reuters (https://en.wikipedia.org/wiki/ResearcherID) - '*ScopusAuthorID*': https://www.scopus.com Scopus IDs for individual authors can be integrated with the open source digital identifier ORCID *Note DOI:* requested in: - "Creator/nameIdentifierScheme" (2.2.1) for 'experiment' (via "experiment_experimentalist_uid")

						Note DOI: a correpondance table will give the corresponding 'URI of the name identifier scheme' requested in "schemeURI"
*experimentalist*_alternate_identifier_code	CS-varchar(255)	S2 [O!!_m]	Exper L0	F	--	Code that uniquely identify the experimentalist in this scheme *Note DOI:* requested in: - "Creator/nameIdentifier" (2.2) for 'experiment' (via "experiment_experimentalist_uid") *Ex:* 'A-1064-2009' (ResearcherID)
*experimentalist*_status [to be added in v0.9.0a]	enum(text)	S3 [!!_md]	Exper	F	--	General status of the experimentalist Enum: {active, inactive, retired, deceased} *default* = 'active' *Definitions*: - '*active*': currently actively working in one of the fields linked with the database - '*inactive*': previously active but no more working in one of the fields linked with the database - '*retired*': previously actively working in one of the fields linked with the database, but currently retired - '*deceased*': deceased *Ex:* - a PhD student that went to secondary school teaching will be tagged 'inactive'
Experimentalist laboratories						
experimentalist_laboratories	***List [L1]***	[!!]				£: laboratory(ies) of the experimentalist *Condition:* absolute mandatory
*experimentalist*_laboratory_state	flag (text)	S1 [!!_m]	Exper	F	--	Flag telling if this laboratory is the previous or current one of the experimentalist.

			L1			Enum: {previous, current} *Condition:* absolute mandatory Constraint: "*experimentalist*_laboratory_state" = 'current' only when "*experimentalist*_status" = {active} [to be added in v0.9.0a] *Definitions:* - 'previous': laboratory where the experimentalist previously worked - 'current': laboratory where the experimentalist currently works *Note:* several 'current' laboratories are allowed *Note xml:* this KW is a flag at each block "*experimentalist*_laboratory"
*experimentalist*_laboratory_uid [*]	varchar(255)	S1 [!!_m]	Exper Labo L1	F	--	Link to the existing UID(s) of the current or previous laboratory(ies) of the experimentalist Note: i.e. link to "*laboratory*_uid" *Note xml*: for occasional external experimentalists you can create a "laboratory" with information just limited to the laboratory name, acronym, and country + DB_manager (set all others to 'NULL')
*experimentalist*_laboratory_status	enum(text)	S1 [!o_m]	Exper L1	F	--	Status of the experimentalist in this laboratory Enum: {researcher, engineer, post-doc, PhD student, master student, undergraduate student} *Condition:* mandatory only when "*experimentalist*_laboratory_state" = {current}
*experimentalist*_laboratory_date_begin	date	S2 [!!o_m]	Exper L1	F	YYYY-MM-DD	Beginning date of the experimentalist in this laboratory *Ex:* '1995-10-01' *Condition:* absolute mandatory only when "*experimentalist*_laboratory_state" = {current}
*experimentalist*_laboratory_date_e	date	S2	Exper	F	YYYY-MM-	Ending date of the experimentalist in this laboratory

nd		[!!o_m]	L1		DD	*Condition:* absolute mandatory only when "*experimentalist*_laboratory_state" = {previous} *Note:* for the current lab, keep it void. *Ex:* '1999-10-05',
*experimentalist*_laboratory_comments	blob	U [m]	Exper L1	F	--	Additional information on the experimentalist in this laboratory.
Experimentalist contacts						
*experimentalist*_email	varchar(255)	S2 [!_m]	Exper	F	--	Current e-mail address of the experimentalist *Note:* this email is used as 'login'
*experimentalist*_phone	varchar(255)	S2 [m]	Exper	F	--	Current phone number of the experimentalist (+ country code) *Ex:* +33(0)476514150
experimentalist_links	***List [L3]***	[O]				£: Current web pages of the experimentalist
*experimentalist*_link_name [*xxx*_link_name]	varchar(255)	U [m]	Exper L3	F	--	Name of the web site(s) of the experimentalist *Ex:* 'Professional web page', 'GhoSST database web page', …
*experimentalist*_link_url [*xxx*_link_url]	CS-varchar(255)	S3 [O!_m]	Exper L3	F	--	URL address of the experimentalist web page *Ex:* http://ipag.osug.fr/~schmitt, …
*experimentalist*_comments	blob	U [m]	Exper	F	--	Additional information on the experimentalist. e.g. to which info should be asked if he/she is no more available.

4. JOURNALS - PUBLICATIONS

4.1 Description

* The **"Journal"** table is intended to provide various equivalent names and acronyms to the official journal name.

- The 'journal' table record the official name of the journal together with lists of alternate or abbreviated names and acronyms.

The *'publication'* table refers to this 'journal' table.

* The **"Publication"** table provide complete information and links on all types of official or internal publications (papers, books, proceedings, PhD, reports, …)

- The 'publication' table contain its types, publication state and rights as well as the complete reference (authors, year, title, journal, volume, issue, pages) and its abstract, or equivalent/supplementary information for conference procceedings (conference name, location, date), book (editor, publisher, …) or external database (name, url). It is completed with relevant content and keyword lists and a set of codes (doi, bibcode, …) and links (publication url, ads, local storage, …) are provided. Additional links to spectra, bandlists and other publications allow to connect the publication with the data they use.

Most of the keywords and some enumerations are similar to BibTeX format (http://en.wikipedia.org/wiki/BibTeX) for better interoperability with the online tool (SSHADE providers interface) designed to facilitate the preparation and ingestion of publication data.

The *"publication", "molecule",* all *"phases", "objects"* and *"matters", "sample", "material", "instrument", "experiment", "spectrum", "bandlist",* and *"band"* as well as the future *"band parameters"* and *"mode parameters"* tables refer to this 'publication' table.

4.2 Journal Table

Root of the table: ***journal***

Data type: 'Journal'

Key-word	Type	Level	Table	Exp	Unit	Description
Journal import mode						
*journal*_import_mode	enum(text)	P [!!_m]	Journ	F	--	Mode of import of the "journals" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*journal*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Journ	(V)	--	Name of the storage copy of the xml import file of the journal metadata ➔ determined automatically during import (from "*journal*_uid"?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Journal indexes and type						
*journal*_index [**][-xml]	int(10)	B [!!_g]	Journ	--	--	Automatic random but unique number (internal) given to new journal
*journal*_uid [**]	varchar(255)	S0 [!!_m]	Journ	--	--	Unique identifier code given to the journal table (to be created) *Nomenclature:* Create this code name with 'JOURNAL_' followed by the acronym of the journal *Note*: It should be of the style 'JOURNAL_JournalAcronym' where 'JournalAcronym' is the simplified acronym of the journal (replace all 'space' by '_' and all non alphanumeric characters by basic ASCII or '_', '-') *Ex:* 'JOURNAL_Adv_Space_Res', 'JOURNAL_MNRAS'

Journal names and acronyms

*journal*_name [tag WoS: SO !]	varchar(255)	S0 [!!_m]	Journ	--	--	Full official name of the journal *Ex:* Advances in Space Research, Applied Optics, Astronomical Journal, Astronomy and Astrophysics, Astronomy and Astrophysics Supplement Series, The Astrophysical Journal, Astrophysical Journal Letters, Atmospheric Chemistry and Physics, Chemical Engineering Journal, Chemical Physics, Clays and Clay Minerals, Earth and Planetary Science Letters, Eos - Transactions American Geophysical Union, Faraday Discussions, Geochimica et Cosmochimica Acta, Geophysical Research Letters, Icarus, Journal of the American Chemical Society, Journal of Chemical Engineering Data, Journal of Chemical Physics, Journal of Geophysical Research - Planets, Journal of Molecular Spectroscopy, Journal of Physical and Chemical Reference Data, Journal of Physical Chemistry, Journal of Physical Chemistry A, Journal of Physical Chemistry B, Journal of Quantitative Spectroscopy and Radiative Transfer, Meteoritics, Meteoritics and Planetary Science, Meteoritics and Planetary Science Letters, National Bureau of Standards, Nature, Physical Chemistry Chemical Physics, Planetary and Space Science, Remote Sensing Review, Science, Spectrochimica Acta A, Vibrational Spectroscopy, …} *Note*: this list should follow the official name of the journal
*journal*_abbreviated_name	varchar(255)	S0 [!!_m]	Journ	--	--	Official abbreviated name of the journal *Ex:* Adv. Space Res., Astron. Astrophys., Astron. Astrophys. Suppl. Ser., Astron. J., Astrophys. J., Astrophys. J. Lett., Appl. Opt., Atm. Chem. Phys., Chem. Eng. J., Chem. Phys., Clays Min., Faraday Disc., Icarus, J. Am. Chem. Soc., J. Chem. Eng. Data, J. Chem. Phys., J. Mol. Spectrosc., Data, J. Phys. Chem., Meteor., Nature, Rem. Sens. Rev., Science, Spectrochim. Acta A, Vib. Spec., … *Note*: - this list should follow the ISO 4 norm (Rules for the abbreviation of title words and titles of publications). - see List of Title Word Abbreviations (LTWA): http://www.issn.org/services/online-services/access-to-the-ltwa/

- see search tool at: http://cassi.cas.org/search.jsp
- or: http://www.journalabbr.com/ (Journal Abbreviation database)

*journal*_alternative_names	***List [L1]***	[m]				£: List of the alternative names of the journal
*journal*_alternative_name	varchar(255)	S1 [m]	Journ L1	--	--	Alternative name of the journal *Note*: provides all the variants of the full and abbreviated names of the journal *Ex:* Astrophysical Journal
journal_acronyms	***List [L2]***	[m]				£: List of the acronyms of the journal
*journal*_acronym	varchar(255)	S1 [m]	Journ L2	--	--	Acronym of the journal *Note*: provides all the acronyms of the journal and their variants *Ex:* AA, A&A, AASS, ApJ, EOS, EPSL, GCA, GRL, Icarus, JGR E, JPCA, JPCB, JQSRT, MAPS, MAPSL, NBS, PCCP, PSS, …
*journal*_url	varchar(255)	S2 [!_m]	Journ	--	--	URL of the main page of the journal *Note:* For the case of no paper DOI, nor identifier, nor direct url to allow to send to the journal main page
*journal*_comments	blob	U [m]	Journ	--	--	Any comment about the journal

4.3 Publication Table

Root of the table: ***publication***

Data type: 'Publication'

Note: [w] in the 'Level' column means that the value will be taken from a BibTeX bibliographic file when available.

Key-word	Type	Level	Table	Exp	Unit	Description
Publication import mode						
*publication*_import_mode	enum(text)	P [!!_m]	Publi	F	--	Mode of import of the "publications" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*publicaion*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Publi	(V)	--	Name of the storage copy of the xml import file of the publication metadata ➔ determined automatically during import (from "*publication*_uid" ?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Publication indexes and type						
*publication*_index [**][-xml]	int(10)	B [!!_g]	Publi	--	--	Automatic random but unique number (internal) given to new publication
*publication*_uid [**]	varchar(255)	S0 [!!_m]	Publi	-	--	Unique identifier code given to the publication table (to be created) *Nomenclature:* Create this code name with 'PUBLI_' followed by the name of the first author and the publication year, plus possibly a letter *Note*: It should be of the style 'PUBLI_FirstAuthorName_Year(Letter)' where 'FirstAuthorName' is the last name of the first author (with capital first letter), 'Year' the year of the publication and 'Letter' an optional small case letter ('a', 'b', …) in case of two or more publications with same first author and same

year.

Ex: PUBLI_Schmitt_2002', 'PUBLI_Quirico_1997b'

Publication

*publication*_type [tag WoS: PT !]	enum(text)	S1 [!!_mw]	Publi	--	--	Type of publication Enum: {journal, book, conference proceeding, abstract booklet, thesis, report, manual, catalog, database, other} *Definitions:* - '*journal*': standard journal publishing individual papers, generally reviewed - '*book*': book either commonly written by single/multiple authors or with several chapters independently written by different authors. - '*conference proceeding'*: proceedings of a conference (reviewed or not) - '*abstract booklet'*: booklet containing the abstracts (short or extended) of a conference - '*thesis*': PhD and Master's thesis manuscript - '*report*': scientific or technical internal or external report, generally without any review - '*manual*': manual containing technical documentation - '*catalog*': catalog describing a set of materials, such as cosmic grains, lunar sample, … - '*database*': database containing documents or web pages - '*other*': any other type of publication
*publication*_document_type [tag WoS: DT (rare)]	enum(text)	S1 [!!_mw]	Publi	--	--	Type of document Enum: {article, review article, discussion paper, discussion, correction, book, book chapter, conference paper, conference abstract, phd thesis, master thesis, scientific report, technical report, technical documentation, catalog of data, catalog of objects, database, numerical data set, other} *Definitions:* - '*article*': an article from a journal or magazine, also include 'letters'

- ‘*review article’*: an article whose aim is to review a sujct, and published as such.
- ‘*discussion*’: discussion of a paper published in a journal
- ‘*correction*’: correction on a paper published in a journal
- ‘*book*’: whole book with an explicit publisher
- ‘*book chapter’*: book chapter or section
- ‘*conference paper’*: a conference paper published either in a printed conference proceeding or on-line. Conference papers published in special issues of journals are ‘article’
- ‘*conference abstract’*: a conference abstract published either in an abstract booklet or on-line
- ‘*phd thesis’*: a PhD thesis
- ‘*master thesis’*: a master’s thesis
- ‘*catalog of data*’: catalog describing a set of data, such as various types of observations or properties: orbits, spectra, observation from instrument or spacecraft, …
- ‘*catalog of objects*’: catalog describing a set of objects, such as astronomical objects: comets, cosmic dust grains, lunar samples, …
- ‘*scientific report’*: printed and bound scientific report but witout named publisher
- ‘*technical report’*: printed and bound technical report but witout named publisher
- ‘*technical documentation’*: technical manual
- ‘*database*’:
- ‘*other*’: if none of the above document types fit

Note: see ‘entry type’ in http://en.wikipedia.org/wiki/BibTeX

*publication*_state	enum(text)	S1 [!!_m]	Publi	--	--	Publication state of the document Enum: {published, in press, submitted, internal, unpublished} *Definitions:* - ‘*published*’: published (widely enough) by an official publisher - ‘*in press’*: in press by an official publisher - ‘*submitted*’: submitted to an official publisher - *‘internal*’: printed document with very limited distribution (sometimes

						restricted) - '*unpublished*': unpublished document
*publication*_access_right	enum(text)	S1 [!!_m]	Publi	--	--	Publisher right on the document Enum: {publisher copyright, publisher free, free, restricted} *Definitions:* - '*publisher copyright'*: copyrighted publication with access through publisher - '*publisher free'*: copyrighted publication but put in free access at publisher web site - '*free*': publication in free access - '*restricted*': document in restricted access
*publication*_access_free_date	date	S2 [m]	Publi	--	YYYY-MM-DD	Date at which the document will be freely acessible, in case of publisher copyrights *Note:* This date will allow a routine to change "*publication*_access_right" to {publisher free} after this date. It will be used to inform the users.
publication_authors	***List [L1]***	[!!]				£: Ordered list (as in the publication) of the authors of the publication *Note xml:* the authors should be entered in the xml file in the same order as in the publication *Note:* the first authors and rank of the other authors will be calculated with this ordered list. *Note*: it can be the authors of a dataset in an external database when "*publication*_document_type" = {database, numerical data set}
*publication*_author_first_name [tag WoS: AU !]	varchar(255)	S2 [!!_mw]	Publi L1	--	--	Initial(s) of the first name (given name) of all authors of the publication. Plus possible type of group/team of authors *Note:* a 'dot' and a 'space' should be put between multiple initials: (ex: 'J. F. K.'), except for linked composed names (e.g. Jean-Jacques: 'J.-J.') *Ex:* 'B.', 'E.', 'F.-R.', 'J. F. K.', 'Team' for ''OMEGA Team''

*publication*_author_family_name [tag WoS: AU !]	varchar(255)	S0 [!!_mw]	Publi L1	--	--	Family name (last name) of all authors of the publication. Plus possible name of group/team of authors *Ex:* 'Spectroman', 'Raman', 'Fluogirl', 'OMEGA' for ''OMEGA Team''
*publication*_year [tag WoS: PY !]	int(4)	S1 [!!_mw]	Publi	--	--	Year of publication (or, if unpublished, the year of creation) e.g.: '2010'
*publication*_title [tag WoS: TI !]	varchar(255)	S1 [!!_mw]	Publi	--	--	Full title of the publication (article, book chapter, thesis, …) *Note*: it can be the title of a dataset in an external database when "*publication*_document_type" = {database, numerical data set} *Note:* isotope numbers and ion charges will be written in parenthesis before the atom and after the species, respectively. Or in LaTeX. *ex:* 'C3H4(+)', '(13)CO2(2-)'
*publication*_journal	varchar(255)	S0 [!!o_m]	Publi	--	--	Full official or common name or acronym of the journal *Condition:* Only and absolute mandatory when *publication*_type" = 'journal' *Notes:* - use either a commonly accepted written form of the journal name or of the acronym (listed in "*journal*_name", "*journal*_abbreviated_name", "*journal*_alternative_name", and "*journal*_acronym") - the official journal name and the official abbreviated name will be determined using the "Journal" table.
*publication*_volume [tag WoS: VL !]	varchar(10)	S2 [!!o_mw]	Publi	--	--	Volume number of the journal of the publication, or of a multi-volume book *Note:* some journals have volume number including a letter (ascii) *Ex:* '125' ou 'E47' *Condition:* absolute mandatory only when "*publication*_type" = 'journal' and when "*publication*_state" = 'published'

*publication*_number [tag WoS: IS ! sauf Conf]	varchar(20)	S2 [mw]	Publi	--	--	Issue number of the journal of the publication *Note:* for JGR issue number is of the type 'E12'
*publication*_first_page [tag WoS: BP !] [tag WoS: AR]	varchar(10)	S2 [!!o_mw]	Publi	--	--	First page of the publication or publication code *Note:* with the new web reference system there is now a "publication code" (ascii) and no more first-last pages. This "publication code" will be also stored in "*publication*_first_page". *Condition:* absolute mandatory only when "*publication*_state" = 'published' *Ex:* '143' ou 'E12008'
*publication*_last_page [tag WoS: EP !]	int(10)	U [mw]	Publi	--	--	Last page of the publication *Note:* with the new web reference system ("publication code") this "*publication*_last_page" should be empty
*publication*_pages_number [tag WoS: PG]	int(10)	U [mw]	Publi	--	--	Number of pages of the publication *Note:* with the new web reference system ("publication code") the number of pages of the publication replace the last page information.

Publication abstract and Keywords

*publication*_abstract [tag WoS: AB !]	Blob	S2 [!o_mw]	Publi	--	--	Full abstract text of the publication *Condition:* mandatory only when "*publication*_document_type" = {article, review article, book, book chapter, phd thesis} *Note:* special symbols can be converted in LaTeX, or written in ascii. In that case for exemple the isotope number and the ion charge will be written in parenthesis before the atom and after the species, respectively *ex:* LaTex: $C_3H_4^+$, $^{13}CO_2^{2-}$ Ascii: 'C3H4(+)', '(13)CO2(2-)'
publication_keywords	***List [L2]***	[!]				£: Keywords describing the publication

*publication*_keyword
[tag WoS: ID x]
	varchar(255)	S0
		[!_m]
			Publi
			L2
				--	--	Keyword(s) describing the publication subject and content.
						Note: These keywords should be quite general and focused on the subject of the database (solids, spectra, ...) + some other general keywords.
						A complete list is available in a separate file: 'publications_keywords_content.xml'
						List (short): cf. file
						Instruments and spectra:
						- '*General KW'*: 'spectroscopy', 'thermodynamics', 'optics', 'photometry', 'polarization', 'instrument', 'sample cell', 'numerical model', …
						- '*Microscopy – imaging'*: any argument of the "*instrument*_microscopy_imaging" Enum
						- '*Instrument type'*: any argument of the "*instrument*_type" Enum
						- '*Spectroscopic technique'*: any argument of the "*instrument*_technique" Enum.
						- '*Spectra'*: any argument of the '*spectrum*_type' and '*bandlist*_spectrum_type' Enum followed by 'spectra'.
						  o Ex: 'Raman spectra'
						- '*Band list'*: 'band position', 'band width', 'band intensity', 'band integrated intensity', 'band vibration mode'
						- '*Spectral range'*: any argument of the '*parameters_instrument*_spectral_range_type' Enum.
						  o Ex: 'NIR', …
						- Samples, matters and species:
						- '*Processes'*: any argument of the '*sample*_processing_type' Enum followed by 'process'. Ex: 'irradiation process'
						- '*Matters'*: any matter family ("*matter_xxx*_family") but without ending by 'matter') and simple matter name ("*matter*_name").
						  o Ex: *ex:* 'snow', 'meteorite', 'Smectite Swy-2',
						- '*Atoms'*: any atom symbol ("*atom*_symbol") preceded by isotope "*atom*_mass_number_a" if not natural
						- *'Chemical function':* any chemical function formula (~ "*chemical_function*_formula")
						- '*Molecules'*: any molecule formula (~"*molecule*_formula")

- '*Minerals'*: any mineral name ("*mineral*_ima_name")
- '*adsorption*': 'absorption', 'interlayer'
- *Note:* the isotope number and the ion charge will be written in parenthesis before the atom and after the species, respectively

ex: 'C3H4(+)', '(13)CO2(2-)'

Applications:

- '*Planetary sciences'*: any category or name (except numeric codes) of solar system objects. Ex: Triton, Pluto, Mars, Comets, meteorite…
- '*Other sciences'*: any generic word characterizing the application
- Type of application: 'radiative transfer simulation', '…'
- Type of application object: 'surface', 'aerosols', 'grains'…,
- *'Observations (mission/observatory - instrument)': Ex*: 'Mars Express - OMEGA', 'UKIRT - CGS4', …

Conferences

Note: For conferences some of the KW of "book" may also be needed:'title', 'publisher', 'publisher_city':

*publication*_conference_name [tag WoS: CT]	varchar(255)	S0 [!o_mw]	Publi	--	--	Name of the conference of the publication *Condition:* mandatory only for "*publication*_type" = {conference proceeding, abstract booklet} *Note:* may be also needed for books coming from a conference
*publication*_conference_location [tag WoS: CL]	varchar(255)	S3 [o_mw]	Publi	--	--	Location of the conference of the publication (town, state, country) *Note:* only for "*publication*_type" = {conference proceeding, abstract booklet}
*publication*_conference_date [tag WoS: CY]	varchar(255)	U [o_mw]	Publi	--	--	Dates of the conference of the publication *Note:* only for "*publication*_type" = {conference proceeding, abstract booklet} *Note:* no special date format. Rather of type '25-28 September 2012'

Books

*publication*_book_chapter_number [tag WoS: ?]	varchar(255)	U [o_m]	Publi	--	--	Chapter number of the book *Note:* only for "*publication*_document" = {book chapter} *Note*: can be numeral or roman number
*publication*_book_title [tag WoS: ?]	varchar(255)	S1 [!o_m]	Publi	--	--	Title of the book containing the publication *Condition:* mandatory only for "*publication*_type" = {book} *Note:* also used for "*publication*_type" = {conference proceeding, catalog}
*publication*_book_series [tag WoS: ?]	varchar(255)	S0 [o_m]	Publi	--	--	Title of the book series in which the book was published *Notes:* - for "*publication*_type" = {book} - may also be used for "*publication*_type" = {conference proceeding, catalog}
*publication*_book_edition_number	varchar(255)	U [o_m]	Publi	--	--	Alphabetic number ('first', 'second', …) of the edition of the publication *Note:* only for "*publication*_type" = {book}

Publication editor and publisher

*publication*_editor [tag WoS: ?]	varchar(255)	S3 [o_m]	Publi	--	--	Name(s) of the editor(s) of the book *Notes:* - only for "*publication*_type" = {book, conference proceeding} - It is the laboratory for Master and PhD 'thesis' - all editors in one line if several *Ex:* E. Ditor, C. Oeditor and K. Iferien
*publication*_publisher [tag WoS: PU]	varchar(255)	S3 [!o_mw]	Publi	--	--	Name of the publisher of the publication *Condition:* mandatory only for "*publication*_type" = {book, conference proceeding, thesis} *Note:* It is mostly an university for Master and PhD 'thesis'

*publication*_publisher_city [tag WoS: PI]	varchar(255)	U [o_mw]	Publi	--	--	Name of the city and country of the publisher of the publication *Note:* only for "*publication*_type" = {book, conference proceeding, thesis}
Databases and numerical data sets						*Note*: a 'numerical data set' can be fully defined with "publication_title", "publication_doi" and "publication_url"
*publication*_dataset_database_name	varchar(255)	S0 [!o_m]	Publi		--	Name of the external database containing the data set *Condition:* only and mandatory for "*publication*_document_type" = {database, numerical data set}
*publication*_dataset_database_url	varchar(255)	S2 [!o_m]	Publi		--	Uniform Resource Identifier of the external database containing the data set *Condition:* only and mandatory for "*publication*_document_type" = {database, numerical data set}
Publication identifiers and links						
*publication*_doi [tag WoS: DI ! sauf Conf.]	CS-varchar(255)	S1 [!o_mw]	Publi	--	--	Digital Object Identifier of the publication (doi:) *Condition:* mandatory only for "*publication*_type" = 'journal' and when "*publication*_state" = 'published' *Notes*: - it can be the doi of a dataset in an external database when "*publication*_document_type" = {database, numerical data set} - its URL can be obtained from doi by adding 'https://doi.org/ (the recommended addresses changed from 'http://dx.doi.org' to 'https://doi.org/' (2017)). *Ex:* 10.1029/2008JE003197 *Ex:* https://doi.org/10.1029/2008JE003197
*publication*_url [-xml]	CS-varchar(255)	S2 [!o_cm]	Publi	--	--	URL of the publication (direct web link to publication at publisher web site) *Condition:* mandatory only for "*publication*_type" = 'journal' and when "*publication*_state" = 'published'

➔ Calculated from ”*publication*_doi”:
⇨ ‘https://doi.org/’”*publication*_doi”

Note:
- the recommended address root changed from ‘http://dx.doi.org/’ to ‘https://doi.org/’ (2017)
- it can be the url of a dataset in an external database when “*publication*_document_type” = {database, numerical data set}

publication_identifiers	***List [L3a]***	[O]				£: Other official identifiers of the publication
*publication*_identifier_type	varchar(255)	S1 [!!o_m]	Publi L3a	--	--	Acronym of the type of official identifier of the publication Enum: {ARK, arXiv, bibcode, EISSN, HAL, Handle, ISBN, ISSN, ISTC, PMID, TEL, URL, no} *Condition:* absolute mandatory when “*publication*_identifier_code” ≠ Ø *Definitions:* - ‘*ARK*’: (Archival Resource Key) is an identification system that can identify any type of digital object but also physical: books, publications and scientific articles. The BnF (Bibliothèque natioanle de France) is one of the Name Assigning Authority: http://gallica.bnf.fr/ark:/ - ‘*arXiv*’: repository of electronic preprints ⇨ https://arxiv.org/abs *cf.* https://arxiv.org/ - ‘*bibcode*’: compact identifier used by several astronomical data systems (ADS, …) ⇨ http://cdsads.u-strasbg.fr/abs/ (ADS, CDAS, Strasbourg, France) or http://adsabs.harvard.edu/abs (ADS, Harvard-Smithsonian, Cambridge, USA) *cf.* http://adsabs.harvard.edu/abs_doc/bibcodes_help.html http://en.wikipedia.org/wiki/Bibcode *Note:* useful for “publication_type” = ‘book’ and 'conference' for which ADS may have a scanned version and that may have no direct publisher link - ‘*EISSN*’: (or e-ISSN) standard label for "Electronic ISSN", the ISSN

for the electronic media (online) version of a serial.
    - ⇨ Simple identifier?
- '*HAL*': French open archive where authors can deposit scholarly documents from all academic fields (https://hal.archives-ouvertes.fr/)
    - ⇨ https://hal.archives-ouvertes.fr
- '*Handle*': assign persistent identifiers, or handles, to information resources
    - ⇨ https://en.wikipedia.org/wiki/Handle_System
- '*ISBN*': The International Standard Book Number (ISBN) is a unique numeric commercial book identifier. It is assigned to each edition and variation (except reprintings) of a book
    - ⇨ Simple identifier, findable with a search engine such as http://www.bookfinder.com/isbn_search/
- '*ISSN*': International Standard Serial Number (ISSN) is an eight-digit serial number used to uniquely identify a serial publication (magazines, …).
    - ⇨ Simple identifier, findable with a search engine such as the ISSN register (fee): https://www.issn.org/understanding-the-issn/the-issn-international-register/
- '*ISTC*': unique identifier for text-based works
    - ⇨ Simple identifier
- '*PMID*': PubMed Identifier
    - ⇨ https://www.ncbi.nlm.nih.gov/pubmed
- '*TEL*': 'Thèses En Ligne', the repository of the French PhD thesis
    - ⇨ https://tel.archives-ouvertes.fr
      cf. https://tel.archives-ouvertes.fr/
- *'URL':* for publications that have no official identifier code but have a stable URL at an alternative repository or web site
- *'no':* for publications that have neither an identifier, nor a stable URL.

Notes:

- some of these identifiers also play the role of official repository for all types of publications (ARK, arXiv, HAL, …) or part of the publications (bibcode, …) or some types only (TEL, …)
- description and properties of most of these identifiers:

						http://licence.rnbm.org/doc_utile/identifiants-docs-numeriques - publications that have neither an identifier, nor a stable URL (‘no’) should be stored as pdf files in SSHADE. Note DOI: relatedIdentifierType
*publication*_identifier_code	varchar(255)	S1 [!o_m]	Publi L3a	--	--	Identifier code of the publication (except DOI) *Condition:* mandatory when “*publication*_identifier_type” = {ARK, arXiv, bibcode, EISSN, HAL, Handle, ISBN, ISSN, ISTC, PMID, TEL} *Notes*: - this code should be an official one and correspond to the type described in “*publication*_identifier_type” (arXiv, HAL, ISBN, TEL, ...) - for some of them the URL can be constructed using this code and the URL root associated to the identifier type. *Ex:* - ‘1806.08056’ for arXiv:1806.08056v1 [astro-ph.EP] - ‘2012Icar..218..364B’ for bibcode - ‘hal-01132273’ for HAL: hal-01132273v1 - ‘tel-01010519’ for TEL: tel-01010519, version 1 - ‘URN:ISBN:0-395-36341-1’ for URN: ISBN:0-395-36341-1 Note DOI: relatedIdentifier
*publication*_identifier_url	varchar(255)	S2 [!o_cm]	Publi L3a	--	--	URL of the publication at this official repository *Condition:* mandatory when “*publication*_identifier_type” = {ARK, EISSN, ISBN, ISSN, ISTC, URL} *Condition:* calculated when “*publication*_identifier_type” = {arXiv, bibcode, HAL, PMID, TEL} ➔ calculated: the URL is constructed using the URL root associated to the type and the code: - ‘arXiv’: https://arxiv.org/abs/"*publication*_identifier_code" (code without ‘arXiv:’) - ‘bibcode’: http://cdsads.u-strasbg.fr/abs/"*publication*_identifier_code" or http://adsabs.harvard.edu/abs/"*publication*_identifier_code"

- ‘HAL’: https://hal.archives-ouvertes.fr/"*publication*_identifier_code"
- ‘Handle’: http://hdl.handle.net/"*publication*_identifier_code"
- ‘PMID’: https://www.ncbi.nlm.nih.gov/pubmed/"*publication*_identifier_code"
- ‘TEL’: https://tel.archives-ouvertes.fr/"*publication*_identifier_code"

Note:

- For “_type” = {ARK, EISSN, ISBN, ISSN, ISTC, URL} the url should be filled manually
- this URL should be stable, i.e. the publication file is stored in a stable repository or local web site.

Ex:

- ‘https://arxiv.org/abs/1806.08056’ for arXiv:1806.08056v1
- ‘http://cdsads.u-strasbg.fr/abs/2012Icar..218..364B’ for bibcode
- ‘https://hal.archives-ouvertes.fr/hal-01132273’ for HAL: hal-01132273v1
- ‘http://hdl.handle.net/10.1000/182’ for Handle
- ‘https://www.ncbi.nlm.nih.gov/pubmed/30409907’ for PMID 30409907
- ‘https://tel.archives-ouvertes.fr/tel-01010519’ for TEL: tel-01010519, version 1

Note DOI: identifier

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*publication*_filename	varchar(255)	S2 [!o_m]	Publi	--	--	Name of the pdf file of the publication *Condition:* mandatory only for “*publication*_access_right“ = {publisher free, free} *File formats:* .pdf *Notes:* - only for publications with ‘unrestricted’ rights, and some scanned publications impossible to found on the web (ex: proceedings, ESA-SP, …) or without publisher link (a few journals). - We also put in the database the pdf files of the publications on lab data with “*publication*_access_right” = ’publisher copyright’, but with

access limited to data managers (to verify that all publication infos are correctly entered).
- preprints, internal reports, … can also be uploaded.
- this file will be imported in the database

SSHADE data in the publication

publication_contents	***List [L4]***	[!]				£: publication content(s)
*publication*_content	enum(text)	S0 [!_m]	Publi L4	--	--	Publication content(s). Enum: {instrument-technique, numerical model, species, phase, sample, material-matter, object, spectral data, band list data, BRDF data, thermodynamic data, spectral data use, band list data use, BRDF data use, thermodynamic data use, astrophysics, planetary sciences, earth sciences, remote sensing, experimental physics, theoretical physics, applied physics, materials sciences, chemistry, optics, other application, ...} *Definitions:* - For Lab data publications: tell if the publication describes instrument and techniques, lab spectral data, sample or material preparation, matter: {instrument-technique, sample, material-matter, spectral data, band list data, BRDF data} - For publications of users of lab data: tell first the type(s) of lab data used {spectral data use, band list data use, BRDF data use} and in addition the category(ies) of application: {astrophysics, planetary sciences, earth sciences, experimental physics, theoretical physics, applied physics, materials sciences, chemistry, optics, other application, ...}
publication_cited_publications	***List [L5]***	[O]				£: Experimental publications cited in the paper
*publication*_cited_publication_uid [*]	varchar(255)	U [$o_m]	Publi Publi L5	F	--	Link(s) to the UID(s) of the experimental publications cited in the paper *Recommendation:* Strongly recommended when already exist in the database. *Condition:* only for papers which have data in the database

						Note: equivalent to reference list of the paper but limited to the experimental publications in the database
publication_used_experiments	***List [L6]***	[O]				£: SSHADE spectral data used or cited in 'data user' paper
*publication*_used_experiment_uid [*]	varchar(255)	S2 [$o_m]	Publi Spectr L6	F	--	Link(s) to the UID(s) of the experiment in the database that is used or cited in the paper *Recommendation:* Strongly recommended when already exist in the database. *Restriction:* only for experiment-spectra in the database that are used in a 'data user' paper or in a 'data provider' paper reefering to another experiment than the one described in the paper *Note:* if only one or a few spectra are used: link to their experiments *Note:* the experiments-spectra published in an experimental paper and entered in the database will be directly linked to their publication with "*experiment_/spectrum*_publication_uid" (their publications should be entered in the database before the spectrum, or corrected after).
publication_used_bandlists	***List [L7]***	[O]				£: SSHADE bandlist data used or cited in 'data user' paper
*publication*_used_bandlist_uid [*]	varchar(255)	US2 [$o_m]	Publi BandLi L7	F	--	Link(s) to the UID(s) of a bandlist in the SSHADE database that is used or cited in the paper *Recommendation:* Strongly recommended when already exist in the database. *Restriction:* only for band lists in the database that are used in an 'data user' paper or in a 'data provider' paper reefering to another experiment than the one described in the paper. *Note:* the bandlist published in an experimental paper and entered in the database will be directly linked to their publication with "*bandlist*_publication_uid" (their publications should be entered in the database before the bandlist, or corrected after).
*publication*_comments	blob		U	Publi	--	--	Any comment about the publication

[m]

5. Fundamental Species (molecular, atomic, chemical bonds & functions)

5.1 Definition

The "Fundamental Species" are the basic building pieces of the constituents of the samples and matters. They are grouped in 3 main families because they share most of their properties: **'atomic'** and **'molecular' species**. An additional virtual species called ‘chemical functions’ (including ‘bond’, ‘functional groups’, ‘anionic radicals’ in minerals, as well as some part of molecules) is added in order to allow to describe them, and their vibration, in molecules and in some minerals. Each of these families includes several types of species:

- Atoms and Ions
  - Atoms (neutral)
  - Atomic ions

- Chemical functions
  - Chemical bonds
  - Functional groups
  - Molecule parts
  - mineral anionic radicals (minerals)

- Molecular species
  - Molecules
  - Molecular ions
  - Radicals

Molecules, and chemical functions refer to atoms for their elemental and isotopic compositions.

Molecules refer also to chemical functions to describe their chemical bonds and functional groups.

The “Extraterrestrial matters” also refer to “atoms” for their elemental analysis and to “chemical functions” for their chemical analysis.

5.2 Description

The **Fundamental species** are either ***atomic, molecular,*** or ***mineral.*** The two last families of species are composed of the first one, i.e., ***atoms*** *and/*or ***ions.***

*** Atomic species** includes ***atoms*** and ***ions***.

As for molecules we also consider, for convenience, virtual atoms consisting of the "natural isotopic mix" of the isotopes of the atom.

- Each ***atomic species*** is defined by *"name and identifiers", “atomic numbers”, “natural isotopic composition”* and some *"physical properties"*.

**** Chemical functions*** (or ***Functional groups***) allow us to partly describe the molecular content of *complex organic solids*, in addition to elemental composition. They can also provide useful information for the other *molecular species*. For minerals they describe the chemical functions of anionic radicals. They allow to search molecules or minerals by one or more of their chemical functions.

Each ***chemical function*** is defined by *"names and identifiers", “chemical structure and atomic composition”*.

*** Molecular species** includes ***molecules, molecular ions*** and ***radical****s.*

Isotopic molecular species: Molecular species are mostly defined as pure isotopic species, but we also consider here, for convenience, virtual molecules consisting of the "natural isotopic mix" of the isotopomers (and of the spin isomers) of the molecule, although formally this mix should be classified as a "constituent" made of a homogeneous molecular mixture of isotopic and isomer species in natural abundances. Partially isotopically substituted molecules

(i.e. only part of the atoms are pure isotopic species, the others being in their natural abundances) can also be defined as virtual molecules. Any other isotopic or spin isomer mixture has to be described at the constituent level as a mixture of pure molecular species.

- **Molecules, molecular ions, radicals** have common key-words to describe them. Each ***molecular species*** is defined by *"names and identifiers"*, *"chemical structure, atomic and spin isomer compositions"* and *"physical properties"*. Natural isotopic mixtures are defined by their *"isotopic composition"*. The *"symmetries and normal vibration modes"* of the free molecular species are also described.

5.3 Atoms and Ions Table

Root of the table: ***atom***

Data type: 'Species'

For "*specie*_family" = {atom, element}

Key-word	Type	Level	Table	Exp	Unit	Description
Atom import						
*atom*_import_mode [*species*_import_mode]	enum(text)	P [!!_m]	Atom	(V)	--	Mode of import of the atom data Enum: {first import, (use existing), ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*atom*_xml_filename [-xml] [*species*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	Atom	(V)	--	Name of the storage copy of the xml import file of the atom metadata ➔ determined automatically during import (from "*atom*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Atom indexes and type						
*atom*_index [**][-xml] [*species*_index]	int(10)	B [!!_g]	Atom	F	--	Automatic random but unique number (ID) given to new atom
*atom*_uid [**] [*species*_uid]	CS-varchar(255)	S0 [!!_m]	Atom	F	--	Unique identifier code (UID) given to the atom table (to be created) *Note:* It should be of the style 'ATOM_(Z)Symbol' or 'ATION_(Z)SymbolCharge' where 'Z' is the atomic number Z (for pure isotopic atoms, none for natural mixtures), 'Symbol' is the atom symbol and 'Charge' is the ion charge (charge sign '-' or '+' after the charge number). *Ex:* 'ATOM_Kr', 'ATOM_13C' or 'ATION_Fe2+'

*atom*_type [*species*_type]	enum(text)	S1 [!!_m]	Atom	F	--	Type of atomic species. Enum: {atom, atomic ion}

Atom names and identifiers

*atom*_name [*species*_name]	varchar(256)	S0 [!!_m]	Atom	F	--	Generic name of the atom or ion (independent of isotope) *Notes:* - for ions: ending with explicit type and level of ion: cation, dication, trication, quadrication, …, anion, dianion, trianion, quadrianion, pentaanion, … - there are specific official names for the isotopic species of Hydrogen: 'Deuterium' and 'Tritium' and of hydrogen ion: 'Proton', 'Deuteron' and 'Triton' - It is used as the title of the mineral page on the SSHADE interface - ion names: http://www.geocities.ws/profmokeur/chimie/tableions.htm
*atom*_iupac_name [*species*_official_name]	varchar(255)	S0 [!!_m]	Atom	F	--	IUPAC unique name of the atom or ion (different for each isotopic species) *Note:* extention of this nomenclature to ions (+ same ending as for 'name') *Ex:* carbon-13, hydrogen-2, iron dication…
*atom*_inchi [*species*_inchi]	CS-varchar(255)	S1 [m]	Atom	F	--	Standard InChI sequence: IUPAC international chemical identifier, unique, of the atom (natural), ion (natural) or isotopic species. *Notes*: - for simplicity the InChI code must be entered without 'InChI='. This part will be added automatically during import. *Ex:* 'InChI=1S/H' (H)
*atom*_inchikey [*species*_inchikey]	CS-varchar(255)	S1 [m]	Atom	F	--	Standard InChI Key number, unique, of the atom or ion *Note:* can be found at http://cactus.nci.nih.gov/chemical/structure (http://www.chemspider.com/) (search for ex 'Carbon-12' for isotopes) *Ex:* 'YZCKVEUIGOORGS-UHFFFAOYSA-N' (H)

*atom*_cas_number [*species*_cas_number]	varchar(255)	S1 [m]	Atom	F	--	CAS registry number, unique, of the atom (natural and isotopic species?) or ion *Note:* can be found on French wiki at atom page *Ex:* '1333-74-0' (H)

Atom symbol and fundamental properties

*atom*_symbol [*species*_chemical_formula]	CS-varchar(5)	S0 [!!_m]	Atom	F	--	Symbol of the atom or ion (with charge) 2 letters: the first is upper case, the second is optional and lower case The charge can be added with '+' or '-' sign followed by the charge number. *Note:* Symbol did not include isotopes (no 'D' and 'T' => 'H') *Ex*: Fe, Fe3+
*atom*_formula [*species*_formula]	CS-varchar(255)	U [!!_m]	Atom	F	--	Developed formula of the atomic species *Syntax:* LaTeX format *Ex:* '$\= ^{13}C{2+}$' for: $=^{13}C^{2+}$ *Note:* contain isotopic and ionic information *Note:* 'D' and 'T' can be used for deuterium and tritium isotopes
*atom*_elemental_formula [-xml] [*species*_elemental_formula]	CS-varchar(255)	S0/S0c/ S1 [!_c]	Atom	F	--	Empirical elemental formula of the atom, including isotope ➔ Calculated: concatenation of 'atom_mass_number_a'+'atom_symbol' *Ex:* '16O' for pure isotope
*atom*_atomic_number_z	int(3)	S0 [!!_m]	Atom	F	*no*	Atomic number Z (or nuclear charge) of the atom or ion: number of protons in the atomic nucleus. Uniquely identify a chemical element.
*atom*_mass_number_a	int(3)	S0 [!!o_m]	Atom	F	*no*	Atomic mass number A: number of nucleons (protons and neutrons) in the atomic nucleus. Uniquely identify an isotopic atomic species. *Condition*: only for isotopic species: Absolute Mandatory when "*atom*_isotope_mixture_type" = 'pure isotope'.

						Note: no value is given for natural mixtures
*atom*_nuclear_spin_qn_i [*species*_nuclear_spin]	enum(text)	S2 [!_m]	Atom	F	--	Value of the nuclear spin quantum number I of the atom or ion isotope Enum: {0, 1/2, 1, 3/2, 2, 5/2, 3, 7/2, 4, 9/2, 5, 11/2, 6, 13/2, 7, 15/2} *Condition:* only if "*atom*_isotope_mixture_type" = 'pure isotope'. *Notes:* - Should be positive or negative multiple of 1/2 - no value is given for natural mixtures
atom_absorption_edges	***List [L1]***	[!o_m]				£: Web pages describing the atom or ion and its properties. *Condition*: mandatory when "*atom*_type" = 'atom' AND when "*atom*_isotope_mixture_type" = 'terrestrial abundance'
*atom*_absorption_edge_type	enum(text)	S2 [!o_m]	Atom L1	F	-	Type of absorption edge of the element Enum: {K, L1, L2, L3, M1, M2, M3, M4, M5, N1, N2, N3, N4, N5, N6, N7, O1, O2, O3, O4, O5, O6, O7}
*atom*_absorption_edge_energy	float	S3 [!o_m]	Atom L1	F	keV	Energy at absorption edge of the element *Unit:* keV *Note:* did not depend on isotope *Note:* values from http://skuld.bmsc.washington.edu/scatter/AS_periodic.html
*atom*_electronegativity [*species*_electronegativity]	float	S3 [!_m]	Atom	F	Pauling	Electronegativity of the atom (Pauling scale) • stored in the database and provided to user in 'Pauling' unit *Note:* did not depend on isotope *Note:* values from http://en.wikipedia.org/wiki/Electronegativity
*atom*_charge [*species*_charge]	int(2)	S2 [!!_m]	Atom	F	*no*	Charge number (positive or negative) of the atom or ion *Note:* = '0' for atoms, > '0' or < '0' for ions

*atom*_ion_atom_uid [*]	varchar(255)	S1i [!!o_m]	Atom Atom	F	--	Link to the existing UID of the element (neutral atom) that compose the ion *Condition:* Absolute Mandatory when "*atom*_type" = {atomic ion} *Constraint:* only when "*atom*_type" = {atomic ion} (only for ions) *Notes:* - mostly used for search of an element defined by its cation (for mineral phases) - for an atom its 'element' is itself.

Atom natural isotopic composition

*atom*_isotope_mixture_type [*species*_isotope_mixture_type]	enum(text)	S1 [!!_m]	Atom	F	--	Type of isotopic mixture of the atom or ion Enum: {pure isotope, terrestrial abundance} *Definitions:* – *'pure isotope'*: only a single isotopic species of the atom – *'terrestrial abundance*': mixture of all its isotopic species of the atom in 'standard' natural terrestrial abundance. Its natural isotopic composition is given by default in the natural 'generic mixture' (i.e. the 'non-isotopic species') entered in the SSHADE database with "*atom*_isotope_uid" and "*atom*_isotope_mole_fraction" of each isotopic species as by IUPAC (2009). *Notes:* - The fundamental atom species stored in the database will be either with natural terrestrial abundance or as pure isotopes. - Atoms with 'specific isotopic abundance' in sample or matters will be described using the main pure atomic isotopologues ("*(constituent_)species*_uid" = 'ATOM_xxx').
*atom*_isotope_atoms	***List [L4]***	[!o]				£: isotopic species contributing to the isotopic mixture of atoms *Condition*: mandatory bloc when "*atom*_isotope_mixture_type" = {terrestrial abundance} *Constraint* only when "*atom*_isotope_mixture_type" = {terrestrial abundance}

*atom*_isotope_atom_uid [*] [*species*_isotope_specie_uid]	varchar(255)	S1i [!o_m]	Atom Atom L4	F	--	Link to the existing UID of a pure isotopic atomic species contributing to the isotopic atomic mixture *Condition*: mandatory when "*atom*_isotope_mixture_type" = {terrestrial abundance}
*atom*_isotope_atom_mole_fraction [+] [*species*_isotope_specie_mole_fraction]	float	U [!o_m]	Atom L4	F	--	Mole fraction of the isotopic atomic species *Condition*: mandatory when the bloc is used *Notes:* – value between 0 and 1, the sum should be = '1' – for "*atom*_isotope_mixture_type " = 'terrestrial abundance' the mole fractions is given by IUPAC (2009) (www.chem.qmul.ac.uk/iupac)

Atom properties + references

*atom*_molar_mass [*species*_molar_mass]	float	S3 [!_m]	Atom	F	*g/mol*	Atomic molar mass. • stored in the database and provided to user in 'g/mol' (= amu) unit *Note:* – For isotopes this "atomic molar mass" is equivalent (in number) to the "atomic mass" in unified atomic mass units (u). This "atomic mass" is not defined for natural mixtures. – For a mixture it is determined by the sum of "atom_molar_mass" weighted by their "atom_isotope_atom_mole_fraction" for all isotopic atomic species composing the natural mixture. – For the standard terrextrial mixture values to be taken from IUPAC 2009 (www.chem.qmul.ac.uk/iupac)
*atom*_state_stp	enum(text)	S1 [!_m]	Atom	F	--	State of the atomic species in standard (STP) conditions Enum: {gas, liquid, solid} *Note:* – STP conditions (IUPAC): 273.15K (0°C), 100kPa (1 bar) – It is the state (homonuclear gas, liquid or solid) of the atom when it is

						put as a pure species in STP conditions
atom_links	***List [L2]***	[O]				£: Web pages describing the atom or ion and its properties.
*atom*_link_name [*species*_link_name]	varchar(255)	U [m]	Atom L2	F	--	Name of the web page(s) describing the atom or ion and its properties.
*atom*_link_url [*species*_link_url]	CS-varchar(255)	U [m]	Atom L2	F	--	URL address(es) of web page(s) describing the atom or ion and its properties. *Reference*: https://en.wikipedia.org/wiki/Periodic_table *Notes*: - you can link to a publication by giving its url address, preferably through its DOI. Ex: https://doi.org/10.1002/ejic.200700067
*atom*_comments [species_comments]	blob	U [m]	Atom	F Aj	--	Additional information on the atom or ion (major isotopic atom, radioactive stability, …)

5.4 Chemical bonds Table

Root of the table: ***chemical_bond***

Data type: 'Species'

For "*specie*_family" = 'chemical bond'

Notes:

- here we describe specific isotopic species or isotopic mixtures for chemical bonds and molecule parts. Chemical bonds are mostly used to describe vibrations.
- a specific point is that we describe a chemical bond as two atoms linked with a bond type (single, double, triple), but also considering the type of bonds (no, one or more) connecting these two atoms to the rest of the molecular species.

Key-word	Type	Level	Table	Exp	Unit	Description
Chemical bond import						
*chemical_bond*_import_mode [*species*_import_mode]	enum(text)	P [!!_m]	ChemB	(V)	--	Mode of import of the chemical bond data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*chemical_bond*_xml_filename [-xml] [*species*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ChemB	(V)	--	Name of the storage copy of the xml import file of the chemical bond metadata ➔ determined automatically during import (from "*chemical_bond*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Chemical bond indexes and type						
*chemical_bond*_index [**][-xml] [*species*_index]	int(10)	B [!!_g]	ChemB	F	--	Automatic random but unique number (ID) given to new chemical bond
*chemical_bond*_uid [**] [*species*_uid]	CS-	S0	ChemB	F	--	Unique identifier code (UID) given to the chemical bond or bond table (to be created)

varchar(255) [!!_m]

Nomenclature: Create this UID with ‘BOND_’ (for single bond) or ‘MOLECPART_’ (for part of a molecule) followed with the atomic numbers Z (for isotopic variants), the atom symbols separed by the Bond symbol (‘d’ or ‘t’, or nothing for single bond) and the ion charge (charge sign '-' or '+' after the charge number), if not null:
‘BOND_ZAtom1(BondSymbol)ZAtom2(Charge)’

Note: It should be unique. Each prefix corresponds to one specific “*chemical_bond*_type”.

Ex: ‘MOLECPART_CH2CH2CH3’, ‘BOND_CdO' , ‘BOND_13Cd18O'

Notes:

- The *vibrational* ‘bonds’ (BOND_) and ‘molecule parts’ (MOLECPART_) are either natural (used for terrestrial isotopic mix of a molecule) or made only of single isotopic atomic species (for isotopic molecules, and for band list) so it is necessary to describe them for all possible isotopes (or at least the mains).
  Ex: ‘BOND_CdO' , ‘BOND_13Cd18O',
  Ex: ‘MOLECPART_CH3’, ‘MOLECPART_13C1HD2’, ...
- ‘MOLECPART_’ is only used to describe vibrations involving more than 2 atoms of the molecule (not used to describe bonds in a molecule)

Notations:

- For *vibrational* bonds (BOND_, and MOLECPART):
  - a single bond: nothing
  - a double bond: will be noted with ‘d’,
  - a triple bond: with ‘t’ (because xml did not like ‘=’ and ‘#’ !)
  - a hydrogen bond: ‘h’
  - a ionic bond: ‘i’
  - a ring: ‘ring’ at the end
  - a cation: ’+’
  - an anion: ‘-‘
  - a radical’r’ (after the atom)
- Bond will have also their ‘surrounding’ bonds noted for better

discrimination (but single bonds are omitted):

Ex: C-C bonds:
- for -C-C-, -=C-C-, -=C-C=-, #C-C=-, #C-C#: 'BOND_CC', '_dCC', '_dCCd', 'tCCd', 'tCCt'
- for -C#C-: 'BOND_CtC'

Ex: 'O...H hydrogen bond': BOND_OhH
Ex: Na^{+}•Cl^{-} bond: BOND_Na+iCl-
Ex: part of molecule C_6 ring: 'MOLECPART_C6ring'
Ex: for CH3OH-nat:
- Natural 'bonds = 'BOND_CH3'
- Isotopic 'bonds = 'BOND_12CH', '_12CD', '_13CH', '_13CD', '_12C16O', '_13C16O', '_12C17O', ('_13C17O'), '_12C18O', ('_13C18O',) '_16OH', '_16OD', '_17OH', ('_17OD',) '_18OH', ('_18OD')

*chemical_bond*_type [*species*_type]	enum(text)	S1 [!!_m]	ChemB	F	--	Type of chemical bond Enum: {bond, molecule part} *Definitions:* Bonds and parts of a molecule used to describe vibrations - '*bond'*: for bonds between 2 atoms - '*molecule part'*: for molecules that can have part (but not all) of its atoms involved in some vibration modes (bending, …). It mostly consists of 3 atoms, but can have more such as in rings. *Note:* 'molecule part' may be also used to describe a known part of a unknown complex molecule (more complete information than just its individual functional groups). *Note*: If all atoms are involved in a vibration mode, the molecule (MOLEC_) will be used instead to describe vibrations.

Chemical bond names

*chemical_bond*_name [*species*_name]	varchar(255)	S0	ChemB	F	--	Generic name of the chemical bond

		[!!_m]				*Notes:* - same name for all isotopic species and for all types of surrounding bonds - did not include ionic information (atom charge) - It is used as the title of the chemical bond page on the SSHADE interface *Nomenclature:* - '*bond*': describe both atoms and end with 'bond' (for single bond), 'double bond' or 'triple bond' *Ex:* =C-O: 'CO bond', >C=O: 'CO double bond', … =C=O: 'CO double bond', … -C#O: 'CO triple bond' -O-H: 'OH hydrogen bond' Na+◦Cl-: 'NaCl ionic bond' - '*molecule part'*: describe the atoms of the molecule part, and end with 'simple-simple bonds', 'double-simple bonds', 'double-double bonds' or 'triple-simple bonds'. *Ex:* #C-CH2-C-: 'CCH2C simple-simple bonds' =C=C=C<: 'CCC double-double bonds' -C#C-C≤: 'CCC triple-simple bonds' -C=C-C=C-C=C-(ring): 'C6 ring simple-double bonds' *Note:* for vibration/rotations bands implying the whole molecule with more than 2 atoms, the vibration will directly refer to the molecule ("*molecule*_uid") as the vibration 'molecule part'
*chemical_bond*_secondary_name [*species*_secondary_name]	varchar(255)	S0 [m]	ChemB	F Aj	--	Alternative used name(s) of the chemical bond *Notes:* - use same ending as in 'name' - same name or different for isotopic species - start with a capital letter

- separate each name by a semicolon

*chemical_bond*_explicit_name	varchar(255)	S3 [!!_m]	ChemB	F	--	Explicit developed name of the chemical bonds

Notes:

- different for each isotopic species
- includes ionic information
- with same ending as in '*chemical_bond*_name' except the type and level of ion is explicit: cation, dication, trication, quadrication, …, anion, dianion, trianion, quadrianion, pentaanion, …
- it is some sort of extension to chemical bonds of the official IUPAC naming convention of molecules

Nomenclature:

- '*bonds*': describe both atoms preceded with their isotopic variant (if any) with their internal and surrounding bonds (nothing for simple, '=' for double, '=,=' for 2 double, '#' for triple, '…' for hydrogen bond, '.' for ionic bond) and end with 'bond', 'double bond', 'triple bond', 'hydrogen bond' or 'ionic bond'

  Ex:

  =C-O: 'CO bond',
  >C=O: 'C=O double bond', …
  =C=O: '=C=O double bond', …
  -C#O: 'C#O triple bond'
  -16OD: '(2H,16O)OH bond'
  =12C=16O: '(12C,16O)=C=O bond'
  -O-H: 'O...H hydrogen bond'
  Na+Cl-: 'Na+.Cl- ionic bond'

- '*molecule part'*: describe the atoms of the molecule part with their internal and surrounding bonds (nothing for simple, = for double, == for 2 double, # for triple) and end with 'simple-simple bonds', 'double-simple bonds', 'double-double bonds' or 'triple-simple bonds'.

  Ex:

  #C-CH2-C-: '#CCH2C simple-simple bonds'
  =C=C=C<: '=C=C=C double-double bonds'
  -C#C-C<-: 'C#CC triple-simple bonds'

-C=C-C=C-C=C-(ring): ‘C6 ring simple-double bonds’

Chemical bond structure and atomic composition

*chemical_bond*_formula [*species*_formula]	varchar(255)	U [!!_m]	ChemB	F	--	Semi-developed (linear) chemical formula of the chemical bond *Syntax:* LaTeX format *Notes:* - contain isotopic, radical and ionic information - D and T can be used for deuterium and tritium isotopes - isotopes only for bonds and molecule parts - cf. http://en.wikipedia.org/wiki/Functional_group Latex writing of bonds: - radical '•': $\bullet$ - hydrogen bond ‘···': $\dots$ - ionic bond ‘·’: $\cdot$ - 1 simple bond ‘–‘: $-$ - 2 simples bonds ‘>‘ or ‘<’: $>$ or $<$ - 3 simples bonds ‘≥ ‘ or ‘≤’: $\geq$ or $\leq$ - 4 simples bonds ‘>|‘ or ‘|<’: $>\mid$ or $\mid <$ - 1 simple + 1 double bonds ‘- =’: $\eqslantgtr$ or $\eqslantless$ - 2 simples + 1 double bonds ‘> =‘or ‘= <’: $\geqq$ or $\leqq$ - 1 double bond ‘=’: $=$ - 2 double bond ‘>> ‘ or ‘<<’: $\gg$ or $\ll$ - 3 double bond ‘=>> ‘ or ‘<<=’: $=\gg$ or $\ll =$ - 1 simple + 2 double bond ‘->> ‘ or ‘<<-’: $-\gg$ or $\ll -$ - triple bond ‘≡’ or ‘#’: $\equiv $ - quadruple bond ‘$’: $\supset$ or $\subset$ - LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf *Ex:* bond '$> ^{13}C = ^{18}O^{2-}$' for $>^{13}C=^{18}O^{2-}$ bond
*chemical_bond*_chemical_formula [*species*_chemical_formula]	CS-varchar(255)	S0 [!!_m]	ChemB	F	--	Simple chemical formula of the chemical bond *Ex:* CO, SO, CO-, O2, Na+Cl- …

						Note: do not contain isotopic, radical, and conformational information but contains ionic information.
*chemical_bond*_chemical_structure_filename	CS-varchar(255)	P/U [m]	ChemB	F	--	File name (with extension) of the plot with 2D or 3D representation of the chemical and isotopic structure of the bond *Image formats:* .png, .jpg, (.gif) *Notes:* - contain isotopic, radical and ionic information - this file will be imported in the database
*chemical_bond*_stoichiometric_formula [-xml] [*species*_atomic_formula]	CS-varchar(255)	S0 [!_c]	ChemB	F	--	Stoichiometric chemical formula of the bond ➔ calculated from "*chemical_bond*_atom_uid" and "*chemical_bond*_atom_number" *Note:* Suite of the atomic elements followed by the total number of their occurrence. The isotope mass number can be added before each atom, the charge can be added at the end with '+' or '-' sign followed by the charge number. This atom information is separated by a 'space' *Ex:* – 'C H3' for -C-H_3 – '13C H2' for $=^{13}$C-H_2 – 'SO4-2' for $\bullet SO_4^{2-}$ *Note:* Bonds contain only 2 types of atoms but one atom can have multiple occurrences (*Ex*: A Hn). Molecule parts can have multiple atoms. *Notes:* – do not contain any radical or conformational information. – when there is only one occurrence (atom or charge) the '1' can be omitted – when the chemical bond is natural there is no isotopic information *Note:* For easier search this stoichiometric chemical formula is also stored in tables listing: – the atom => "*chemical_bond*_atom_uid"

						– the total number of each atom => "*chemical_bond*_atom_number" – the charge is stored in '*chemical_bond*_charge'
*chemical_bond*_structural_formula [*species*_structural_formula]	CS-varchar(255)	S2 [!_m]	ChemB	F	--	Semi-developed SMILES structural chemical formula of the bond *Note:* This formula includes the description of the isotopic atoms (but use [2H] for D, [3H] for T), the charge and radical(s) of the chemical function. *Note:* We use the explicit SMILES formula with grouped H with heavier atoms and all in bracket (but no explicit simple bond except for multiple ones above 2). *Note:* Extension of semi-developped SMILES (see "*molecule*_structural_formula") to define the chemical functions and bonds. - We express also the 'external bonds': *Ex:* R=C=O => =[C]=[O] - For radical: use '.' *Ex:* •SO_4^{2-} => .[O-][S]([O])([O])[O-] - For hydrogen bond: '…' - For ionic bond: '.' *Ex:* Na^+°Cl^-: [Na+].[Cl-] - For multiple external single bonds, n-1 of these bonds are expressed as branched '(-)'. If there is a single and a double bond then only (=) is expressed and no single bonds (n-1=0).
chemical_bond_chemical_bonds	***List [L2]***	[!o]				£: Chemical bond (s) of the molecule part *Condition:* mandatory if "*chemical_bond*_type" = {molecule part}
*chemical_bond*_chemical_bond_uid [*] [*species*_chemical_bond_uid]	varchar(255)	S1i [!o_m]	ChemB ChemB L2	F	--	Link to the existing UID of the chemical bonds of the molecule part *Condition:* mandatory if "*chemical_bond*_type" = {molecule part} *Note*: – Describe the 'bonds' inside the 'molecular part' – The chemical bonds are either 'generic terrestrial mixture' or fully isotopic. – For isotopic mixtures of a molecule part in terrestrial abundance, the

						chemical bonds are the ‘generic terrestrial abundance mixture’ ones. – For an isotopic substituted molecule part made of at least one purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope atomic species of the others *Ex:* for CH2OH-nat: ‘bonds’ = 2 x ‘BOND_CH’, ‘BOND_CO’, ‘BOND_OH’ *Ex:* for HD32S: ‘bonds’ = ‘BOND_32SH’, ‘BOND_32SD’
*chemical_bond*_chemical_bond_number [+] [*species*_chemical_bond_number]	varchar(255)	U [!o_m]	ChemB L2	F	--	Number of bonds of each type composing the molecule part *Condition:* mandatory if “*chemical_bond*_type” = {molecule part} *Note:* For molecule part of natural isotopic molecules (and most minerals) this number is the total number of this bond (no specific isotope).
chemical_bond_atoms	***List [L2]***	[!!]				£: Description of the atomic composition of the chemical bond.
*chemical_bond*_atom_uid [*] [*species*_atom_uid]	varchar(255)	S0b [!!_m]	ChemB Atom L2	F	--	Link to the existing UID of the atom(s) (isotopic atomic species) composing the chemical bond *Notes:* – for chemical bonds of natural molecular mixtures (and most minerals) the "atom_uid" should refer to the one of the "atom in natural terrestrial abundance" – Generally, no ions as charge is frequently not localized on one atom *Note xml:* practically the "atom_uid" can also be unambiguously found using “atom_symbol”, “atomic_number_z” and “mass_number_a”
*chemical_bond*_atom_number [+] [*species*_atom_number]	int(11)	S0b [!_m]	ChemB L2	F	--	Number of atoms of each type (isotopic atomic species) composing the chemical bond For chemical bonds of natural molecular mixtures (and most minerals) this number is the total number of this chemical element (no specific isotope).

*chemical_bond*_electronegativity [*species*_electronegativity]	float	S2/S0b [m]	ChemB	F	Pauling	Electronegativity difference of the bond (Pauling scale) • stored in the database and provided to user in 'Pauling' unit *Definition*: it is the electronegativity difference between the 2 atoms *Note:* did not depend on isotopes *Note:* values for atoms from http://en.wikipedia.org/wiki/Electronegativity
*chemical_bond*_charge [*species*_charge]	int(2)	S2/S0b [!!_m]	ChemB	F	*no*	Charge (positive or negative) of the chemical bond *Notes:* - the charge of a chemical bond is frequently global (not on a specific atom) - charge = 0 for neutral chemical bond, > 0 or < 0 for ionic chemical bond *Ex.*: '+1', '-1'
*chemical_bond*_unpaired_electrons [*species*_unpaired_electrons]	int(2)	S3 [!_m]	ChemB	F	*no*	Number (positive) of unpaired electrons of the chemical bond *Notes:* – = 0 for molecule or ion chemical bond, – > 0 for radicals and ionic radical chemical bond

Chemical bond natural isotopic composition

*chemical_bond*_isotope_mixture_type [*species*_isotope_mixture_type]	enum(text)	S1 [!!_m]	ChemB	F		Type of isotopic mixture of the chemical bond Enum: {pure isotope, partly substituted, terrestrial abundance} *Definitions:* see "*molecule*_isotope_mixture_type" *Notes:* - The fundamental bonds stored in the database will be either with natural terrestrial abundance or as pure isotopes. - Some of the partly isotopically substituted bonds (the most important ones) may be also entered as fundamental species in the database.

						- Bonds with ‘specific isotopic abundance’ in sample or matters species (mostly to describe complex organics) will be described using the main pure isotopologue bonds (“*(constituent_)species*_uid” = ‘BOND_xxx’).
*chemical_bond*_isotope_*chemical_bonds*	***List [L4]***	[!o]				£: isotopic bond contributing to the isotopic mixture of chemical bonds *Condition:* mandatory only when “*chemical_bond*_isotope_mixture_type“ = {partly substituted, terrestrial abundance}
*chemical_bond*_isotope_chemical_bond_uid [*] [*species*_isotope_specie_uid]	varchar(255)	S1i [!o_m]	ChemB ChemB L4	F	--	Link to the existing UID of a pure isotopic bond contributing to the isotopic mixture of bonds *Condition:* mandatory only when “*chemical_bond*_isotope_mixture_type“ = {partly substituted, terrestrial abundance} *Notes:* – The list of all the isotopic species composing an isotopic mixture (with ‘terrestrial abundance’ or ‘partly substituted’) should be determined "by hand" as it depends on some symmetry elements of the chemical bond. – For big molecule parts composed of atoms having large numbers of isotopic species the list can be limited to the main isotopic species (above some threshold value in abundance).
*chemical_bond*_isotope_chemical_bond_mole_fraction [+] [*species*_isotope_specie_mole_fraction]	float	U [!o_m]	ChemB L4	F	--	Mole fraction of the isotopic bond *Condition*: mandatory when the bloc is used *Note:* – value between 0 and 1 – For “*chemical_bond*_isotope_mixture_type“ = ‘terrestrial abundance’ the mole fractions should be determined using the standard terrestrial atom mole fractions given by IUPAC (2009) (www.chem.qmul.ac.uk/iupac) – These abundances should be determined "by hand" as they depend on some symmetry elements of the molecule part. The sum should be = '1'

- For simple bonds (2 atoms) it is simply the product of the é isotopic abundances of the aroms
- For big molecule parts composed of atoms having large numbers of isotopic species, if not all species are listed the sum will be < '1.0' (but close to 1). Not a major problem.

Chemical bond properties

*chemical_bond*_polarity	enum(text)	S1 [!_m]	ChemB	F	--	Polarity of the chemical bond Enum: {nonpolar, polar, ionic} *Definitions:* Bond polarity is typically divided into three groups that are loosely based on the difference in electronegativity between the two bonded atoms. According to the Pauling scale: – '*nonpolar*': generally occur when the difference in electronegativity between the two atoms is less than 0.4 – '*polar*': generally occur when the difference in electronegativity between the two atoms is roughly between 0.4 and 1.7 if a metal is involved, and between 0.4 and 2.0 if only nonmetals are involved – '*ionic*': generally occur when the difference in electronegativity between the two atoms is greater than 1.7 if a metal is involved, and greater than 2.0 if only nonmetals are involved From: https://en.wikipedia.org/wiki/Chemical_polarity https://en.wikipedia.org/wiki/Electronegativity https://chem.libretexts.org/Bookshelves/General_Chemistry/Electronegativity
*chemical_bond*_dipole	float	S3 [m]	ChemB	F	*D*	Dipole moment of the chemical bond • stored in the database and provided to user in 'debye (D)' unit

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Chemical bond references + comments

chemical_bond_links	***List [L3]***	[O]				£: Web pages describing the chemical bond and its properties.
*chemical_bond*_link_name [*species*_link_name]	varchar(255)	U [m]	ChemB L3	F	--	Name of the web page(s) describing the chemical bond and its properties.
*chemical_bond*_link_url [*species*_link_url]	CS-varchar(255)	U [m]	ChemB L3	F	--	URL address(es) of web page(s) describing the chemical bond and its properties. *Reference*: https://en.wikipedia.org/wiki/Chemical_bond *Notes*: - you can link to a publication by giving its url address, preferably through its DOI. Ex: https://doi.org/10.1002/ejic.200700067
*chemical_bond*_comments [*species*_comments]	blob	U [m]	ChemB L3	F	--	Additional information on the chemical bond

5.5 Chemical functions Table

Root of the table: ***chemical_function***

Data type: 'Species'

For "*specie*_family" = 'chemical function'

Notes:

- all 'chemical functions' are with natural terrestrial isotopic abundances, or without specification.
- they are also called 'functional groups'

Key-word	Type	Level	Table	Exp	Unit	Description
Chemical function import						
*chemical_function*_import_mode [*species*_import_mode]	enum(text)	P [!!_m]	ChemF	(V)	--	Mode of import of the chemical function data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*chemical_function*_xml_filename [-xml] [*species*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ChemF	(V)	--	Name of the storage copy of the xml import file of the chemical function metadata ➔ determined automatically during import (from "*chemical_function*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Chemical function indexes and type						
*chemical_function*_index [**][-xml] [*species*_index]	int(10)	B [!!_g]	ChemF	F	--	Automatic random but unique number (ID) given to new chemical function
*chemical_function*_uid [**] [*species*_uid]	CS-varchar(255)	S0 [!!_m]	ChemF	F	--	Unique identifier code (UID) given to the chemical function table (to be created) *Nomenclature:* Create this UID with 'GROUPMOLEC_', 'GROUPION_',

‘GROUPRAD_’, ‘MINION_', followed by ‘R’ (except for MINION_). Each prefix corresponds to one specific “*chemical_function*_type”.

It should be of the style ‘GROUPMOLEC_RChemicalFormula’, ‘GROUPION_RChemicalFormulaCharge’, ‘GROUPRAD_RChemicalFormula(Charge)’. ‘MINION_ChemicalFormula_Charge’ (did not include ‘R’) where ‘ChemicalFormula’ is the chemical formula of the chemical function, and ‘Charge’ is the ion charge (charge sign '-' or '+' after the charge number), if not null.

Ex: ‘GROUPMOLEC_RCH3’, ‘GROUPION_RCOO-’, ‘GROUPRAD_RCO’, 'MINION_MoO4_2-'

Notes:

- The ‘anionic radicals’ (MINION_) are specific to minerals, and defined as the molecular ions included in the mineral structures. They UID are all of the form ‘MINION_AOn_x-’
- The *chemical* ‘functional groups’ (‘GROUPMOLEC_’, ‘GROUPION_’ and ‘GROUPRAD_’) and ‘mineral anionic radicals’ (MINION_) are independent of isotopes

Notations:

- The descriptor of the UID of the *chemical* ‘functional groups’ (‘GROUPMOLEC_Rxx’, ‘GROUPION_Rxx, ‘GROUPRAD_Rxx’) allways start with ‘_R’ and can also end with ‘R’. R is not only an alkyl but is extended to be any part of a molecule, but connected to the group by a C atom, or it can be simply H.

  Ex: for CH3OH-nat:

  - ‘functional groups’ = ‘GROUPMOLEC_RCH3’ and ‘GROUPMOLEC_ROH’

Notes:

- In complex matters when a complex functional group is known, such as ‘R-CH2-CH2-CH3’ it can be described here. It will be itself described in term of simple groups (e.g. R-CH2-R, R-CH3)
- for list of functions see: http://en.wikipedia.org/wiki/Functional_group
- https://en.wikibooks.org/wiki/Organic_Chemistry/Overview_of_Functional_Groups

– http://www.chemistry-drills.com/functional-groups.php?q=simple

*chemical_function*_type [*species*_type]	enum(text)	S1/S2s [!!_m]	ChemF	F	--	Type of chemical function Enum: {functional group, ionic functional group, radical functional group, mineral anionic radical} *Definitions:* - '*functional group'*: for neutral group of molecules - '*ionic functional group'*: for charged group of molecules - '*radical functional group'*: for radical group of molecules - *' mineral anionic radical'* specific for ionic group in minerals

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Chemical function names

*chemical_function*_name [*species*_name]	varchar(255)	S0/S1bs [!!_m]	ChemF	F	--	Generic name of the chemical function *Notes:* - the same for all isotopic species and of surrounding bonds - It is used as the title of the chemical function page on the SSHADE interface *Nomenclature:* - '*functional group'*: end with 'group'. *Ex:* 'Carbonyl group' - '*ionic functional group'*: end with 'anion/cation group'. *Ex:* 'Carboxylate ion group', … - '*radical functional group'*: end with 'radical group' *Ex:* - 'mineral *anionic radical'*: end with 'anion'. *Ex:* 'Hydroxide anion', 'Carbonate anion' …
*chemical_function*_secondary_name [*species*_secondary_name]	varchar(255)	S0/S1bs [m]	ChemF	F	--	Alternative used name(s) of the chemical function (functional group) *Notes:* – use same ending as in 'name' – start with a capital letter

						– separate each name by a semicolon
*chemical_function*_explicit_name	varchar(255)	S3 [!!_m]	ChemF	F	--	Explicit developed name of the functional groups *Notes:* - no isotopic species - with same ending as in '*chemical_function*_name' except the type and level of ion is explicit: cation, dication, trication, quadrication, …, anion, dianion, trianion, quadrianion, pentaanion, … - it is some sort of extension to chemical functions of the official IUPAC naming convention of molecules *Ex*: 'Carboxylate anion group', 'Hydroxide anion group', … *Note:* cf. http://en.wikipedia.org/wiki/Functional_group http://www.chemistry-drills.com/functional-groups.php?q=simple

Chemical function structure and atomic composition

*chemical_function*_formula [*species*_formula]	varchar(255)	U [!!_m]	ChemF	F	--	Semi-developed (linear) chemical formula of the chemical function (functional group, …) *Syntax:* LaTeX format *Notes:* - contain radical and ionic information - cf. http://en.wikipedia.org/wiki/Functional_group *Ex:* '$\bullet SO_4^{2-}$' for $\bullet SO_4^{2-}$ mineral anionic radical Latex writing of bonds: see "*chemical_bond*_formula"
*chemical_function*_chemical_formula [*species*_chemical_formula]	CS-varchar(255)	S0 [!!_m]	ChemF	F	--	Simple chemical formula of the chemical function (functional group, …) *Ex:* CH3O, SO4, COO-, O2, OO, … *Note:* do not contain isotopic, radical, and conformational information but contains ionic information.

*chemical_function*_chemical_structure_filename	CS-varchar(255)	P/U [!_m]	ChemF	F	--	File name (with extension) of the plot with 2D or 3D representation of the chemical structure of the functional group. *Image formats:* .png, .jpg, (.gif) *Note:* contain radical and ionic information *Note:* this file will be imported in the database
*chemical_function*_stoichiometric_formula [-xml] [*species*_atomic_formula]	CS-varchar(255)	S0 [!_c]	ChemF	F	--	Stoichiometric chemical formula of the functional group. ➔ calculated from => "*chemical_function*_atom_uid" and "*chemical_function*_atom_number" *Note:* Suite of the atomic elements followed by the total number of their occurrence. The charge can be added with '+' or '-' sign followed by the charge number. This atom information are separated by a 'space' *Ex:* – 'C H3' for -C-H_3, – 'S O4-2' for •SO_4^{2-} *Notes:* – do not contain any radical or conformational information. – when there is only one occurrence (atom or charge) the '1' can be omitted – the chemical function is only described using the atoms with their natural terrestrial isotopic composition *Note:* For easier search this stoichiometric chemical formula is also stored in tables listing: – the atom => "*chemical_function*_atom_uid" – the total number of each atom => "*chemical_function*_atom_number" – the charge is stored in '*chemical_function*_charge'
*chemical_function*_structural_formula [*species*_structural_formula]	CS-varchar(255)	S2 [!_m]	ChemF	F	--	Semi-developed SMILES structural chemical formula of the functional group. *Note:* This formula includes the description of the atoms (no specific isotope), the charge and radical(s) of the chemical function. *Note:* We use the explicit SMILES formula with grouped H with heavier

						atoms and all in bracket (but no explicit simple bond except for multiple ones above 2). *Note:* Extension of semi-developped SMILES (see "*molecule*_structural_formula") to define the chemical functions and bonds. We express also the 'external bonds': *Ex:* R=C=O => =[C]=[O] For radical: use '.' *Ex:* •SO_4^{2-} => .[O-][S]([O])([O])[O-] For multiple external single bonds, n-1 of these bonds are expressed as branched '(-)'. If there is a single and a double bond then only (=) is expressed and no single bonds (n-1=0).
chemical_function_chemical_functions	***List [L1]***	[O]				£: Description of the functional groups of complex chemical functions
*chemical_function*_chemical_function_uid [*]	varchar(255)	U [m]	ChemF ChemF L1	F	--	Link to the existing UID of the functional groups of complex chemical function *Note:* – permits to describe a complex chemical function in terms of simpler chemical functions (or moieties). *Ex:* 'R-CH(NH2)-COOH' (amino acid): simple groups 'R-COOH', 'R-NH2' 'R-CH2-CH2-CH3' (propyl): simple groups 'R-CH2-R', 'R-CH3'
*chemical_function*_chemical_function_number [*species*_chemical_function_number]	varchar(255)	U [m]	ChemF L1	F	--	Number of functional groups of each type composing the complex chemical function
chemical_function_chemical_bonds	***List [L2]***	[!]				£: Chemical bond (s) of the chemical function
*chemical_function*_chemical_bond_uid [*]	varchar(255)	S2 [!_m]	ChemF ChemB	F	--	Link to the existing UID of the chemical bonds (natural species only) of the chemical function

[*species*_chemical_bond_uid]			L2			*Note*: – These "*chemical_bond*_uid" should only refer to the generic bonds (with natural terrestrial abundance) *Ex:* for RCH2OH: 'bonds' = 2 x 'BOND_CH', 'BOND_CO', 'BOND_OH'
*chemical_function*_chemical_bond_number [+] [*species*_chemical_bond_number]	varchar(255)	S3 [!_m]	ChemF L2	F	--	Number of bonds of each type composing the chemical function *Note:* - for all functional groups this number is the total number of this bond (no specific isotope). - although it is a 'varchar(255)' format, uses mostly integer, float or 'n' to allow calculation constituent and phase bond numbers with it.
chemical_function_atoms	***List [L2]***	[!!]				£: Description of the atomic composition of the chemical function.
*chemical_function*_atom_uid [*] [*species*_atom_uid]	varchar(255)	S0b [!!_m]	ChemF Atom L2	F	--	Link to the existing UID of the atom(s) (natural species only) composing the chemical function *Note*: These "atom_uid" should only refer to the generic atoms (with natural terrestrial abundance) *Note:* – 'R' is not included (not an atom!) – no ions, as charge is frequently not localized on one atom *Note xml:* practically the "atom_uid" can also be unambiguously found using "atom_symbol", "atomic_number_z" and "mass_number_a"
*chemical_function*_atom_number [+] [*species*_atom_number]	int(11)	S0b [!_m]	ChemF L2	F	--	Number of atoms of each type (natural species only) composing the chemical function *Note*: Chemical functions being natural molecular (or mineral) mixtures this number is the total number of this atom (no specific isotope).
*chemical_function*_charge [*species*_charge]	int(2)	S2/S0b	ChemF	F	*no*	Charge (positive or negative) of the chemical function

		[!!_m]				*Notes:* - the charge of a chemical function is frequently global (not on a specific atom) - = 0 for neutral chemical functions, > 0 or < 0 for ionic chemical functions *Ex.*: '+1', '-1'
*chemical_function*_unpaired_electrons [*species*_unpaired_electrons]	int(2)	S3 [!_m]	ChemF	F	*no*	Number (positive) of unpaired electrons of the chemical function *Note:* = 0 for molecule or ion chemical functions, > 0 for radicals and ionic radical chemical functions
Chemical function natural isotopic composition						
*chemical_function*_isotope_mixture_type [*species*_isotope_natural_mixture]	enum(text)	U [!!_m]	Chem F	F		Type of isotopic mixture of the chemical function Enum: {terrestrial abundance} = default *Note*: the chemical function is only described without specific isotopic composition. So, the atoms used are those with their natural terrestrial isotopic composition
Chemical function references + comments						
chemical_function_links	***List [L3]***	[O]				£: Web pages describing the chemical function and its properties.
*chemical_function*_link_name [*species*_link_name]	varchar(255)	U [m]	ChemF L3	F	--	Name of the web page(s) describing the chemical function and its properties.
*chemical_function*_link_url [*species*_link_url]	CS-varchar(255)	U [m]	ChemF L3	F	--	URL address(es) of web page(s) describing the chemical function and its properties. *Reference*: https://en.wikipedia.org/wiki/Functional_group *Notes*: - you can link to a publication by giving its url address, preferably

						through its DOI. Ex: https://doi.org/10.1002/ejic.200700067
*chemical_function*_comments [*species*_comments]	blob	U [m]	ChemF	F	--	Additional information on the chemical function

5.6 Molecules, Molecular Ions and Radicals Table

Root of the table: ***molecule***

Data type: 'Species'

For "*specie*_family" = 'molecule'

Note: Only all the pure isotopic species, some substituted isotopic mixtures and the natural terrestrial isotopic mixture (with natural terrestrial composition) will be entered in the database as fundamental species. All other isotopic mixtures will need to be generated by data providers using a mixtuee of the pure isotopic species.

Key-word	Type	Level	Table	Exp	Unit	Description
Molecular species import						
*molecule*_import_mode [*species*_import_mode]	enum(text)	P [!!_m]	Molec	(V)	--	Mode of import of the molecule data Enum: {first import, (use existing), ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*molecule*_xml_filename [-xml] [*species*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	Molec	(V)	--	Name of the storage copy of the xml import file of the atom metadata ➔ determined automatically during import (from "*molecule*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Molecular species indexes and type						
*molecule*_index [**][-xml] [*species*_index]	int(10)	B [!!_g]	Molec	F	--	Automatic random but unique number (ID) given to new molecular species
*molecule*_uid [**] [*species*_uid]	CS-varchar(255)	S0 [!!_m]	Molec	F	--	Unique identifier code given (UID) to the molecular species table (to be created) *Nomenclature:* Create this UID with 'MOLEC_', 'MOLION_', 'MOLRAD_', 'MOLRADION_' depending on the molecular species type, followed by the molecule formula (or by the name for complex molecules) and then the ion

charge, if any. It should be unique. If a possible confusion exists between 2 species then add a small letter after (first letter of name, ...). For stereoisomers add its cap letter type (‘R-‘, ‘S-‘, …) before.

Note: It should be of the style

- ‘MOLEC_(Isotopic)ChemicalFormula(Letter)’
- ‘MOLRAD_(Isotopic)ChemicalFormula(Letter)’,
- ‘MOLION_(Isotopic)ChemicalFormulaCharge(Letter)’
- ‘MOLRADION_(Isotopic)ChemicalFormulaCharge(Letter)’

where ‘(Isotopic)ChemicalFormula’ is the chemical formula of the molecular species, including the isotope mass number (preceding atom) for pure isotopic atoms and ‘Charge’ is the charge of the ion or ionic radical (charge sign '-' or '+' after the charge number), if not null.

Ex: ‘MOLEC_CO2’, ‘MOLEC_13C16O18O’, ‘MOLEC_C3H4a', ‘MOLEC_C3H4p', ‘MOLEC_D-malic_acid’, 'MOLION_CO2+', 'MOLRAD_OH'

Note:

- All the pure isotopic species and one ‘natural isotopic mixture’ (defined to have natural terrestrial composition) will be entered in the fundamental SSHADE database.
- Some substituted isotopic mixtures (the most important/commercially available ones) may be entered as fundamental species in the SSHADE database.
- All other natural, synthetic, labeled or substituted isotopic mixtures will be directly built in their “Sample” with “*constituent*_specie_molecule” using the fundamental pure isotopic species (at least the most abundant) to provide their effective isotopic atomic and molecular composition.

Ex: fundamental species: ‘MOLEC_CO’ (‘generic isotopic mixture’), ‘MOLEC_12C16O’, ‘MOLEC_12C17O’, ‘MOLEC_12C18O’, ‘MOLEC_13C16O’, ‘MOLEC_13C17O’, ‘MOLEC_13C18O’.
Ex: ^{13}CO (with O as an isotopic mixture) will refer to ‘MOLEC_CO’

*molecule*_type [*species*_type]	enum(text)	S1 [!!_m]	Molec	F	--	Type of molecular species. Enum: {molecule, molecular ion, molecular radical, molecular ionic radical} *Definitions*: - '*molecule*': neutral molecule - '*molecular ion*': molecule with a negative or positive charge - '*molecular radical*': molecular radical. It also includes 'mer', the building unit of a polymer - '*molecular ionic radical*': molecular radical with a negative or positive charge

Molecule names and identifiers

*molecule*_name [*species*_name]	varchar(255)	S0 [!!_m]	Molec	F	--	Generic name of the molecule, molecular ion, radical or ionic radical (the same for all isotopic species) *Notes*: – start with a capital letter – it is used as the title of the molecule page on the SSHADE interface – it has no isotopic information – for amino acid and sugar enantiomers, add 'D-' or 'L-' before the name – for the other enantiomers, add 'R-' or 'S-' before the name – for some specific diastereomers the '*cis*-', '*trans*-' or '*alpha*-', '*beta*-' (anomers) prefixes are used. – for the other diastereomers, add 'Z-', 'E-', 'P-', or 'M-' before the name – for conformers the following prefixes are used: '*syn*-', '*anti*-', '*clinal*-', '*periplanar*-', '*synperiplanar*-', '*synclinal*-', '*anticlinal*-', or their corresponding symbols: 's-', 'a-', 'c-', 'p-', 'sp-', 'sc-', 'ac-', 'ap-' (cf. '*molecule*_stereoisomer_conformer_synanti') – a molecule name with '*racem-*' prefix is a racemate (racemic mixture) of the 2 types of isomers. It will be only used in constituents as a 1:1 mixture of the 2 species. – for spin isomers, add '*para*-', '*ortho*-', '*meta*-', '*para-ortho*-'...,

						before the name *Ex.:* 'Water', 'Dioxygen', 'Dinitrogen', 'Methanol', 'Ethanol', … *Ex*: 'L-Malic acid', 'D-Malic acid', 'para-Water' *Note:* ion names: http://www.geocities.ws/profmokeur/chimie/tableions.htm
molecule_secondary_names	***List [L0]***	[O]				£: Alternative used names of the molecular species.
*molecule*_secondary_name [*species*_secondary_name]	varchar(255)	S0 [m]	Molec L0	F Aj	--	Alternative used name of the molecular species (same or different for isotopic species) *Notes*: – start with a capital letter – For isotopes add the mass number before the substituted atom(s) – For enantiomers alternative names use '(+)-', '(-)-' or add them after 'L-', 'D-' *Ex*: 'L-(+)-tartaric acid' for dextrotartaric acid – A molecule name without isotopic mass number or stereoisomer prefix has the 'standard atomic composition' (IUPAC 2009) and is a racemic mixture of all possible types of isomers *Ex.:* 'Oxygen', 'Nitrogen', 'Water', 'Methanol', 'Good gnole' ... *Ex:* '13CO2', 'Carbon-13C dioxide' for $^{13}CO_2$
*molecule*_iupac_name [*species*_official_name]	varchar(255)	S0 [!!_m]	Molec	F	--	IUPAC unique name of the molecule, molecular ion, radical or ionic radical *Notes*: - it is different for each isotopic species and each stereoisomer - no IUPAC nomenclature currently exists for nuclear spin isomers but is under study by IUPAC. *Ex:* '(1H2,18O)Water' for $^{1}H_2{}^{18}O$ *Ex:* '(H2,18O)Water' for $H_2{}^{18}O$
*molecule*_inchi [*species*_inchi]	blob	S1 [!o_m]	Molec	F	--	Standard InChI sequence:

Condition: Mandatory only when "*molecule*_type"='molecule'

Definition: IUPAC international chemical identifier, unique, of the molecule, ion, radical or ionic radical, natural or any type of isotopic composition.

Notes:

- Currently InChI did not take into account conformational isomers and nuclear spin isomers
- for simplicity the InChI code must be entered without 'InChI='. This part will be added automatically during import.
- when the molecule is a mixture of all isotopic species in natural or any other abundances there is no isotopic information, except if one atom is fully substituted.

Ex:

- (InChI=)'1S/CO2/c2-1-3' for CO_2
- (InChI=)'1S/CO2/c2-1-3/i1+1' for $^{13}CO_2$
- (InChI=)'1S/H2O/h1H2/i1+2/hH2' for $H_2{}^{18}O$
- (InChI=)'1S/HO/h1H' or InChI='1S/H2O/h1H2/p-1' for hydroxyl radical •OH
- (InChI=)'1S/H2O/h1H2/p-1' for hydroxide ion H_2O^-
- (InChI=)'1S/C3H6O3/c1-2(4)3(5)6/h2,4H,1H3,(H,5,6)/t2-/m0/s1' for (S)-(+)-lactic acid enantiomer

Notes:

- cf. http://www.vamdc.eu/documents/standards/inchi/index.html#the-inchikey
- a software that can generate the InChI sequence and the InChIKey: "ACD/ChemSketch Freeware" (http://www.acdlabs.com/resources/freeware/chemsketch/)

*molecule*_inchikey [*species*_inchikey]	CS-varchar(255)	S1 [!o_m]	Molec	F	--	Standard InChI Key: InChI sequence coded over 25 characters (hash) *Condition:* mandatory only when "*molecule*_type"='molecule' *Ex:* 'LELOWRISYMNNSU-UHFFFAOYSA-N' for HCN 'TUJKJAMUKRIRHC-UHFFFAOYSA-N' for hydroxyl radical •OH

Note: when one atom is fully substituted the inchikey is different from the one of the isotopic mixture of the molecule. (ex: $^{13}CO_2$)

*molecule*_cas_number [*species*_cas_number]	varchar(255)	S1 [m]	Molec	F	--	CAS registry number, unique, of the molecule, molecular ion, radical or ionic radical (natural and isotopic species) *Ex:* '74-90-8' for HCN *Notes:* - change with isotopic species but also for substituted isotopic mixtures. - change with enantiomer - did not take into account nuclar spin isomers - the problem is to found them !!! no registry, not systematic! See "Chemical Identifier Resolver" (inchi, inchikey, smiles, CAS, IUPAC name, chemical structure (gif), …: http://cactus.nci.nih.gov/chemical/structure

---

Molecule chemical structure and atomic composition

*molecule*_formula [*species*_formula]	varchar(255)	U [!!_m]	Molec	F	--	(Semi)-developed chemical formula of the molecule, molecular ion, radical or ionic radical *Syntax:* LaTeX format (always put only a $ at beginning and end of formula) *Ex:* trans-$(^{13}CDH_2)_2^{18}O^{2-}$ for trans-($^{13}CDH_2)_2{}^{18}O^{2-}$ *Ex:* $(COOH)CH_2CHOH(COOH)$ for Malic acid *Notes:* – contain isotopic, radical, conformational, spin isomer and ionic information. – For large molecules it is best to condense the formula (semi-developed) but keep visible the functional groups *Ex*: $(C_6H_6)_c(CH_3)_3CH=CHC(CH_3)=CHCH=CHC(CH_3)=CH(=O)$ for $(C_6H_6)_c(CH_3)_3CH=CHC(CH_3)=CHCH=CHC(CH_3)=CH(=O)$ – D and T can be used for deuterium and tritium isotopes – when the molecule is a mixture of all isotopic species in natural or any other abundances there is no isotopic information, except if one (or more) atom is fully substituted

- dot • (\bullet) for radicals
- dot · (\cdot) between ions
- ‘molecule mers’ should be put between bracket with radicals at both ends
  Ex: $\bullet[CH(C_4H_6NO)CH_2]\bullet$ for Vinylpyrrolidone mer
- For stereo-isomers use either the CIP notation by adding ‘X-‘ in front of the formula, where ‘X’ can be {R, S, E, Z, P, M)
- For enantiomers alternative writing use ‘D-‘, ‘L-‘, or ‘(+)-‘, ‘(-)-‘ and sometimes both
  Ex: D-$(COOH)CH_2CHOH(COOH)$ for D-Malic acid
- For some specific diastereomers the ‘cis-‘, ‘trans-‘ or ‘alpha-‘, ‘beta-’ (anomers) notations are used. Old notations are: ‘threo’ and ‘erythro’.
- For conformers the following prefixes are used: ‘syn-‘, ‘anti-‘, ‘clinal-‘, ‘periplanar-‘, ‘synperiplanar-‘, ‘synclinal-‘, ‘anticlinal-‘, or their corresponding symbols: ‘s-‘, ‘a-‘, ‘c-’, ‘p-‘, ‘sp-‘, ‘sc-‘, ‘ac-‘, ‘ap-’ (cf. ‘*molecule*_stereoisomer_conformer_synanti’)
- for spin isomers, add ‘para-‘, ‘ortho-‘, ‘meta-‘... before the name
- a molecule formula without isotopic mass number or stereoisomer prefix has the ‘standard atomic composition’ (IUPAC 2009) and is a racemic mixture of all possible types of isomers
  Ex: $(^{13}CO_2)$: C is only (mostly) ^{13}C, O is a mixture of the isotopic species
- LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf

*molecule*_chemical_formula [*species*_chemical_formula]	CS-varchar(255)	S0 [!!_m]	Molec	F	--	Simple chemical formula of the molecule, molecular ion, radical or ionic radical *Ex:* CH3OH, C3H8, COOH, OCN-, or (CH3CH3O)2- (pour: trans-($^{13}CDH_2)_2{}^{18}O^{2-}$) *Note:* - only written with simple ascii characters - do not contain isotopic, radical, spin isomer, stereoisomeric and conformational information but contains global ionic information. - do not display the types of bonds

- only display internal ionic bonds with ·, without the charges
  Ex: Na·Cl (not $Na^+ \cdot Cl^-$)
- display hydration with • (ascii #149)
  Ex: Na·CO3•2H2O
- this formula can be sometimes ambiguous for ions
  Ex: (CH3CH3O)2- can be $(CH_3CH_3O)^{2-}$ or $(CH_3CH_3O)_2^-$

*molecule*_chemical_structure_file name	CS-varchar(255)	P/U [!_m]	Molec	F	--	Image file name (with extension) with 2D or 3D representation of the chemical and isotopic structure of the molecule, molecular ion, radical or ionic radical *Image formats:* .png, .jpg, (.gif) *Notes:* – contain isotopic, radical, conformational and ionic information. – different for each enantiomer (mirroring) – isotopic mixtures will refer to the 'non-isotopic' structure even with one (or more, but not all) atom(s) fully substituted [note: too complex to generate all structures for all substitution cases!] – when the molecule is an equilibrium between two configuration: draw both configurations *Ex*: N2O: $N\#N^+-O^-$ <=> $N^-=N^+=O$ – isotopic species and mixtures will refer to the 'non-isotopic' structure *Notes:* – this file will be imported in the database – 3D active representation of the chemical structure of the molecule, molecular ion, radical or ionic radical will be obtained using InChI. => URL giving the 3D jmol http://chemapps.stolaf.edu/jmol/jmol.php or http://cactus.nci.nih.gov/chemical/structure choice: TwirlyMol(3D)
*molecule*_stoichiometric_formula [-xml] [*species*_atomic_formula]	CS-varchar(255)	S0 [!_c]	Molec	F	--	Stoichiometric chemical formula of the molecule, molecular ion, radical or ionic radical. ➔ calculated from => "*molecule*_atom_uid" and "_atom_number" *Definition:* suite of the atomic elements followed by the total number of their occurrence. The isotopic number is added before each atom. The global charge of an ion can be added at the end (after a 'space') with '+' or '-' sign followed

by the charge number. This atom information is separated by a ‘space’

Ex.: ‘O2’, ‘N2’, ‘13C H4 18O’, ‘C2 H6 O’, ‘N2+’, ‘C O2-2’, …

Notes:

- do not contain any radical or conformational information.
- when there is only one occurrence (atom or charge) the ‘1’ should be omitted
- when the molecule is a mixture of all isotopic species in natural or any other abundances there is no isotopic information, except if one (or more) atom is fully substituted (ex: 13C O2: C is only (mostly) 13C, O is a mixture of the isotopic species)

Note: For easier search this stoichiometric chemical formula is also stored in tables listing:

- the atom => “*molecule*_atom_uid”
- the total number of each atom => “*molecule*_atom_number”
- the global charge of the molecule is stored in ‘*molecule*_charge’

*molecule*_structural_formula [*species*_structural_formula]	blob	S2 [!_m]	Molec	F	--	Semi-developped SMILES structural chemical formula of the molecule, molecular ion, radical or ionic radical.

Notes:

- This formula includes the description of the isotopic atoms, the charge, the radicals and conformation of the molecular species
- We use the semi-explicit SMILES formula with bonded H within the braquet of the ‘heavier atoms’. All in braquet (no simple ‘organic’ atoms without H)
  Ex: methane = [CH4], ethane = [CH3] [CH3], methanol = [CH3][CH2][OH], sulfur dioxide = [O][S][O], water = [OH2]
- For aromatic structure we adopt the semi-explicit Kékulé form
  Ex: Benzene: [C1H]=[CH][CH]=[CH][CH]=[C1H]
  Semi-condensed form: C1=CC=CC=C1
  Condensed form: c1ccccc1
- when the molecule is an equilibrium between two configurations: give one of the two
  Ex: N2O: N#[N+][O-] and [N-]=[N+]=O

						– when the molecule is a mixture of all isotopic species in standard terrestrial abundances there is no isotopic information, except if one (or more) atom is fully substituted *Ex:* [O]=[13C]=[O]: C is only (mostly) ^{13}C, O is a mixture of the isotopic species – Isomerism: uses @ which means 'the other three atoms are listed anti-clockwise'; or @@ which means 'clockwise'. *Reference*: http://www.daylight.com/meetings/summerschool98/course/dave/smiles-isomers.html *Reference document:* http://www.opensmiles.org/spec/open-smiles-3-input.html#3.1
molecule_chemical_functions	***List [L1]***	[!]				£: Chemical function(s) (or functional group(s)) of the molecular species.
*molecule*_chemical_function_uid [*] [*species*_chemical_function_uid]	CS-varchar(255)	S2 [!_m]	Molec ChemF L1	F	--	Link to the existing UID of the chemical function(s) of the molecular species *Note:* – these chemical functions should be already in the database. – the chemical functions are independent of isotopes *Ex:* for CH3OH-nat: 'functional groups' = 'GROUPMOLEC_RCH3', 'GROUPMOLEC_ROH' *Ex:* for 13CH3OD: 'functional groups' = 'GROUPMOLEC_RCH3', 'GROUPMOLEC_ROH',
*molecule*_chemical_function_number [+] [*species*_chemical_function_number]	varchar(255)	S3 [!_m]	Molec ChemF L1	F	--	Number of functional groups of each type composing the molecular species *Note:* although it is a 'varchar(255)' format, uses mostly integer, float or 'n' to allow calculation constituent and phase function numbers with it.
molecule_chemical_bonds	***List [L2]***	[!]				£: Chemical bond (s) of the molecular species.
*molecule*_chemical_bond_uid [*] [*species*_chemical_bond_uid]	CS-varchar(255)	S2 [!_m]	Molec ChemB	F	--	Link to the existing UID of the chemical bonds of the molecular species *Note:* these chemical bonds should be already in the database.

			L2			*Note*: – The chemical bonds are either ‘generic mixture’ or fully isotopics. – For mixtures of isotopic molecules, the chemical bonds are the ‘generic mixture’ ones. – For isotopic substituted molecules made of at least one purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope of the others – For band list only the fully isotopic bonds are used (except if no idea of which isotopic species creates this band). – when the molecule is an equilibrium between two configurations: provide bonds of both configurations and give number=0.5 *Ex*: N2O: NtN+ + N+O- and N-dN+ + OdN+ *Ex:* for CH3OH-nat: ‘bonds’ = ‘BOND_CH3’, ‘BOND_CO’, ‘BOND_OH’ *Ex:* for 13CH3OD: ‘bonds’ = ‘BOND_13CH3’, ‘BOND_13C16O’, ‘BOND_16OD’ *Note:* practically the "*chemical_bond*_uid" could also be found using “*chemical_function*_stoichiometric_formula” or “*chemical_function*_structural_formula” but it can be ambiguous and need conversion (not unique way to write them)
*molecule*_chemical_bond_number [+] [*species*_chemical_bond_number]	varchar(255)	S3 [!_m]	Molec L2	F	--	Number of functional groups or bounds of each type composing the molecular species *Notes:* although it is a ‘varchar(255)’ format, uses mostly integer, float or ‘n’ to allow calculation constituent and phase bond numbers with it.
molecule_atoms	***List [L3]***	[!!]				£: Atomic composition of the molecular species.
*molecule*_atom_uid [*] [*species*_atom_uid]	CS-varchar(255)	S0b [!!_m]	Molec Atom L3	F	--	Link to the existing UID of the atom(s) (natural or isotopic atomic species) composing the molecular species *Notes:* – For natural isotopic mixtures ("*molecule*_isotope_mixture_type" = {terrestrial abundance}) the "atom_uid" should refer to the ones of the

						"terrestrial isotopic atom mixture" – For pure isotopic or partly isotopically substituted molecules (one or more atom of the molecule is fully substituted) the "atom_uid" of these substituted atoms will refer to the pure isotopic atom species. *Ex:* for $^{13}CO_2$: 1 atom '13C' and 2 atoms 'O'
*molecule*_atom_number [+] [*species*_atom_number]	int(11)	S0b [!_m]	Molec L3	F	--	Number of atoms of each type (natural or isotopic atomic species) composing the molecular species For natural molecular mixtures ("*molecule*_isotope_mixture_type" = {terrestrial abundance, partly substituted}) this number is the total number of this chemical element (no specific isotope).
*molecule*_charge [*species*_charge]	int(2)	S2/S0b [!!_m]	Molec	F	*no*	Charge (positive or negative) of the molecular species *Note:* = 0 for neutral molecules and molecular radicals, > 0 or < 0 for molecular ions and ionic radicals *Ex.*: '+1', '-1'
*molecule*_unpaired_electrons [*species*_unpaired_electrons]	int(2)	S3 [!o_m]	Molec	F	*no*	Number (positive) of unpaired electrons of radical species *Condition*: mandatory only when "*molecule*_type" = {molecular radical, molecular ionic radical} *Note:* = 0 for molecule or ions, > 0 for radicals and ionic radicals
Molecule: Stereoisomers						
*molecule*_stereoisomer_stereodescriptor	enum(text)	S2 [!o_m]	Molec	F	--	Type of stereoisomer of the molecular species (CIP rules) FreeList: {R, S, E, Z, P, M, cis, trans, alpha, beta, syn, anti, clinal, periplanar, synperiplanar, synclinal, anticlinal, antiperiplanar, and any combination} *Condition:* mandatory and only when "*molecule*_stereoisomer_relation" = {enantiomer, diastereomer, anomer, atropisomer, conformer} *Ex*:

- ‘S,R’, ‘S,S’, …
- ‘2R,3S,4R,5R’, ..

Reference:

- https://en.wikipedia.org/wiki/Cahn%E2%80%93Ingold%E2%80%93Prelog_priority_rules

Definitions:

* R/S enantiomers:

Definition: R-S isomerism (IUPAC) is an absolute stereochemical description of the stereo-centers based on the Cahn–Ingold–Prelog priority rules (CIP rules), is when two stereoisomers are related to each other by a reflection: They are mirror images of each other that are non-superimposable.

Nomenclature:

- The letters R and S are conventionally printed in italic type, within parentheses, and separated from the rest of the name with a hyphen.
- R for « Rectus, right-handed stereoisomer » and S for « Sinister, left-handed stereoisomer »
- For organic molecules with multiple asymmetric carbons, it is necessary to indicate the carbon location for each R or S symbol.

Notes:

- Also known as ‘optical isomers’
- the (S) and (R) designators are used to indicate the absolute stereochemistry.

* cis-trans diastereomer:

Definition: ‘cis’ indicates that the functional groups are on the same side of the carbon chain. *‘trans’* conveys that functional groups are on opposing sides of the carbon chain.

Notes:

- Also known as ‘geometric isomerism’ or ‘configurational isomerism’
- cis/trans notation only describes relative stereochemistry and thus can be used to describe double bonds having only two substituents.
- cis/trans isomerism mostly exists with alkenes (C=C bonds) but also

with Diazenes and related diphosphenes (N=N bonds) and inorganic coordination complexes with octahedral or square planar geometries.

Reference: https://en.wikipedia.org/wiki/Cis%E2%80%93trans_isomerism

*** E/Z stereo-isomers:**

Definition: E–Z isomerism (IUPAC), which is an absolute stereochemical description based on the Cahn–Ingold–Prelog priority rules (CIP rules), is an extension of cis/trans notation to describe the absolute stereochemistry of double bonds having two, three or four substituents.

Nomenclature:

- The letters E and Z are conventionally printed in italic type, within parentheses, and separated from the rest of the name with a hyphen.
- For organic molecules with multiple double bonds, it is sometimes necessary to indicate the alkene location for each E or Z symbol.

Reference: https://en.wikipedia.org/wiki/E-Z_notation

* Anomers:

Definition: 'alpha' (α) or *'axial':* when the anomeric hydroxyl group (-OH) and the terminal CH2OH group are on opposite sides of the cycle. *'beta'* (β) or *'equatorial':* when they are on the same side.

Reference: https://en.wikipedia.org/wiki/Anomer

* P/M atropisomers *:*

Definition: P/M atropisomers, which is an absolute stereochemical description based on the Cahn–Ingold–Prelog priority rules (CIP rules), are stereoisomers arising because of hindered rotation about a single bond, where energy differences due to steric strain or other contributors create a barrier to rotation high enough to allow for isolation of individual conformers.

- Conformers are stereoisomers that can be interconverted exclusively by rotations about formally single bonds).

Nomenclature:

- The letters P and M are conventionally printed in italic type, within parentheses, and separated from the rest of the name with a hyphen.

- P for clockwise and M for counterclockwise

Notes:

- atropisomers is a subclass of conformers which can be isolated as separate chemical species and which arise from restricted rotation about a single bond.

References:

- https://en.wikipedia.org/wiki/Atropisomer

* Conformational isomers:

Definition: conformational isomerism is a form of stereoisomerism in which the isomers can be interconverted exclusively by rotations about formally sp^3-hybridised (single) bonds.

- '*syn*' (s): a torsion angle between 0° and ± 90°
- '*anti*' (a): a torsion angle between ± 90° and 180°
- '*clinal*' (c): a torsion angle between 30° and 150° or between –30° and –150°
- '*periplanar*' (p): a torsion angle between 0° and ± 30° or ± 150° and 180°
- '*synperiplanar*' (sp): a torsion angle between 0° and ± 30°
- '*synclinal*' (sc): a torsion angle between 30° to 90° and –30° to –90°
- '*anticlinal*' (ac): a torsion angle between 90° and 150° or –90° and –150°
- '*antiperiplanar*' (ap): a torsion angle between ± 150° and 180°

Notes:

- also referred to as conformational isomers or conformers and, specifically, as rotamers.
- these stereo-isomers cannot be isolated and always exist as a mixture in dynamical equilibrium

References:

- https://en.wikipedia.org/wiki/Conformational_isomerism

molecule_stereoisomer_relations	***List [L4a]***	[!]				£: Relations of stereo-isomery existing between the molecular species and other molecular species
*molecule*_stereoisomer_relation	enum(text)	S1 [!_m]	Molec L4a	F	--	Relation of stereo-isomery existing with the molecular species Enum: {enantiomer, diastereomer, anomer, atropisomer, conformer, other, no} *Definitions:* – '*enantiomer*': when two stereoisomers are related to each other by a reflection: They are mirror images of each other that are non-superimposable. Also known as 'optical isomers' – '*diastereomer*': when two or more stereoisomers of a compound have different configurations at one or more (but not all) of the equivalent (related) stereocenters and are not mirror images of each other (for ex: when it has one or more double bonds with 2 to 4 substituents). – '*anomer*': when it has a single bonded ring structure – '*conformer*': when the single bond between the two centres is free to rotate – '*atropisomer*': when it has a hindered rotation around single bond – '*other*': for other types of stereo-isomers not listed above. Give the information in "*molecule*_comments" – '*no*': when the molecule has no stereoisomer *Notes*: – When two diastereoisomers differ from each other at only one stereocenter they are called 'epimers'. *Reference*: - https://en.wikipedia.org/wiki/Stereoisomerism

Molecule: Natural isotopic composition

*molecule*_isotope_mixture_type [*species*_isotope_mixture_type]	enum(text)	S1 [!!_m]	Molec	F	--	Type of isotopic mixture of the molecule, molecular ion, radical or ionic radical Enum: {pure isotope, partly substituted, terrestrial abundance}

Definitions:

- *'pure isotope'*: only a single isotopic species of the molecule, i.e. a completely substituted molecule.
- *'partly substituted':* molecule with some atoms in natural isotopic abundance and one or more others that are fully substituted by pure isotopic species
- *'terrestrial abundance*': mixture of all its isotopic species of the molecule in 'standard' natural terrestrial abundance. Its natural isotopic composition is given by default in the natural 'generic mixture' (i.e. the 'non-isotopic species') entered in the SSHADE database by "*molecule*_isotope_uid" and "*molecule*_isotope_mole_fraction" of each isotopic species as calculated using the standard terrestrial atom mole fractions given by IUPAC (2009).

Notes:

- The fundamental molecule species stored in the database will be either with natural terrestrial abundance or as pure isotopes.
- Some of the partly isotopically substituted molecules (the most important/commercially available ones) may be also entered as fundamental species in the database.
- Molecules with 'specific isotopic abundance' in sample or matters will be built with several pure isotopologue molecules ("*constituent*_specie_uid" = 'MOLEC_xxx').

Ex:

- 'pure isotope' for $^{1}H_2{}^{13}C^{16}O$
- 'partly substituted' for $H_2{}^{13}CO$
- 'terrestrial abundance' for H_2CO

molecule_isotope_molecules	***List [L4b]***	[!o]

£: isotopic species contributing to the isotopic mixture of molecular species

Condition: mandatory only when "*molecule*_isotope_mixture_type" = {partly substituted, terrestrial abundance}

*molecule*_isotope_molecule_uid [*] [*species*_isotope_specie_uid]	CS-varchar(255)	U [!o_m]	Molec Molec L4b	F	--	Link to the existing UID of a pure isotopic species contributing to the isotopic molecular mixture *Condition:* mandatory only when "*molecule*_isotope_mixture_type" = {partly substituted, terrestrial abundance} *Notes:* – The list of all the isotopic species composing an isotopic mixture (with 'terrestrial abundance' or 'partly substituted') should be determined "by hand" as it depends on some symmetry elements of the molecule. – For big molecules composed of atoms having large numbers of isotopic species the list can be limited to the main isotopic molecular species (above some threshold value in abundance).
*molecule*_isotope_molecule_mole_fraction [+] [*species*_isotope_specie_mole_fraction]	float	U [!o_m]	Molec L4b	F	--	Mole fraction of the isotopic molecular species *Condition*: mandatory when the bloc is used *Note:* – value between 0 and 1 – For "isotope_mixture_type" = 'terrestrial abundance' the mole fractions should be determined using the standard terrestrial atom mole fractions given by IUPAC (2009) – These abundances should be determined "by hand" as they depend on some symmetry elements of the molecule. The sum should be = '1' – For big molecules composed of atoms having large numbers of isotopic species, if not all species are listed the sum will be < '1.0' (but close to 1). Not a major problem.

Molecule nuclear spin isomer composition

*molecule*_nuclear_spin_type [*species*_nuclear_spin_type]	enum(text)	S2 [!o_m]	Molec	F	--	Nuclear spin isomer of the molecule, molecular ion, radical or ionic radical. Enum: {equilibrated, para, ortho, meta**,** para-para, para-ortho, ortho-para, ortho-ortho, other, unique, unknown} *Condition:* mandatory for "*molecule*_isotope_mixture_type" = 'pure isotope' *Constraint:* only for "*molecule*_isotope_mixture_type" = {pure isotope, partly

substituted}

Definitions:

- 'equilibrated': for equilibrated mixtures of at least 2 spin isomers (with value corresponding to the high temperature limit)
- '*para*': with total nuclear spin I = '0' or '1/2' (singlet)
- '*ortho*': with total nuclear spin I = '1' or '3/2' (triplet)
- '*meta*': with total nuclear spin I = 2 or 5/2 (?) (quintuplet)
- *'para-para':* for cases where the molecule has 2 two different spin symmetries, such as for CH_2D_2. The first spin type refers to the first pair of symmetric atoms in the molecule formula, and the second type to the second pair. "*molecule*_nuclear_spin_qn_i" provides the detailed description

  Ex: ortho-para- CH_2D_2
- *'para-ortho':* same as 'para-para'
- *'ortho-para':* same as 'para-para'
- *'ortho-ortho:* same as 'para-para'
- *'other':* for any other spin type or combination of two or more spin types within a molecular species. "*molecule*_nuclear_spin_qn_i" provides the detailed description
- '*unique*': for the other molecules without spin isomers (with unique atoms, or not symmetric atoms, or with integer atom spin).
- *'unknown'*: unknown spin type

Notes:

- Spin isomers exist only for molecules having at least 2 identical atoms with non-nul spin, indiscernible with a symmetry operation of the molecule (H_2, N_2, H_2O, H_2CO, NH_3, CH_4, C_2H_4, C_2H_6, CH_3OH, …), radical ($\bullet NH_2$, …) or ion (H_3^+, H_2O^+, H_3O^+, …)
- Spin isomers can only be defined for a pure isotopic species, or for some partly substituded species where at least the atoms leading to the isomery are fully substituted.
- Combinaisons of spin isomers can occurs in some isotopologues with multiple symmetric pairs of atoms, for ex CH_2D_2 with ortho-para for both H_2 and D_2

*molecule*_nuclear_spin_qn_i [*species*_nuclear_spin_qn_i]	varchar(255)	S3 [!o_m]	Molec	F	--	Value of the total nuclear spin quantum number I of the nuclear spin isomer. *Condition*: Mandatory when "*molecule*_nuclear_spin_type" = {para, ortho, meta**,** para-para, para-ortho, ortho-para, ortho-ortho, other} *Constraint*: only when "*molecule*_nuclear_spin_type" = {equilibrated, para, ortho, meta**,** para-para, para-ortho, ortho-para, ortho-ortho, other} *Notes:* - The rotational angular momentum (J) has different allowed values for the different spin isomers that forbid their interconversion. Each spin isomer has its own rotational levels - 'I' should be positive and a multiple of ½ *Ex:* - '0, 1, 2' for equilibrated mixture of spin isomers - '0', '1/2' (para), '1', '3/2' (ortho), … for pure spin isomer species - '0 (para-H2), 1 (ortho-D2)', '1/2 (para-H2), 3/2 (ortho-D2)' for para-ortho-CH_2D_2 - '3/2 (ortho-H2), 3/2 (ortho-D2)' for ortho-ortho-CH_2D_2
*molecule*_nuclear_spin_equilibrium_opr [*species*_nuclear_spin_equilibrium_opr]	varchar(255)	S3 [!_m]	Molec	F	--	High temperature equilibrium ortho/para ratio. *Condition*: mandatory when "*molecule*_nuclear_spin_type" = {equilibrated} *Constraint*: only when "*molecule*_nuclear_spin_type" = {equilibrated} *Definition:* it is the equilibrium Ortho/Para mole fraction Ratio (OPR) at high temperature. *Note*: write it as a decimal number folloxed by the ratio of state occurence *Ex*: - '3 (3/1)' for H_2 with high T limit OPR = 3 (3/1) - '4.5 (9/2)' for CH_4 with high T limit OPR = 4.5 (9/2)
*molecule*_nuclear_spin_equilibrium_mpr [*species*_nuclear_spin_equilibrium_mpr]	varchar(255)	S3 [!_m]	Molec	F	--	High temperature equilibrium meta/para ratio. *Condition*: mandatory when "*molecule*_nuclear_spin_type" = {equilibrated} *Constraint*: only when "*molecule*_nuclear_spin_type" = {equilibrated} *Definition:* it is the equilibrium Meta/Para mole fraction Ratio (MPR) at high

						temperature. *Note*: write it as a decimal number folloxed by the ratio of state occurence *Ex*: - 2.5 (5/2) for CH_4 with high T limit MPR = 2.5 (5/2)
*molecule*_nuclear_spin_temperature_half_opr [*species*_nuclear_spin_temperature_half_opr]	float	S3 [m]	Molec	F	*K*	Spin temperature at half the high temperature equilibrium ortho/para ratio. *Constraint*: only when "*molecule*_nuclear_spin_type" = {equilibrated} *Definition:* it is the temperature corresponding to Ortho/Para mole fraction Ratio (OPR) equal to 50% of its high temperature equilibrium value. *Ex*: H_2 with high T limit OPR = 3 has an equilibrium T = 95 K for OPR = 1.5
molecule_nuclear_spin_isomer_molecules [*species*_nuclear_spin_isomer_specie]	***List [L4c]***	[!o]				£: Nuclear spin isomers contributing to the equilibrated (high T equilibrium) mixture of spin isomers *Condition:* mandatory only when "*molecule*_nuclear_spin_type" = {equilibrated}
*molecule*_nuclear_spin_isomer_molecule_uid [*] [*species*_nuclear_spin_isomer_specie_uid]	CS-varchar(255)	U [!o_m]	Molec Molec L4c	F	--	Link to the existing UID of a nuclar spin isomer contributing to the equilibrated mixture of spin isomers *Notes:* – The list of all the spin isomers (pure isotopic species) composing the equilibrated nuclear spin mixture should be determined "by hand" as it depends on some symmetry elements of the molecule.
*molecule*_nuclear_spin_isomer_molecule_mole_fraction [*species*_nuclear_spin_isomer_specie_mole_fraction]	varchar(255)	U [!o_m]	Molec L4c	F	--	Equilibrium molar fraction and fractional abundance of the spin isomer at the high temperature limit *Format*: provide both of them as 'mole fraction (fractional abundance)' *Ex:* 'para-$^{12}C^1H_4$' = '0.125 (2/16)', 'ortho-$^{12}C^1H_4$' = '0.5625 (9/16)', 'meta-$^{12}C^1H_4$' = '0.3125 (5/16)' for $^{12}C^1H_4$ (para:ortho:meta = 2:9:5, idem for NH_4^+) *Notes:* – Molar fraction, value between 0 and 1

- fractional abundance: simple ratio between the number of isomer configurations and the total number of configurations of all isomers
- the sums should be = '1'
- other nuclear spin isomer mixtures (synthetic, at low temperature, …) should be defined in 'sample' by using a molecular mixture of pure spin isomers

---

Molecule symmetries

*molecule*_symmetry [*species*_symmetry]	CS-enum(text)	S2 [!!_m]	Molec	F	--	Symmetry (point group) of the molecule, molecular ion, radical or ionic radical. Enum: {C1, Cs, Ci, Cinfv, Dinfh, C2, C3, C2h, C3h, C2v, C3v, C4v, D2, D3, D2h, D3h, D4h, D5h, D6h, D2d, D3d, D4d, D5d, Td, Oh, Ih, no, unknown} *Notes:* – true writing of Schönflies symbols is with the number/letter after the capital letter put in underscript. *Ex:* 'C2v' => C_{2v} – 'Dinfv' and 'Dinfh' are for $D_{\infty v}$ and $D_{\infty h}$ – for the isotopic mixtures with terrestrial abundance it is given for the main isotopic species (Ex: $^{12}C^{1}H_4$) Cf.: http://en.wikipedia.org/wiki/Symmetry
*molecule*_case	enum(text)	S2 [!!_m]	Molec	F	--	Description of the case category of molecular state for the molecule, molecular ion, radical or ionic radical. Enum: {diatomic, linear-triatomic, nonlinear-triatomic, spherical-top, symmetric-top, asymmetric-top, linear-polyatomic, nonlinear-polyatomic, complex} *Note:* Correspondance with XSAMS cases (we removed the difference between open/closed shell as we did not fully describe the electronic states): '*diatomic'* = 'dcs', 'hunda', 'hundb' '*linear-triatomic'* = 'ltcs', 'ltos' '*nonlinear-triatomic'* = 'nltcs', 'nltos' '*spherical-top'* = 'sphcs', 'sphos'

‘*symmetric-top’* = ‘stcs’
‘*asymmetric-top’* = ‘asymcs’, ‘asymos’
‘*linear-polyatomic’* = ‘lpcs’, ‘lpos’
‘*nonlinear-polyatomic’* = (not XSAMS cases)
‘*complex’* = (not XSAMS cases)

Note:

- no difference between linear and nonlinear polyatomic in XSAMS
- ‘complex’ will be used for complex molecules when there is no possible description of states quantum numbers, but only normal vibration modes.
- the case is used as a constraint on the Quantum Numbers necessary to describe the state of molecules of this type. When a transition will refer to a state its value of “*state*_case” get the value “*molecule*_case” of the molecule subjected to the transition
- for the isotopic mixtures with terrestrial abundance it is given for the main isotopic species (Ex: $^{12}C^{1}H_4$)

Molecule fundamental vibration modes

Note: for the isotopic mixtures with terrestrial abundance they are given for the main isotopic species (Ex: $^{12}C^{1}H_4$)

*molecule*_vibrations_number [*species*_vibrations_number]	int(3)	U [!_m]	Molec	F	--	Number ‘n’ of fundamental internal vibration modes ‘Vi’ (normal modes) of the free molecular species *Note:* did not include the multiplicity of degenerated modes
molecule_vibrations	***List [L5]***	[O]				£: Fundamental internal vibrations of the molecular species. *Condition:* Optional bloc - Mandatory active below when *“molecule*_vibration_mode” ≠ ‘NULL’
*molecule*_vibration_mode	enum(text)	S2 [(!!)do_m]	Molec L5	F	--	Type of fundamental internal vibration mode of the free molecule, molecular ion or radical. Enum: {stretching, stretching sym., stretching antisym., bending, bending in-p, bending out-p, bending sym., bending antisym., bending sym. in-p

(scissoring), bending antisym. in-p (rocking), bending sym. out-p (wagging), bending antisym. out-p (twisting), deformation, other, unknown}

Default = 'NULL'

Condition: (option trigger) the filling of this KW is 'absolute mandatory' when this optional bloc is used. It triggers the 'mandatory' status of several others KW in the optional bloc.

Definitions:

- '*stretching*': a change in the length of a bond
  Ex: C-H, C-C
- '*stretching sym.*': symmetric stretching mode that concerns at least 3 atoms and is symmetric relative to the central atom
- '*stretching antisym.*': antisymmetric stretching mode that concerns at least 3 atoms and is antisymmetric relative to the central atom
- '*bending*': a change in the angle between two bonds
  Ex: the HCH angle in a methylene group
- '*bending in-p*': in-plane bending (can be rocking or scissoring)
- '*bending out-p'*: out-of-plane bending (can be wagging or twisting)
- '*bending sym.*': symmetric bending (can be wagging or scissoring)
- '*bending antisym.*': antisymmetric bending (can be rocking or twisting)
- '*bending sym. in-p (scissoring)*': symmetric in-plane bending
  Note: mostly for bending with symmetric atoms (ex: H2O, …),
- '*bending antisym. in-p (rocking)*': a change in angle between a group of atoms.
  Ex: a ethylene group relative to the rest of the C2H4 molecule
- *'bending sym. out-p (wagging)*': a change in angle between the plane of a group of atoms,
  Ex: a methylene group from the plane through the rest of the C2H4 molecule,
- '*bending antisym. out-p (twisting)*': a change in the angle between the planes of two groups of atoms.
  Note: also called 'torsion' for twisting of a bond in large molecules
  Ex: a change in the angle between the two ethylene groups in C2H4

- '*deformation*': a combination of two or more of the different types of bending modes

  Note: used in particular for bending with asymmetric atoms or in complex molecules
- '*other*': other mode which cannot be described with one or the above term.
- '*unknown*': unknown mode of vibration

Notes:
- '*xxx sym.'*: (symmetric) attribute telling that the vibration concerns at least 3 atoms and is symmetric relative to the central atom
- '*xxx antisym.'*: (antisymmetric) attribute telling that the vibration concerns at least 3 atoms and is asymmetric relative to the central atom
- '*xxx in-p'*: (in-plane) attribute telling that all the changes in the angle of the bonds occurs in the plane defined by the remaining atoms of the molecule
- '*xxx out-p'*: (out-of plane) attribute telling that the change in the angle occurs between any one of the bonds and the plane defined by the remaining atoms of the molecule

  Ex: a change in the angle between any one of the C-H bonds and the plane defined by the remaining atoms of the ethylene molecule.

  Ex: in BF3 when the boron atom moves in and out of the plane of the three fluorine atoms.

Notes on other attributes:

A few additional attributes to vibration modes are generally found in the literature:
- '*ring xxx*': attribute telling that the vibration mode concerns a molecular ring.

  ⇨ this complementary information is given by "*chemical_bond*_formula" of "*molecule*_vibration_chemical_bond_uid"

  Ex: S8, C6H6, …
- '*degenerate xxx*': attribute telling that the vibration mode is doubly, or more, degenerated (and has no other attribute).

  ⇨ this complementary information is given in

					"*molecule*_vibration_degeneracy" *Note:* basic definitions at: http://en.wikipedia.org/wiki/Vibrational_spectroscopy https://en.wikipedia.org/wiki/Molecular_vibration http://chemwiki.ucdavis.edu/Core/Physical_Chemistry/Spectroscopy/Vibrational_Spectroscopy/Vibrational_Modes/Normal_Modes
*molecule*_vibration_chemical_bond_uid [*]	varchar(255)	S1i [!o_m]	Molec ChemB Molec L5	F	--	Link to the existing UID of the bond, part of the molecular species, or whole molecule, subjected to the fundamental vibration *Condition:* Mandatory only if "*molecule*_vibration_mode" ≠ 'NULL' *Note:* the UID starts with either 'BOND_', MOLECPART_', or 'MOLEC_' depending on the number of bonds involved and size of the molecule, see below *Notes:* - The bond (2 bonded atoms) is always a specific isotopic bond whatever for natural terrestrial isotopic mixtures, partially isotopic substituted molecules, a pure isotopic molecules. - In the first case it will be generally the bond made with the major isotopic species of both atoms (if largely dominant, such as for 1H, 12C, 16O, 14N…). In case of atoms with 2 isotopic species of equivalent abundance (ex: 35Cl and 37Cl) it will be necessary to create a partly substituted bond to link with it here (ex: Cl16O, Cl being 'natural'). - For partially isotopic substituted moleculesthe bond will that of the substituted isotopic atom with the major isotopic species of the second atom. *Notes:* - when more than one bond (generally 2 or 3) are involved in the vibration, but not the whole molecule, a 'molecule part' (or its isotopic variant) should be used instead. It is mostly the case for bending, symmetric and antisymetric stretchings, rocking, and deformations. *Ex:* 'MOLECPART_CH3', 'MOLECPART_CCdC', 'MOLECPART_tCCH3', …

- when the vibration involves the whole molecule (case of twisting, some deformations, …) we use:
  - diatomic molecules: the bond ‘BOND_XY’ or its isotopic variant
    Ex: ‘BOND_CO’, ‘BOND_13C18O’, …
  - larger molecules: the molecule ‘MOLEC_XYZ’ or its isotopic variant
    Ex: ‘MOLEC_CH4’, ‘MOLEC_13C16O18O’, ‘MOLEC_CH3OH’, …

*molecule*_vibration_label	varchar(255)	S U [!o_m]	Molec Miner L5	F	F	--	--

Labels of the normal mode of vibrations of the molecular species

Condition: Mandatory only if “*molecule*_vibration_mode” ≠ ‘NULL’

Note: First letter should be ‘V’ followed by an integer: ‘Vi’. When there is only one vibration mode (diatomic molecules) it will be simply ‘V’

Ex: ‘V1’, ‘V2’, …

*molecule*_vibration_symmetry	CS- enum(text)	S U [m]	Molec Miner L5	F	F	--	--

Point group symmetries of the normal modes of vibration of the molecular species

Enum: {A, Ap, As, A1, A1p, A1s, A2, A2p, A2s, B, B1, B2, B3, E, Ep, Es, E1, E1p, E1s, E2, E2p, E2s, E3, F, F1, F2, Sigma+, Sigma-, Pi, Phi, Delta}

Condition: only for isotopic species (if "*molecule*_isotope_mixture_type" = 'pure isotope')

Note: The “prime” in A’, and the “second” in A” are respectivement noted ‘p’ and ‘s’ Ex: {A1p, A1s}

*molecule*_vibration_degeneracy	enum(text)	S S2 [!o_m]	Molec Miner L5	F	F	--	

Degeneracy of the mode of vibration of the free molecule

Enum: {no, double, triple, quadruple}

Condition: Mandatory only if “*molecule*_vibration_mode” ≠ ‘NULL’

Note: degeneracy is function of vibration symmetry:

- *‘no’:* A, A1, A2, (+ p, s), B, B1, B2, B3, Sigma+
- *‘double’:* E, E1, E2 (+ p, s), Pi

– *'triple':* F2
– *'quadruple':*

*molecule*_vibration_fundamental_frequency	float	S [m]	U	Molec Miner L5	F	F	*cm-1*	Fundamental frequency of the normal mode of vibration of the molecular species • stored in the database and provided to user in 'cm-1' unit *Condition:* only for isotopic species (if "*molecule*_isotope_mixture_type" = 'pure isotope') *Note:* The normal modes of the free molecule are given only for the ground electronic state
*molecule*_vibration_observed_frequency	float	S [!o_m]	S3	Molec Miner L5	F	F	*cm-1*	Observed frequency of the normal mode of vibration of the molecular species • stored in the database and provided to user in 'cm-1' unit *Condition:* Mandatory only if "*molecule*_vibration_mode" ≠ 'NULL' *Note:* The observed mode is significantly different from the fundamental mode when there is resonance (Fermi, …) with another mode.
*molecule*_vibration_observed_frequency_2	float	S [m]	S3	Molec Miner L5	F	F	*cm-1*	Second observed frequency of the normal mode of vibration of the molecular species • stored in the database and provided to user in 'cm-1' unit *Note:* a second observed mode frequently appear when there is resonance (Fermi, …) with another mode.
*molecule*_vibration_harmonic_frequency	float	S [o_m]	U	Molec Miner L5	F	F	*cm-1*	Harmonic frequency of the normal mode of vibration of the molecular species • stored in the database and provided to user in 'cm-1' unit *Condition:* only for isotopic species (if "*molecule*_isotope_mixture_type" = 'pure isotope') *Note:* The normal modes of the free molecule are given only for the ground electronic state

*molecule*_vibration_activity_ir	enum(text)	S [!o_m]	U	Molec Miner L5	F	F	--	--	IR activity of the normal modes of vibration of the molecular species Enum: {active, inactive, unknown} *Condition:* Mandatory only if "*molecule*_vibration_mode" ≠ 'NULL' *Note:* for natural mixture it concerns the major isotopic species Can be checked on NIST chemical webbook or here for some molecules: http://www.chem.purdue.edu/gchelp/vibs/index.html
*molecule*_vibration_activity_raman	enum(text)	S [!o_m]	U	Molec Miner L5	F	F	--	--	Raman activity of the normal modes of vibration of the molecular species Enum: {active, inactive, unknown} *Condition:* Mandatory only if "*molecule*_vibration_mode" ≠ 'NULL' *Note:* for natural mixture it concerns the major isotopic species Can be checked on NIST chemical webbook or here for some molecules: http://www.chem.purdue.edu/gchelp/vibs/index.html
*molecule*_vibration_intensity_strength	enum(text)	S [m]	U	Molec Miner L5	F	F	--	--	Arbitratry qualitative (relative) spectroscopic classification of band intensity of the normal modes of vibration of the molecular species Enum: {ia, vvw, vw, w, m, s, vs, vvs} *Definitions*: – This classification is very raw and relative. Here we follow the values provided in NIST Chemistry Webbook, + other complementary references *Note:* typically the strongest fundamental vibration band (IR) of a molecule is 'vs'. The strongest electronic transitions (UV) are 'vvs' *Note:* For 'species with natural terrestrial isotopic abundances it will be the intensity of the mixture of isotopic species, but in general it is dominated by the major isotopic species (>95%).
*molecule*_vibration_comments	blob	S [m]	U	Molec Miner L5	F	F	--	--	Comments on this normal mode of vibration of the molecular species

*molecule*_vibrations_comments	blob	S U [m]	Molec	F	F	-- --	General comments on the normal modes of vibration of the molecular species
molecule_vibrations_publications	***List [L4]***	[O]					£: Publications describing the fundamental vibrations of the molecular species
*molecule*_vibrations_publication_uid [*]	varchar(255)	U [m]	Molec Publi L4	F	--		Link to the existing UID of the publication(s) or database(s) in which information on these normal modes of vibration of the molecular species have been published *Condition:* only for isotopic species (if "*molecule*_isotope_mixture_type" = 'pure isotope')

Molecule properties

*molecule*_molar_mass [*species*_molar_mass]	float	S3 [!_m]	Molec	F	*g/mol*	Molar mass of the molecular species or molar weight of isotopic mixture • stored in the database and provided to user in 'g/mol' unit *Note:* – For isotopes this "molecule molar mass" is equivalent (in number) to the "molecular mass" in unified atomic mass units ('u', formerly noted 'amu'). It is taken from IUPAC tables. – This "molecular mass" is not defined for mixtures. – For an isotopic mixture the molar mass is determined by the sum of "*molecule*_molar_mass" weighted by their "*molecule*_isotope_molecule_mole_fraction" for all isotopic molecular species composing the mixture. – For the terrestrial standard isotopic mixture the "*molecule*_isotope_molecule_mole_fraction" determined using the standard terrestrial atom mole fractions given by IUPAC (2009) is used. *Calculator*: https://www.lenntech.com/calculators/molecular/molecular-weight-calculator.htm

*molecule*_state_stp	enum(text)	S1 [!o_m]	Molec	F	--	State of the molecular species in standard (STP) conditions Enum: {gas, liquid, solid} *Condition*: mandatory only when "*molecule*_type" = {molecule} *Note:* STP conditions (IUPAC): 273.15K (0°C), 100kPa (1 bar) *Ex*:: 'solid' for H_2O as its melting point is 273.153 K
*molecule*_state_ntp	enum(text)	S2 [!o_m]	Molec	F	--	State of the molecular species in normal (NTP) conditions Enum: {gas, liquid, solid} *Condition*: mandatory only when "*molecule*_type" = {molecule} *Note:* NTP conditions (NIST): 293.15K (20°C), 101.325kPa (1 atm) *Ex*:: 'liquid' for H_2O as its melting point is 273.153 K
*molecule*_protic	enum(text)	S1 [!_m]	Molec	F	--	Ability of the molecular species to give a H+ ion and form hydrogen bonds (protic) or not (aprotic) Enum: {protic, aprotic} *Note:* a protic molecule posseses a polar bonding of H with another more electronegative atom (O, N, F, Cl, Br, …): OH, NH, … groups
*molecule*_polarity	enum(text)	S1 [!_m]	Molec	F	--	Polarity of the molecular species Enum: {nonpolar, polar, ionic, amphiphilic} *Definitions:* A molecule may be polar either as a result of polar bonds due to differences in electronegativity as described above, or as a result of an asymmetric arrangement of nonpolar covalent bonds and non-bonding pairs of electrons. – '*nonpolar*': a molecule may be nonpolar either when there is an equal sharing of electrons between the two atoms of a diatomic molecule or because of the symmetrical arrangement of polar bonds in a more complex molecule. – '*polar*': a polar molecule has a net dipole as a result of the opposing

						charges (i.e. having partial positive and partial negative charges) from polar bonds arranged asymmetrically – '*ionic*': a molecule in which the total number of electrons is not equal to the total number of protons, giving the atom or molecule a net positive or negative electrical charge. Also molecules with local positive and negative electrical charges that compensate (salts...) – '*amphiphilic* ': Large molecules that have one end with polar groups (hydrophilic) attached and another end with nonpolar groups (hydrophobic, lipophilic) are described as amphiphilic molecules (or amphiphiles). From: https://en.wikipedia.org/wiki/Chemical_polarity
*molecule*_dipole	float	S3 [m]	Molec	F	*D*	Permanent dipole moment of the molecular species • stored in the database and provided to user in 'debye (D)' unit

Molecule references and comments

molecule_links	***List [L6]***	[O]				£: Web pages describing the molecular species and its properties.
*molecule*_link_name [*species*_link_name]	varchar(255)	U [m]	Molec L6	F	--	Name of the web page(s) describing molecule, molecular ion, radical or ionic radical and its properties. *Ex:* 'Wikipedia', 'NIST Chemistry Webbook', 'HITRAN', …
*molecule*_link_url [*species*_link_url]	CS-varchar(255)	U [m]	Molec L6	F	--	URL address(es) of web page(s) describing the molecule, molecular ion, radical or ionic radical and its properties. *Notes*: - you can link to a publication by giving its url address, preferably through its DOI. Ex: https://doi.org/10.1002/ejic.200700067
*molecule*_comments [*species*_comments]	blob	U [m]	Molec	F	--	Additional information on molecular species (major isotopic molecular

Aj species, …)

6. Fundamental Phases

6.1 Definition

The "Fundamental phases" are the basic building pieces of the materials of the samples and matters. They are grouped in 5 main families with common properties: **'molecular solids', 'ionic solids', 'covalent network solids', 'metallic solids',** and **'minerals'**. We also consider **'liquids'** as a special fundamental constituent.

Definitions:

- 'molecular solids': Made up of atoms or molecules held together by London dispersion forces, dipole-dipole forces, or hydrogen bonds.
- 'ionic solids': Made up of positive and negative ions and held together by electrostatic attractions.
- 'covalent network solids' (glasses, ceramics, and polymeric solids): Made up of atoms connected by covalent bonds in a continuous network extending throughout the material. In a network solid there are no individual molecules, and the entire crystal or amorphous solid may be considered a macromolecule.
- 'metallic solids': Made up of metal atoms that are held together by metallic bonds.
- 'minerals': any of the above type of solid but of natural origin
- 'liquids': any of the above type of solid but in the liquid phase (molecular, ionic, atomic, metallic)

The four classes of solids permit six pairwise intermediate forms

Refs:

- Properties of Solids: http://www.chem.fsu.edu/chemlab/chm1046course/solids.html)
- Bonding in solids: https://en.wikipedia.org/wiki/Bonding_in_solids

In addition there are two main categories of solid phases: Crystalline solids and amorphous solids.

- Crystalline solids are those in which the atoms, ions, or molecules that make up the solid exist in a regular, well-defined arrangement. The smallest repeating pattern of crystalline solids is known as the unit cell, and unit cells are like bricks in a wall—they are all identical and repeating.
- Amorphous solids do not have much order in their structures. Though their molecules are close together and have little freedom to move, they are not arranged in a regular order as are those in crystalline solids.

The "mineral and rock matters" (see ***) as well as some "extraterrestrial matters" refer to the mineral phases to define the fundamental minerals that form them.

6.2 Liquid phase Table

Root of the table: ***liquid***

Data type: 'Fundamental phase'

Notes:

- In "Exp" column 'VL' means a variable key-word of the fundamental liquid phase: when defining a "sample" or a "matter" containing fundamental liquid phases (described in "basic constituents") the VL values in "liquid phase" can be modified (but will not be changed in the fundamental liquid database) to reflect the exact liquid properties (for exemple for liquid solutions). See specific notes in *Variable: liquid in Sample and Matters*
- currently there is no way to define isotopic mixtures of liquids (only natural terrestrial, pure isotopic mixtures or pure isotopic substitution of molecules are possible)

Key-word	Type	Level	Table	Exp	Unit	Description
Liquid import						
*liquid*_import_mode [phase_import_mode]	enum(text)	P [!!_m]	Liquid	(V)	--	Mode of import of the liquid data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*liquid*_xml_filename [-xml] [phase_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	Liquid	(V)	--	Name of the storage copy of the xml import file of the liquid metadata ➔ determined automatically during import (from "*liquid*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Liquid indexes and type						
*liquid*_index [**][-xml] [phase_index]	int(10)	B [!!_g]	Liquid	F	--	Automatic random but unique number (ID) given to new liquid
*liquid*_uid [**] [phase_uid]	varchar(255)	S0/S0c/S0	Liquid	F	--	Unique identifier code given (UID) to the liquid table (to be created) *Nomenclature:* Create this UID with 'LIQUID_', possibly followed by

		[!!_m]				‘SERIES_’ for ‘liquid solution’ series It should be of the style: ⇨ ‘LIQUID_LiquidFormula’ or ‘LIQUID_LiquidName’ ⇨ ⇨ ‘LIQUIDSERIES_SeriesName’ or ‘LIQUIDSERIES_SoluteFormula_SolventFormula(_MoleFraction)’ where: ⇨ ‘LiquidFormula‘ is the liquid chemical formula, ⇨ ‘LiquidName’ is the “*liquid*_official_name” ⇨ ‘SeriesName’ is the liquid solution series name, ⇨ ‘SoluteFormula‘ is the solute chemical formula, ⇨ ‘SolventFormula’ the solvent chemical formula. *Note*: If a possible confusion between 2 solutions (but not for generic solution) then add ‘MoleFraction’ the “*liquid*_specie_mole_fraction” of the solute (in %). *Ex:* - ‘LIQUIDSERIES_HCl_H2O’ for HCl in H2O - ‘LIQUID_HCl_H2O_10’ for 10% HCl in H2O *Note*: The fundamental liquid phases stored in the database will be, by default, with natural terrestrial abundance.

Liquid names and identifiers

*liquid*_official_name [*phase*_official_name]	varchar(255)	S0/S0c/S0 [!!_m]	Liquid	F	--	Official name of the liquid *Ex:* ‘sulfuric acid solution’…
liquid_secondary_names [*phase*_secondary_names]	***List [L0]***	[m]				£: List of the alternative names used for the liquid
*liquid*_secondary_name [*phase*_secondary_name]	varchar(255)	S0/S0c/S0	Liquid L0	F	--	Alternative name(s) used for the liquid *Notes:*

		[m]				- start with a capital letter *Ex.:* 'vitriol', …
*liquid*_cas_number [*phase*_cas_number]	varchar(255)	S1/S1c/S2 [m]	Liquid	F	--	CAS registry number, unique, of the liquid (natural and isotopic species) *Note:* - the problem is to found them !!! no registry, not systematic! - a CAS number is generally not linked to a phase but to composition, so not necessary a specific CAS number for the liquid
Liquid family						
*liquid*_family [*constituent/phase*_family]	enum(text)	S1/S1c/S1 [!!_m]	Liquid	F	--	Phase family (or major class) of liquid Enum: {molecular liquid, atomic liquid, ionic liquid, metallic liquid, molecular and atomic liquid, molecular and ionic liquid, atomic and ionic liquid, liquid solution, complex liquid, other, unknown} [to be changed in v0.9.0a] *Definitions:* see in "*constituent*_family"
*liquid*_class [*constituent/phase*_class]	enum(text)	S1/S1c/S1 [!!_m]	Solid	F	--	Class of liquid Enum: {non polar molecular liquid, polar molecular liquid, hydrogen bonded molecular liquid, molecular liquid solution, atomic liquid, atomic liquid solution, ionic liquid, ionic liquid solution, metallic liquid, metallic liquid solution, mixed liquid solution} *Definitions:* - For molecular liquids: - '*non polar molecular liquid'*: liquid made of non polar molecular species - '*polar molecular liquid'*: liquid made of polar molecular species - '*hydrogen bonded molecular liquid'*: liquid made of hydrogen bonded molecular species - '*molecular liquid solution'*: homogeneous liquid mixture of molecular species

						- For atomic liquids: - '*atomic liquid'*: liquid made of a single atomic species - '*atomic liquid solution'*: homogeneous liquid mixture of atomic species - For ionic liquids: - '*ionic liquid'*: liquid made of ionic species (molten salts) - '*ionic liquid solution'*: homogeneous liquid mixture of ionic and molecular species - For metallic liquids: - '*metallic liquid'*: molten metal - '*metallic liquid solution'*: homogeneous liquid mixture of metallic species - '*mixed liquid solution'*: homogeneous liquid mixture of different types of species *Notes:* - Equivalent to "*constituent*_class"
*liquid*_compound_type [*phase*_compound_type]	openum(text)	S0/S0c/S0 [!_m]	Liquid	F	--	General type of liquid compound OpenEnum: {liquid, liquid solution, weak acid, strong acid, weak base, strong base, liquid salt, organic liquid, other compound} *Definitions:* - '*liquid'*: liquid composed of a single molecular, atomic or ionic species - '*liquid solution'*: homogeneous liquid mixture of species (solute: initially gas, liquid or solid) dissolved in another species (solvent) in the liquid state - '*other compound'*: compounds which cannot be described by one of the above words (describe in "*liquid*_comments") *Notes:* - same compound types for "*constituent*_compound_type". It will be used for main search.
*liquid*_solution_type	enum(text)	S1/S2c	Liquid	F	--	Type of liquid solution

		[!o_m]				Enum: {polar protic solution, polar aprotic solution, apolar solution} *Condition:* Mandatory and only when "*liquid*_family" = {liquid solution} *Definitions:* - '*polar protic solution*': solution with polar solvent containing H atom (dielectric constant > 15) - '*polar aprotic solution*': solution with polar solvent without H atom (dielectric constant > 15) - '*apolar solution*': solution with apolar solvent (dielectric constant < 15)

Liquid endmembers

liquid_endmembers *[phase_endmembers]*	***List [L1]***	[!o]				£: List of the endmember liquids of the series *Condition:* mandatory only when "*liquid*_family" = {liquid solution}
*liquid*_endmember_liquid_uid [*] [*phase*_endmembers_phase_uid]	varchar(255)	U [!o_m]	Liquid Liquid L1	F	--	Link to the existing UID of the endmember liquids of the series *Ex:*
*liquid*_figures	***List [L2]***					£: List of the figures on the liquid
*liquid*_figure_filename [*phase*_figure_filename]	varchar(255)	U [m]	Liquid L2	F	--	File name(s) (with extension) of the figure on the liquid *Image formats:* .png, .jpg, (.gif) *Notes:* - mostly for solution series - can be a liquid-solid phase diagram - can be a (end)members diagram of a liquid solution series … *Note DB:* this file will be imported in the database
*liquid*_figure_caption	varchar(255)	U	Liquid	F	--	Caption(s) or comment(s) on the figure(s) on the liquid

[*phase*_figure_caption]		[m]	L2			

Liquid composition

*liquid*_formula [*phase*_formula]	varchar(255)	U [!!_m] [V: m]	Liquid	VL	--	Developed (empirical) chemical formula of the liquid *Syntax:* Latex format *Ex:* - 'H_2O' for H_2O - '$(N_2) \colon (CH_4)_{n}$' for $(N2):(CH4)_n$ - '$NH_3 \bullet (H_2O)_{n}$' for $NH_3•(H_2O)_n$ *Notations:* – Colon (: or \colon) can separate molecules in liquid solution – Dot • (\bullet) separates hydration – LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf ***Variable: liquid in Sample and Matters*** *Notes*: – Can contain isotopic information when an atom is substituted in a molecule *Ex*: '$^{18}H_2O$'
*liquid*_chemical_formula [*phase*_chemical_formula]	CS-varchar(255)	S0/S0c/ S1 [!!_m] [V: m]	Liquid	VL	--	Developed global chemical formula of the liquid *Ex:* - '(N2:CH4)', or '(N2):0.03(CH4)' for 3% CH_4 in liquid solution in N_2 - 'NH3•(H2O)n' for NH3 hydrated in H2O *Notes:* - can contain ionic information. - liquid solution series are indicated by colon separating the molecules that varies in amount. The more dominant molecule is usually listed first. - big point '•' (ascii=149) separates hydration in ( ) - For liquid with non-natural isotopic abundance, substituted atoms will have their atomic mass between square brackets preceding the atom

						symbol. D can be used for ^{2}H. *Ex:* 'NH3•(D2[18]O)n' ***Variable: liquid in Sample and Matters*** Developed global chemical and structural formula of the actual liquid
Liquid chemical functions						
liquid_chemical_functions	***List [L3a]***	[O] [V: £_m] [V Flag: !!o_m]		VL		£: List of different chemical functions present in the liquid *Note*: this keyword lists all inter-molecular chemical functions, except those already in the molecular species and anionic radicals described as 'species' of the liquid ***Variable: liquid in Sample and Matters*** *Condition:* compulsory to list the new inter-molecular chemical functions and the intra-molecular chemical functions with changing 'number' Flag 'full_definition': {yes, no} *Condition:* Flag absolute mandatory when "*solid*_chemical_function_uid" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of chemical functions defined in the 'fundamental liquid phase'. Need to fully redefine it. - '*no*': only to add new chemical functions to the original list and modify some already defined (they should have the same "*liquid*_chemical_function_uid" than the original chemical function to be modified). *Note:* the flag 'full_definition' allows to control the mode of definition of the chemical functions of the actual liquid.
*liquid*_chemical_function_uid [*] [*phase*_chemical_function_uid]	varchar(255)	S2/S2c [!o_m] [V: ££o_m]	Liquid ChemF	VL	--	Link to the existing UID of the chemical function present in the liquid *Condition*: mandatory when *"liquid*_chemical_function_number" ≠ Ø (i.e. the bloc is used)

				L3a			*Note*: - If the liquid is described in terms of molecular species with "*liquid*_species_uid" their chemical functions (already implicitely taken into account) should not be listed here. - it is mostly used to describe chemical functions when a molecular liquid is described in terms of atoms or when it cannot be fully described in terms of molecules ***Variable: liquid in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used
*liquid*_chemical_function_number [+] [*phase*_chemical_function_number]	varchar(255)	S3/S3c [m] [V: m]	Liquid L3a	VL	--	Number or range of numbers of this chemical function present in the liquid ➔ Calculation for display: *Condition*: when all "*liquid*_specie_mole_fraction" ≠ {Ø, NULL} – n(function_i) = [*liquid*_chemical_function_number(function_i) + $\sum_{molecule_j}$ (*liquid*_specie_mole_fraction(molecule_j) * *specie*_chemical_function_number(molecule_j,function_i) + *liquid*_specie_number_min(function_i))] / [*liquid*_chemical_function_number(function_i) + $\sum_{function_i}$ [$\sum_{molecule_j}$ ("*liquid*_specie_mole_fraction(molecule_j) * *specie*_chemical_function_number(molecule_j,function_i) + *liquid*_specie_number_min(function_i))]] ***Variable: liquid in Sample and Matters*** Actual number of the chemical functions
liquid_chemical_bonds	***List [L3b]***	[!O]				£: List of the inter-molecular bonds and ionic bonds of the liquid, except those already in the molecular species and anionic radicals described as 'species' of the liquid *Condition:* mandatory when "*liquid*_class" = {hydrogen bonded molecular liquid, ionic liquid, ionic liquid solution} *Note*: These bonds are only the inter-molecular bonds (hydrogen bonds, …) and ionic bonds between molecules or atoms. All the other intra-molecular

						chemical bonds are already described in the isolated molecules.
*liquid*_chemical_bond_uid [*] [*phase*_chemical_bond_uid]	varchar(255)	S2/S1c [!o_m]	Liquid ChemB L3b	F	--	Link to the existing UID of the inter-molecular bonds and ionic bonds of the liquid *Note*: – The chemical bonds used for liquids are only 'generic mixture' with terrestrial abundance *Ex:* for liquid H_2O: 2 x 'BOND_HhO' – For isotopic substituted liquids made of at least one molecule with a purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope of the others
*liquid*_chemical_bond_number [+] [*phase*_chemical_bond_number]	varchar(255)	S3/S3c [!o_m]	Liquid L3b	F	--	Number, or minimum number, of inter-molecular bonds and ionic bonds of each type composing the liquid ➔ Calculation of 'n(bond_i)' for display: *Condition*: when all "*liquid*_specie_mole_fraction" ≠ {Ø, NULL} ⇨ n(bond_i) = [*liquid*_chemical_bond_number(bond_i) + $\sum_{specie_j}$ (*liquid*_specie_mole_fraction(specie_j) * *specie*_chemical_bond_number(specie_j, bond_i))] / [*liquid*_chemical_bond_number(bond_i) + $\sum_{function_i}$ [$\sum_{specie_j}$ (*liquid*_specie_mole_fraction(specie_j) * *specie*_chemical_bond_number(specie_j, bond_i))]] *Note*: determined relative to a formula unit *Ex:* '< 2' hydrogen bonds per H_2O molecule for liquid H_2O
Liquid molecular and atomic composition						
*liquid*_isotope_mixture_type [*phase*_isotope_mixture_type]	enum(text)	S1/S1c/ S1 [!!d_m] [V: £o_m]	Liquid	VL	--	Type of isotopic mixture of the liquid Enum: {pure isotope, partly substituted, terrestrial abundance} *Definitions: cf "solid*_isotope_mixture_type" *Notes:*

- The fundamental liquid stored in the database will be, by default, always with natural terrestrial abundance. The other options are only for ‘variable’ (see below)

Variable: liquid in Sample and Matters

Enum: {pure isotope, partly substituted, terrestrial abundance, specific abundance, unknown}

Condition: Compulsory when “*liquid*_isotope_mixture_type” ≠ ‘terrestrial abundance’

Note: isotopic mixtures in liquid with some molecules not in natural isotopic abundance will be set to ‘specific abundance’ or to ‘partly substituted’ (one or more molecule with an atom as a pure isotopic species). Their isotopic abundance will be defined in “*liquid*_specie_isotope_mole_fraction” using the pure isotopologue molecules

Note: define the effectif type of isotopic mixture

*liquid*_species_mole_fraction_unit	enum(text)	U [od_m] [V: m]	Const	VL	--

Unit for the molar fraction or concentration of the species in the liquid

Enum: {mol/mol, mol/g, mol/kg, mol/l}

Default: ‘mol/mol’

Note:

- the ‘mol/g’, ‘mol/kg’ and ‘mol/l’ units are used only in liquid solutions and allow to express the concentration of solutes relative to a solvent
- in liquid solutions, the solvent mole fraction should be expressed in the same unit as the solutes
- used only for “*constituent*_specie_mole_fraction” and “*constituent*_specie_mole_fraction_error”

Variable: liquid in Sample and Matters

- the unit can change only when *liquid_species* ‘full_definition’:= ‘yes’
- otherwise it is necessary to check in which unit is entered the liquid phase and to enter new species in the same unit

liquid_species	***List [L4]***	[!!] [V: £_m] [VFlag: !!o_m]				£: Description of the molecular and/or atomic composition of the liquid ***Variable: liquid in Sample and Matters*** *Condition:* compulsory to list the impurity, or substituted molecules/atoms, as well as the main molecules/atoms of the liquid (defined in the fundamental liquid) with better defined or changing 'number_min/_max' *Notes:* – for isotopic substitution of one or more molecules/atoms, or for liquids with specific abundance (i.e. non-terrestrial), all or at least the main isotopic species present will be listed with same nominal values of "*liquid*_specie_mole_fraction" but with their isotopic fractional abundance given in "*liquid*_specie_isotope_mole_fraction" Flag 'full_definition': {yes, no} or {true, false} *Condition:* flag absolute mandatory when "*liquid*_specie_uid" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of species defined in the 'fundamental liquid phase'. Need to fully redefine it. - '*no*': only to add new species to the original definition of composition and modify some already defined (they should have both the same "*liquid*_specie_uid" and "*liquid*_specie_relevance" than the original specie to be modified). *Note:* the flag 'full_definition' allows to control the mode of definition of the atomic and molecular composition of the actual liquid.
*liquid*_specie_family [-xml] [*phase*_specie_family]	enum(text)	U [!!_c] [V: !_c]	Liquid L4	VL	--	Family of the species composing the liquid Enum: {element, molecule, chemical function} *Note:* equivalent to "*constituent*_specie_family" *Note xml:* determined automatically from the type of the species ***Variable: liquid in Sample and Matters***

						Notes:
*liquid*_specie_uid [*] [*phase*_specie_uid]	CS-varchar(255)	S0/S0c/ S1 [!!_m] [V: !_m]	Liquid Molec Atom L4	VL	--	Link to the existing UID of the molecular or atomic specie(s) (natural or isotopic species) composing the liquid *Notes:* - put all species as atoms for mixed molecular/atomic solids - the links are only to natural molecules/atoms with natural terrestrial isotopic composition (the only possibility for 'fundamental liquids'), i.e., "*liquid*_specie_uid" refers to a species with "*molecule/atom*_isotope_mixture_type" = 'terrestrial abundance' *Note xml:* the same species (same "*liquid*_specie_uid") can occurs several times only if its relevance ("*liquid*_specie_relevance") is different. They are considered as different species. ***Variable: liquid in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used *Notes:* - includes the substituted (isotopic) and impurities molecules/atoms - For liquids as 'pure isotope', and in 'specific abundance' this "specie_uid" should refer only to pure isotopes. - For liquids with a specific isotopic composition, at least the main isotope species should be listed with "*liquid*_specie_uid". - only in specific cases it can refer to partly substituted molecular/atomic species. - for 'partly substituted' liquids "specie_uid" will refer to both 'terrestrial abundance' and 'pure isotope' molecular/atomic species
*liquid*_specie_mole_fraction [+] [*phase*_specie_mole_fraction]	float	U [!_m] [V:!o_ m]	Liquid L4	VL	*var*	Mole fraction of the molecular/atomic species in the liquid *Unit:* in *"liquid*_species_mole_fraction_unit" *Definitions:* – It is the nominal or average value for liquid solutions *Note:*

						– value between 0 and 1 – For a partly substituted liquid the mole fraction of each pure isotopic specie constituting the liquid is its partial abundance relative to the whole liquid, and not relative only to its own specie (where it should be '1'). Ex: N_2 = '0.3', $^{13}CH_4$ = '0.70' for a mixture with 30% N_2 + 70% CH_4 with $^{13}CH_4/^{12}CH_4$ = 1 ***Variable: liquid in Sample and Matters*** *Condition:* mandatory when "*liquid*_specie_uid" ≠ Ø Exact value for the specific liquid. *Note:* – for liquids with a specific isotopic composition (for isotopic substitution of one or more molecule/atom, or for liquids with specific abundance, i.e. non-terrestrial, …), it is the partial abundance of each isotope species in the liquid. – all, or at least the main isotopic species present should be listed. Ex: N_2 = '0.3', $^{12}CH_4$ = '0.35', $^{13}CH_4$ = '0.35' for a mixture with 30% N_2 + 70% CH_4 with $^{13}CH_4/^{12}CH_4$ = 1
*liquid*_specie_mole_fraction_error [*phase*_specie_mole_fraction_error]	float	U [!o_m] [V:!o_m]	Liquid L4	VL	*var*	Absolute uncertainty on mole fraction of the molecular/atomic species in the liquid *Unit:* in *"liquid*_species_mole_fraction_unit" *Condition:* mandatory and only when "*liquid*_specie_mole_fraction" ≠ {Ø, NULL} *Notes:* ***Variable: liquid in Sample and Matters*** *Condition:* mandatory when the bloc is used *Notes:*

*liquid*_specie_state [*phase*_specie_state]	enum(text)	S1/S1c/ S1 [!_m] [V: !o_m]	Liquid L4	VL	--	State of the molecular/atomic species inside the liquid OpenEnum: {constituent element, constituent cation, constituent anion, constituent molecular, pure, mixed, monomers, dimers, multimers, solute, solvent, liquid solution, hydration, hydrated, other, unknown, …} *Definitions:* => See "*constituent*_specie_state" *Note:* This state depends on "*liquid*_compound_type" which gives the type of liquid and tells how the molecular/atomic species are organized at the molecular/atomic level ***Variable: liquid in Sample and Matters*** *Condition:* mandatory when "*liquid*_specie_uid" ≠ Ø *Notes*:
*liquid*_specie_relevance [*phase*_specie_relevance]	enum(text)	S1/S1c/ S1 [!!_m] [V: !!o_m]	Liquid L4	VL	--	Relevance of thr molecule or ions species in the liquid Enum: {main, (substituted, impurity)} *Definitions:* • *'main'*: molecules of the liquid • *'substituted'*: used only for isotopic molecular/atomic species substituting the equivalent "natural molecule/atom" • '*impurity'*: molecules or ions not contributing to the fundamental liquid *Note:* for all molecular species their relevance are all 'main' as the possible 'impurities' are not included in the generic formula of the fundamental liquid. ***Variable: liquid in Sample and Matters*** Enum: {main, substituted, impurity} *Condition:* absolute mandatory when "*liquid*_specie_uid" ≠ Ø *Note*: all molecules not in the fundamental liquid will be 'impurity'

*liquid*_composition_comments	blob	U [m] [V: m]	Liquid	VL	--	Any additional information or comments on the composition of the liquid ***Variable: liquid in Sample and Matters*** Flag 'replace': {yes, no} *Definitions*: see "*mineral*_comments" *Note:* the flag 'replace' allows to control if the comment replace the original one ('yes') or is added to the original one ('no').
Liquid phase						
*liquid*_phase_type [*phase*_phase_type]	enum(text)	S1/S1c/Liquid F S1 [!!_m] [V: £_m]	Liquid	VL	-- --	Type of phase of the solid Enum: {liquid, supercooled liquid, supercritical fluid, unknown} *Definitions:* cf. "*constituent*_phase_type" *Notes:* ***Variable: solid in Sample and Matters*** *Condition:* compulsory for supercooled liquid of equivalent liquid. *Notes:*
Liquid properties						
*liquid*_ph	varchar(255)	S3 [m] [V: m]	Liquid	VL	*no*	pH (value or range) of liquid solution *Constraint:* only for liquid aqueous solutions *Notes:* - mostly for aqueous solution (solvent = H_2O) - provide T° conditions in parenthesis *ex:* '2.5 – 7', '8.5 (350K)' ***Variable: liquid in Sample and Matters*** Exact value for specific solution

*liquid*_molar_mass [phase_molar_mass]	varchar(255)	S3 [m] [V: m]	Liquid	VL	g/mol	Molar mass (value or range) of the liquid • Provided in 'g/mol' unit *Notes:* - for liquid solution it is determined per mole of solvent - for liquid solution series the range go from the minimum value for pure solvent to the maximum value determined with solute at full solubility (or the reverse if solute is lighter than solvent) *ex:* '160.3', '160.2 - 162.5' ***Variable: liquid in Sample and Matters*** Exact value for specific liquid or liquid solution.
*liquid*_density [phase_density]	varchar(255)	S3 [m] [V: m]	Liquid	VL	*g/cm3*	Density (value or range) of the liquid • provided in 'g/cm^3' unit *Notes:* - provide T & P conditions in parenthesis - for liquid solution depend on mole fraction of solute(s) and solvent - range of density for solution series *ex:* '1.236 (300K, 1 bar)', '1.23 - 1.34' ***Variable: liquid in Sample and Matters*** Exact value for specific liquid solution. Minor changes with impurities molecules or elements.

Liquid thermodynamic properties

*liquid*_state_ntp [*phase*_state_ntp]	enum(text)	S1/S1c [!_m]	Liquid	F	--	State of the liquid phase in NTP conditions Enum: {solid, metastable liquid - solid, liquid, gas} *Definitions:* - *'solid':* this liquid phase cannot exist at NTP conditions but its constituting species are stable in solid phase at NTP conditions - *'metastable liquid - solid':* this liquid phase can exist at NTP

						conditions under some conditions but it is outside its thermodynamic stability zone. A solid phase is stable at NTP conditions. - *'liquid':* this liquid phase is stable at NTP conditions - *'gas':* neither this liquid phase nor any solid phases can exist at NTP conditions. The gas is the only stable phase at NTP conditions. *Note:* NTP conditions (NIST): 293.15K (20°C), 101.325kPa (1 atm) *Ex*: - 'solid' for liquid sulphur - 'liquid' for liquid H_2O as its melting point is 273.15 K - 'gas' for liquid N_2
*liquid*_phase_transitions	***List [L5]***	[O]				£: Description of the main phase transitions of the liquid
*liquid*_phase_transition_type [*phase*_phase_transition_type]	enum(text)	U [m]	Liquid L5	F	--	Type of phase transition of the liquid Enum: {solid-liquid, liquid-gas, triple point solid-solid-liquid, triple point solid-liquid-gas, quadruple point, liquid decomposition} *Notes:* - only the most important transition points need to be given (i.e. triple points, solid-liquid at ambient pressure …) - the solid-liquid phase diagram can be given in "*liquid*_figures"
*liquid*_phase_transition_other_phases [*phase*_phase_transition_phases]	varchar(255)	U [m]	Liquid L5	F	-	Name(s) of the other phase(s) implied in the phase transition of the liquid *Notes:* - it can be one solid (solid-liquid) or two solids (triple point solid-solid-liquid), or more (quadruple point) - the full name and type of phase should be given *Ex:* 'Water ice Ih' for liquid Water, 'water ice Ih, liquid, gas' for triple point of water
*liquid*_phase_transition_temperature [*phase*_phase_transition_temperat	varchar(255)	U [m]	Liquid L5	F	K Pa,	Temperature (value(s) or range) of the phase transition of the liquid at defined pressure, or average value when variable • temperature should be provided in 'K' unit, with the unit written after

ure]					bar	the numbers • pressure should be provided in parenthesis after the temperature and in 'Pa' or 'bar' unit (or their (sub-)multiples), with the unit written after the numbers *Notes:* – range of temperature for variable liquid. – No requested value for liquid solutions and hydrated liquids. *Ex:* '35.4 K (100 mbar)', '273.2 - 273.5 K (100 MPa)', '272.3 K (1 bar) – 275.2 K (100 bar)'
*liquid*_phase_transitions_comments [*phase*_phase_transitions_comments]	blob		U [m]	Liquid	F	--	Additional information on liquid phase transitions (unknown limits of transition, …)
Liquid optical properties							
*liquid*_refraction_index_n	varchar(255)		S3 [m] [V: m]	Liquid	VL	*no*	Refraction index, n, (value or range) of the liquid (at 589.3 nm) *Definition:* Standard refractive index measurements are taken at yellow doublet sodium D line, with a wavelength of 589.29 nm. *Note:* range of refraction index for solution series *ex:* '1.532', '1.456 - 1.583' ***Variable: liquid in Sample and Matters*** Exact value for specific solution. Minor changes with impurities elements.
*liquid*_dispersion_v	varchar(255)		U [m] [V: m]	Liquid	VL	*no*	Abbe number V (value or range) expressing the visible dispersion of a transparent liquid *Definition:* dispersion is defined as $V = (n_d-1)/(n_F-n_C)$ using the Fraunhofer lines d, F and C at 587.6 nm (d), 486.1 (F) and 656.3 nm (C). cf wiki: en.wikipedia.org/wiki/Abbe_number

						Note: range of Abbe number for liquid solution series *Ex:* ’32, ‘40-65' ***Variable: liquid in Sample and Matters*** Exact value for specific solid solution. Possible significant changes with impurities elements
*liquid*_pure_color [*phase*_pure_color]	enum(text)	S2 [m]	Liquid	F	--	Color of the pure liquid (without any impurity) FreeList: {colorless, white, blue, bluish, azure, green, greenish, emerald, olive, turquoise, yellow, yellowish, orange, pink, pinkish, red, reddish, lilac, violet, indigo, purple, brown, brownish, beige, gray, grayish, black, blackish, bronze, lead, silver, steel, copper, tin, various, …}
*liquid*_diaphaneity [*phase*_diaphaneity]	enum(text)	S2 [m] [V: m]	Liquid	VL	--	Capacity of the liquid to transmit light Enum: {transparent, transparent to translucent, translucent, translucent to opaque, opaque, various, unknown} ***Variable: liquid in Sample and Matters*** actual diaphaneity of the liquid

Liquid references and comments

liquid_publications	***List [L6a]***	[O]				£: Publications on the fundamental liquid phase and its properties.
*liquid*_publication_uid [*] [*phase*_publication_uid]	varchar(255)	U [m]	Liquid Publi L6a	F	--	Link to the existing UID of the publications on the liquid *Note:* these papers should be in the bibliography database, with “*publication*_content” = ‘phase’
liquid_links *[phase_links]*	***List [L6b]***	[O]				£: Web pages describing the liquid and its properties.
*liquid*_link_name [*phase*_link_name]	varchar(255)	U	Liquid	F	--	Name of the web page(s) describing the liquid and its properties.

		[m]	L6b			*Ex:* ‘Wikipedia’, …
*liquid*_link_url [*phase*_link_url]	CS-varchar(255)	U [m]	Liquid L6b	F	--	URL address(es) of web page(s) *Notes*: - you can link to a publication by giving its url address, preferably through its DOI. Ex: https://doi.org/10.1002/ejic.200700067
*liquid*_comments [phase_comments]	blob	U [m]	Liquid	VL Aj	--	Additional information on the liquid *Ex:* impurities, … ***Variable: liquid in Sample and Matters*** Flag ‘replace’: {yes, no} *Definitions*: see “*mineral*_comments” *Note:* the flag ‘replace’ allows to control if the comment replace the original one (‘yes’) or is added to the original one (‘no’).

6.3 Mineral phase Table

Root of the table: ***mineral***

Data type: 'Fundamental phase'

In "Exp" column 'VM' means a variable key-word of the fundamental mineral: when defining a "sample" or a "matter" containing fundamental mineral phases (described in "basic constituents") the VM values in "mineral phase" can be modified (but will not be changed in the fundamental mineral database) to reflect the exact mineral properties (for exemple for solid solutions and n-hydrated minerals). See specific notes in *Variable: mineral in Sample and Matters*

To found info on minerals: http://www.webmineral.com, https://www.mindat.org, https://www.mineralienatlas.de/, https://en.wikipedia.org/wiki/List_of_minerals, ...

Key-word	Type	Level	Table	Exp	Unit	Description
Mineral phase import						
*mineral*_import_mode [phase_import_mode]	enum(text)	P [!!_m]	Miner	(V)	--	Mode of import of the mineral data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*mineral*_xml_filename [-xml] [phase_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	Miner	(V)	--	Name of the storage copy of the xml import file of the mineral metadata ➔ determined automatically during import (from "*mineral*_uid" ?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Mineral phase indexes and type						
*mineral*_index [**][-xml] [phase_index]	int(10)	B [!!_g]	Miner	F	--	Automatic random but unique number (ID) given to new mineral
*mineral*_uid [**] [phase_uid]	varchar(255)	S0 [!!_m]	Miner	F	--	Unique identifier code (UID) given to the mineral table (to be created) *Nomenclature:* Create this code name with 'MINERGROUP_'

						(*mineral*_classification_level = {mineral group, mineral subgroup}), 'MINERSERIES_' (= {solid solution series}) or 'MINER_' (= {variable mineral, unique mineral}). It should be of the style 'MINERGROUP_GroupName', 'MINERSERIES_SeriesName' or 'MINERSERIES_EndmemberName1_EndmemberName2' or 'MINER_MineralName' where 'Group/SeriesName' are the Dana group/series names, and 'EndmemberName'n'' and 'MineralName' are the "*mineral*_ima_name". *Note*: use only lowercase for the mineral name *Note*: The fundamental mineral phase stored in the database will be, by default, with natural terrestrial abundance. Ex: MINER_calcite, MINERSERIES_fayalite_forsterite, MINERGROUP_smectites
Mineral names						
*mineral*_ima_name [*phase*_official_name]	varchar(255)	S0/S0c/ S1 [!!_m]	Miner	F	--	IMA unique name of the mineral (or series) *Notes:* ⇨ Start with capital letter *Ex:* 'Brucite' ⇨ for solid solutions series the name should be built as: 'nom_IMA1'-'nom_IMA2' series *Ex:* 'Diopside-Hedenbergite series' ⇨ It is used as the title of the mineral page on the SSHADE interface ⇨ IMA names are defined by CNMNC of IMA (http://nrmima.nrm.se)
*mineral*_secondary_name [*phase*_secondary_name]	varchar(255)	S0/S0c/ S1 [m]	Miner	F	--	Alternative name(s) used for the mineral *Notes:* – start with a capital letter – if several, separate each name by a semicolon

*mineral*_cas_number [*phase*_cas_number]	varchar(255)	S1/S1c/S2 [m]	Miner	F	--	CAS registry number, unique, of the mineral (natural or synthetic) *Note:* the problem is to found them !!! no registry, not systematic! => some (mostly with equivalent synthetic) in Wikipedia http://www.chemindustry.com/chemicals/

Mineral type and (end)members

*mineral*_family [-xml] [*constituent/phase*_family]	enum(text)	U/S0c/S1 [!!d_m]	Solid	F	--	Phase family (or major class) of 'mineral' Enum: {mineral} *Default* = 'mineral' - '*mineral*': single naturally occurring mineral phase (include natural salts, and native elements) *Notes:* fixed value, equivalent to "*constituent*_family"
*mineral*_class [*phase*_class]	enum(text)	S1/S1c/S1 [!!_m]	Miner	F	--	Class of mineral phase. Enum: {native element, silicate mineral, non-silicate mineral, organic mineral} *Note*: - same classes for "*constituent*_class" - corresponds to some grouping of old Dana major classes (*mineral*_dana_major_class) and Dana classes (*mineral*_dana_class): o 'native element': major class I, class 01 o 'silicate mineral': major class II to VII, class 02 to 49 o 'non-silicate mineral': major class VII, class 51 to 78 o 'organic mineral': major class IX, class 50
*mineral*_compound_type [*phase*_compound_type]	enum(text)	S0/S0c/S0 [!_m]	Miner	F	--	Type of mineral compound Enum: {metal, metallic alloy, elemental mineral, carbon allotrope, oxide, hydroxyde, oxide-hydroxide, antimonate, antimonite, arsenate, arsenite, borate, carbide, carbonate, chromate, fluoride, halide, iodate, molybdate, nitrate, nitride, phosphate, phosphide, phosphite, silicide, selenate, selenide, selenite, sulfate, sulfide, sulfite, sulfosalt, tellurate, tellurite, tungstate,

						vanadate, vanadium oxysalt, silicate, cyclosilicate, inosilicate, nesosilicate, phyllosilicate, sorosilicate, tektosilicate, organic salt, hydrocarbon, organic mineral} *Definitions:* - ‘metal’: - ‘metallic alloy’: - ‘elemental mineral’: - carbon allotrope - oxide, hydroxyde - ‘oxide-hydroxide’: - ‘antimonate, antimonite, arsenate, arsenite, borate, carbide, carbonate, chromate, fluoride, halide, iodate, molybdate, nitrate, nitride, phosphate, phosphide, phosphite, silicide, selenate, selenide, selenite, sulfate, sulfide, sulfite, sulfosalt, tellurate, tellurite, tungstate, vanadate, vanadium oxysalt’ => cf. “*solid*_compound_type” - ‘silicate’: - ‘nesosilicate’: - ‘sorosilicate’: - ‘cyclosilicate’: - ‘inosilicate’: - ‘phyllosilicate’: - ‘tektosilicate’: - ‘organic salt’: - ‘hydrocarbon’: - ‘organic mineral’: *Notes:* - same compound types for “*constituent*_compound_type”. It will be used for main search. - corresponds to some inter- and intra-grouping of Dana classes (*mineral*_dana_class)
*mineral*_classification_level [*phase*_classification_level]	enum(text)	S1/S2c/ S2	Miner	F	--	Level of mineral classification Enum: {mineral group, mineral subgroup, mineral polymorphs, solid solution

[!!_m]

---

series, variable mineral, unique mineral}

Definitions:

- *'mineral group'*: General group of mineral, with at least 2 variable elements
  Ex: Spinel group AE2O4 (A=Fe, Zn, Mg, Mn, Ni, Ti, +Al) (E=Al, Fe, Cr)
- *'mineral subgroup'*: subgroup of a mineral group, with one element of the group fixed, and at least 1 other variable element
  Ex: Iron spinel subgroup AFe2O4 (A=Fe, Mg, Ni, +Mn, +Zn)
- '*mineral polymorphs'*: minerals with exactly same composition but different crystalline structures
  Ex: Calcite & Aragonite ($CaCO_3$)
- *'solid solution series':* series between 2 endmembers of a group, or subgroup, with one variable between 2 elements
  Note: for solid solutions of cations (Fe, Mg, …) or anions (OH, F, Cl, O…)
  Note: glasses will be always classified as 'solid solution series'
  Ex: Magnesioferrite-Magnetite series (Iron Spinel subgroup): (Mg,Fe)2+(Fe3+)2O4
- *'variable mineral'*: mineral with still at least one variable element.
  Note: Can be an endmember. It did not includes minerals only with variable hydration.
  Ex: Cuprospinel (Cu,Mg)Fe+++2O4, Galaxite (Mn,Mg)(Al,Fe3+)2O4
  Ex: Montmorillonite (Na,Ca)0,3(Al,Mg)2Si4O10(OH)2•n(H2O)
  Nontronite Na0.3(Fe3+)2(Si,Al)4O10(OH)2•n(H2O)
- *'unique mineral'*: mineral with a fully defined formula.
  Note: Can be with variable hydration.Can be an endmember.
  Ex: Magnesioferrite Mg2+(Fe3+)2O4, spinel MgAl2O4

---

mineral_endmembers
[phase_endmembers]

List [L1]

[!o]

£: List of the endmember minerals of the series

Condition: Mandatory when "*mineral*_classification_level" = {mineral group, mineral subgroup, solid solution series}

*mineral*_endmember_mineral_uid [*] [phase_endmember_phase_uid]	varchar(255)	U [!o_m]	Miner Miner L1	F	--	Link to the existing UID of the endmember minerals of the series *Ex:* Olivine $(Mg,Fe^{2+})SiO_4$ - Forsterite Mg_2SiO_4 - Fayalite $Fe_2^{2+}SiO_4$
mineral_members	***List [L1b]***	[O]				£: List of the intermediate members of the mineral series
*mineral*_member_name [phase_member_name]	varchar(255)	S0 [o_m]	Miner L1b	F	--	Name(s) of the intermediate member(s) of the mineral series *Condition:* not if "*mineral*_classification_level" = {unique mineral} *Ex:* Fayalite-Forsterite series $(Mg,Fe^{2+})SiO_4$: Forsterite; Chrysotile (Olivine); Hyalosiderite; Hortonolite; Ferrohortonolite; Fayalite.
*mineral*_member_composition [phase_member_composition]	varchar(255)	U [o_m]	Miner L1b	F	mole%	Composition range(s) of the intermediate member(s) of the mineral series *Unit:* mole% *Note:* not if "*mineral*_classification_level" = {unique mineral} *Ex:* Fayalite-Forsterite series $(Mg,Fe^{2+})SiO_4$: - Forsterite: Fe=100-90% (Mg=0-10%) - Chrysolite (Olivine): Fe=90-70% - Hyalosiderite: Fe=70-50% - Hortonolite: Fe=50-30%; - Ferrohortonolite: Fe=30-10% - Fayalite: Fe=10-0%
mineral_polymorphs [*phase_polymorphs*]	***List [L2a]***	[!o]				£: List of the mineral polymorphs *Condition:* Mandatory when "*mineral*_classification_level" = {mineral polymorphs} *Note:* For monoatomic minerals the polymorphs are called 'allotropes'
*mineral*_polymorph_mineral_uid [*] [*phase*_polymorph_phase_uid]	varchar(255)	U [!o_m]	Miner Miner	F	--	Link to the existing UID of mineral polymorph *Ex:* MINER_calcite & MINER_aragonite

			L2a			
*mineral*_polymorph_comments [*phase*_polymorph_comments]	varchar(255)	U [m]	Miner L2a	F	--	Additional information on the mineral polymorph *Note:* to provide some information on the P-T stability domain of the polymorph
mineral_polytypes [*phase_polytypes*]	***List [L2b]***	[O]				£: List of the polytypes of the mineral *Constraint:* only when "*mineral*_classification_level" = {mineral polymorphs, solid solution series, variable mineral, unique mineral} ***Variable: mineral in Sample and Matters*** *Note*: keep only the actual polytype, if it is known. *Note xml*: when filled, it will replace the full list of polytypes (equivalent to a "*mineral_polytypes*_full_definition" = 'yes')
*mineral*_polytype_name [*phase*_polytype_name]	varchar(255)	S0/S0c/ S1 [m]	Miner L2b	VM	--	Name of the polytype of the mineral *Notes:* - provide a list of the polytypes using their names or names and symbols whatever they are (still) considered as separate IMA minerals or not. - If they are considered as separate IMA minerals they need to be also listed in "*mineral*_polymorph_mineral_uid" with a note in "*mineral*_polymorph_comments" - Tell which polytype is used to give the 'optical properties' (if *Ex:* 'Heterogenite-2H', 'Heterogenite-3R' *Ex:* 'Chrysotile', 'Parachrysotile', 'Clinochrysotile', 'Orthochrysotile' ***Variable: mineral in Sample and Matters*** *Note*: put the name of the actual polytype (taken amoung the list of polytypes, if present)
*mineral*_polytype_comments	varchar(255)	U	Miner	VM	--	Additional information on the mineral polytype

[*phase*_polytype_comments]		[m]	L2b			*Note:* ***Variable: mineral in Sample and Matters*** *Note*: copy the 'comment' given in "*mineral*_polytype_comments" for the actual polytype, if still relevant. Possibly add another comment.
*mineral*_figures *[phase_figures]*	***List [L2c]***					£: List of the figures on the mineral
*mineral*_figure_filename [*phase*_figure_filename]	varchar(255)	P/U [m]	Miner L2c	F	--	File name(s) (with extension) of the figure on the mineral *Image formats:* .png, .jpg, (.gif) *Notes:* - mostly for polymorphs and series - can be a phase diagram of the polymorphs, or the (end)members diagram of a solid solution series … *Note DB:* this file will be imported in the database
*mineral*_figure_caption [*phase*_figure_caption]	varchar(255)	U [m]	Miner L2c	F	--	Caption(s) or comment(s) on the figure(s) on the mineral

Mineral chemical composition

*mineral*_formula [*phase*_formula]	varchar(255)	U [!!_m] [V: m]	Miner	VM	--	Developed empirical chemical and structural formula of the mineral *Syntax:* Latex format *Ex:* $(Fe^{2+}_{1.5},Mg_{0.5}).Si_2O_6$ 'for '$(Fe^{2+}_{1.5},Mg_{0.5}).Si_2O_6$' Clinoferrosilite $((Fe^{2+}_{1.5},Mg_{0.5}).(SiO_3)_2)$ $(Mg_xFe^{2+}_{1-x}).SiO_4$ for Olivine $(Mg_xFe^{2+}_{1-x}).SiO_4$ *Note:* – Contain ionic information for multiple valences ions *Notations:* – Small point (.) can separate structural units – Dot • (\bullet) separates hydration

						– LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf ***Variable: mineral in Sample and Matters*** *Notes*: – Includes replacement and impurities elements, as well as values of x,y,z fractions and n-hydration number – Can contain isotopic information when an atom is substituted Ex: $^{29}SiO_2$
*mineral*_hydration [*phase*_hydration]	boolean	S2/S2c/ S2 [!!_m]	Miner	F	--	Flag to telling if the mineral contains structural and/or interlayer H_2O BoolEnum: {yes, no} or {true, false}
*mineral*_hydration_series [*phase*_hydration_series]	boolean	U [!!o_m]	Miner	F	--	Flag to telling if the mineral is an isostructural series of n-hydrated minerals ('true') BoolEnum: {yes, no} or {true, false} *Condition*: absolute mandatory when "*mineral*_hydration" = {true} *Notes:* n-hydrated minerals have variable amount of H_2O molecules, either structural (limited range of n: min-max, or incremental) or interlayer (variable 'n' from 0 to some maximum value. *Ex*: phylosilicates…)
*mineral*_hydration_number [*phase*_hydration_number]	varchar(255)	S3/S3c/ S3 [!o_m] [V: m]	Miner	VM	--	Number or range of numbers of H_2O (structural and/or interlayer) in the mineral *Condition*: Mandatory when "*mineral*_hydration" = 'true' *Note:* for hydration series put the current value (if well defined and known), or a range (if not well defined or known) either fixed and continuous ('1 - 6'), or incremental ('2, 3, 4, 6, 12') for some groups, or with one limit unknown ('2 - ?', '? – 6'), or open with no upper limit in 'n' ('2 - n'), or 'n' if fully unknown or undefined. *Ex:* '2', '4 - 6', '0 - 20', '0 - n' (if no real limit to 'n'), '2, 3, 4, 6, 12' ***Variable: mineral in Sample and Matters*** *Note:* It will take into account the level of (de)hydration of the matter. Put the

						value, but if not well known then put some range. *Note:* To change the hydration number when a matter is processed to make a sample or when a sample is processed before experiment (heated, …), or during experiment (adsorption, …), with the interlayer H_2O varying: make a sample (or a new sample) with a composition similar to the matter (or to the previous sample) but with 'n' changed in the mineral (VM) and make a link to the "mineral_matter" (or parent sample) in 'processes'.
*mineral*_chemical_formula [*phase*_chemical_formula]	CS-varchar(255)	S0/S0c/S1 [!!_m] [V: m]	Miner	VM	--	Developed global chemical and structural formula of the mineral *Ex:* '(Fe2+,Mg)2Si2O6' for Clinoferrosilite 'Ca2(Fe2+)3Al2(Si6Al2)O22(OH)2' 'Ca6(AsO4)(AsO3OH)3(PO4)0.7(SO4)3.15(H2O)' for Machatschkiite '([ ],Fe,Mg)(Mg,Al,Fe)5Al4Si2(Si,Al)2(B,Si,Al)(O,OH,F)22' *Note:* - contain ionic information. - individual radicals are in ( ), such as OH, CO3, SO4, PO4, SiO4, … - Mineral series are indicated by comma separating the elements that varies in amount.The more dominant element is usually listed first. - Anytime there is more than one valence for an atom in a mineral, the valence is written after the element symbol and put in ( ) - big point '•' (ascii=149) separates hydration in ( ) - 'n' give a variable value for structural hydration. *Ex:* Min•n(H2O) - a range of hydration number 'n' can be given with 'n1-n2': *Ex:* Min•8-12(H2O) - Square brackets with a 'blanc' [ ] are used in the formula to signify a vacancy (hole). - For minerals with isotopic atomic substitution (non-natural isotopic abundance), substituted atoms will have their atomic mass between square brackets preceding the atom symbol. D can be used for ^2H. *Ex:* '(Fe2+,Mg)2.Si2[18]O6' *Note:* Definition of this type of formula: cf http://webmineral.com/help/ChemicalFormula.shtml ***Variable: mineral in Sample and Matters***

Developed global chemical and structural formula of the actual mineral

Mineral chemical functions and bonds

mineral_chemical_functions	***List [L3a]***	[!]				£: List of different chemical functions present in the mineral, except those already in the molecular species and anionic radicals described as 'species' of the mineral. *Note*: - These chemical functions are mostly the anionic radicals. They should be listed except if they are already described as ‘species’ rather than atoms (in that case their chemical functions are already included in the specie)
*mineral*_chemical_function_uid [*] [*phase*_chemical_function_uid]	varchar(255)	S2/S2c [!_m]	Miner ChemF L3a	F	--	Link to the existing UID of the chemical function present in the mineral *Exhaustive list:* - mineral anionic radicals: OH^-, AsO_4^{3-}, BO_3^{3-}, BO_4^{4-}, CO_3^{2-}, CrO_4^{2-}, MoO_4^{2-}, NO_3^-, PO_4^{3-}, SO_4^{2-}, SiO_4^{4-}, VO_4^{3-}, WO_4^{2-}, UO_2^{4-} *Note:* These UID are all of the form ‘MINION_AOn_x-’ (n=3, 4; x=1, 2, 3, 4)
*mineral*_chemical_function_number [+] [*phase*_chemical_function_number]	varchar(255)	S3/S3c [m]	Miner L3a	F	--	Number, or minimum number, of this chemical function present in the mineral. ➔ Calculation of ’n_min(function_i)’ for display: ⇨ *See “solid*_chemical_function_number”
mineral_chemical_bonds	***List [L3b]***	[!]				£: List of the chemical bond(s) of the mineral except those already in the molecular species and anionic radicals described as 'species' of the mineral *Note*: – These chemical bonds are only the molecular bonds between atoms, in SiOx groups, in anionic radicals, and in H2O (or other interlayer molecules) except if these anionic radicals are already listed as ‘species’ rather than atoms (in that case their chemical bonds are

						already included in the specie)
*mineral*_chemical_bond_uid [*] [*phase*_chemical_bond_uid]	varchar(255)	S2/S2c [!_m]	Miner ChemB L3b	F	--	Link to the existing UID of the chemical bonds of the mineral *Note*: – The chemical bonds used for minerals are only 'generic mixture' with terrestrial abundance *Ex:* for $(Mg,Fe)SiO_4$: 4 x 'BOND_SiO' – For isotopic substituted mineral made of at least one purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope of the others
*mineral*_chemical_bond_number [+] [*phase*_chemical_bond_number]	varchar(255)	S3/S3c [!_m]	Miner L3b	F	--	Number, or minimum number, of bonds of each type composing the mineral ➔ Calculation of 'n_min(bond_i)' for display: ⇨ *See "solid*_chemical_bond_number" *Note*: determined relative to a formula unit *Ex:* '4' S-O' for $MgSO_4$

Mineral atomic and molecular composition

*mineral*_elemental_formula [-xml] [*phase*_elemental_formula]	CS-varchar(255)	S0/S0c/S1 [!_c] [V: c]	Miner	VM	--	Empirical elemental formula of the mineral ➔ Calculated: see "*constituent*_elemental_formula" *Notations:* see "*constituent*_elemental_formula" *Ex:* 'Fe1.5 Mg0.5 Si2 O6' for Clinoferrosilite 'Ca2 (Fe2+)3 Al4 Si6 O24 H2' for Ca2(Fe2+)3Al2(Si6Al2)O22(OH)2 Notes: – most mineral are natural, so there is generaly no isotopic information ***Variable: mineral in Sample and Matters*** ➔ Calculated for each 'atom_i' excepted those with "*mineral*_specie_relevance" = {impurity} when one or more "*mineral*_specie_uid" is added or changed

						⇨ see "*constituent*_elemental_formula" This formula includes substitution molecules or elements plus replacement elements in the actual mineral. *Ex:* 'Fe1.3 Mg0.7 Si2 O6' for Clinoferrosilite
*mineral*_isotope_mixture_type [*phase*_isotope_mixture_type]	enum(text)	S1/S1c/ S1 [!!d_m] [V: £o_m]	Miner	VM	--	Type of isotopic mixture of the mineral Enum: {(pure isotope, partly substituted), terrestrial abundance, (specific abundance)} *Default* = 'terrestrial abundance' *Definitions: cf* "*constituent*_isotope_mixture_type" *Notes:* – The fundamental mineral stored in the database will be, by default, always with natural terrestrial abundance. The other options are only for 'variable' (see below) ***Variable: mineral in Sample and Matters*** Enum: {pure isotope, partly substituted, terrestrial abundance, specific abundance, unknown} *Condition:* Compulsory when "*mineral*_isotope_mixture_type" ≠ 'terrestrial abundance' *Note:* isotopic mixtures in mineral with some atoms not in natural isotopic abundance will be set to 'specific abundance' or to 'partly substituted' (one or more atom as a pure isotopic species). Their abundance will be defined in "*mineral*_specie_isotope_mole_fraction" using the pure isotopologue atoms *Note*: define the effectif type of isotopic mixture
mineral_species	***List [L4]***	[!!o] [V: £_m] [VFlag: !!o_m]		VM		£: Description of the atomic composition of the mineral *Condition:* absolute mandatory when "*mineral*_classification_level" = {mineral subgroup, solid solution series, variable mineral, unique mineral} *Notes*: – Structural H2O hydration will be described by "molecular species". It

will thus provide direct link to their bonds.
- there is also a few 'minerals' that may be described by "molecular species", such as 'CH_4 clathrate hydrate', 'H_2O ice', …
(note: they will be also described in "solids")
- anionic radical will be described directly instead by their atoms, as it will provide direct link to their bonds.

Variable: mineral in Sample and Matters

Condition: compulsory to list the replacement, impurity, or substituted atoms or molecules as well as the main atoms/molecules of the mineral with changing 'number_min/_max'

Notes:
- for isotopic substitution of one or more atom, or for minerals with specific abundance (i.e. non-terrestrial, e.g. for meteorites, …) all, or at least the main isotopic species present will be listed with same nominal value of "*mineral*_specie_number(_min)" but with their isotopic fractional abundance given in "*mineral*_specie_isotope_mole_fraction"

Flag 'full_definition': {yes, no} or {true, false}

Condition: flag absolute mandatory when "*mineral*_specie_uid" ≠ Ø

Definitions:
- '*yes*': fully replace the original list of species defined in the 'fundamental mineral phase'. Need to fully redefine it.
- '*no*': only to add new species to the original definition of composition and modify some already defined (they should have both the same "*mineral*_specie_uid" and "*mineral*_specie_relevance" than the original specie to be modified).

Note: the flag 'full_definition' allows to control the mode of definition of the atomic and molecular composition of the actual mineral.

*mineral*_specie_family [*phase*_specie_family] [-xml]	enum(text)	U [!!_c] [V:	Miner L4	VS	--	Family of the species composing the mineral Enum: {element, molecule, chemical function} *Notes:*

		!o_c]				- equivalent to "*constituent*_specie_family" - 'molecule' will be mostly used for H2O of hydration, but in also in a few special cases CH4, CO2, - "chemical functions"='anionic radical' will be described directly instead by their atoms - this will allow to directly heritate the molecule 'bonds' *Note xml:* determined automatically from the type of the species ***Variable: mineral in Sample and Matters*** *Condition:* mandatory when "*mineral*_specie_uid" ≠ Ø *Notes*:
*mineral*_specie_uid [*] [*phase*_species_uid]	varchar(255)	S0/S0c/ S1 [!!_m] [V: ££o_m]	Miner Atom L4	VM	--	Link to the existing UID of the atomic/molecular/function species composing the mineral. *Notes:* - if a cation can exist in more than one valence, then it is necessary to define the different ions with different valences *Ex:* 'Fe^{2+}', 'Fe^{3+}', 'Mn^{2+}', 'Mn^{3+}', 'Mn^{4+}', 'V^{2+}', 'V^{3+}', 'V^{4+}', 'V^{5+}', 'Cr^{2+}', … and thus call them with 'ATION_xxx' instead of 'ATOM_xx' *Ex*: 'ATOM_Mg', 'ATION_Fe3+', … - anionic radicals (MINION_) must be used instead of their atoms - the link for mineral is only to natural atomic/molecular species (natural mixtures of the isotopologues with terrestrial abundance). ***Variable: mineral in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used *Notes*: - includes the replacement, substituted and impurities elements - this "atom_uid" refers to particular isotopes only for isotopicaly substituted minerals. *Note xml:* the same atomic/molecular species (same "*mineral*_specie_uid") can occurs several times only if its relevance ("*mineral*_specie_relevance") is

						different. They are considered as different atoms. It will allow to have one atom present as ‘main’ constituent but also present as ‘impurity’ or ‘replacement’ element at another place of the mineral.
*mineral*_specie_number_min [*phase*_specie_number_min]	float or ‘n’	S0b/S0cb [!_m] [V:!o_m]	Miner L4	VM	*no*	Nominal or Minimum total number of this atomic/molecular species composing the mineral *Definitions:* - It is the nominal value when “*mineral*_classification_level” = {unique mineral} - It is the nominal or minimum value when “*mineral*_classification_level” ≠ {unique mineral} *Notes:* For ‘unique mineral’ - Interlayer (variable) n-hydration is not taken into account in the H2O count. But it is necessary to count OH and fixed structural hydration. For all other minerals: - Minimum value only for atomic/molecular species with variable abundance (x,y,z) in the mineral, in solid solutions or in n-hydrated minerals (H2O). Also for mineral groups and subgroups. - For solid solution and variable mineral this minimum value is found by putting all variable composition atomic/molecular species to their minimum. - If there is specific information on a limitation in the minimum number of an atomic/molecular species in variable abundance, then put this number. - For n-hydrated minerals the minimum number for H2O is the minimum fixed structural hydration value, excluding interlayer (variable) n-hydration in the H2O count. ***Variable: mineral in Sample and Matters*** *Condition:* mandatory when “*mineral*_specie_uid” ≠ Ø *Notes:* For ‘unique mineral’: - total number of atomic/molecular species composing the mineral,

						including replacement, substituted and impurities elements, OH and fixed structural hydration including interlayer (variable) n-hydration in the H2O count. When an essential (main) atomic/molecular species of a variable mineral, or mineral (sub-)group is not present, its number has to be set to ‘0’. For all other minerals: - minimum number of atomic/molecular species composing the mineral, including replacement, substituted and impurities elements, OH and fixed structural hydration including interlayer (variable) n-hydration in the H2O count (TBD: à homogénéiser)
*mineral*_specie_number_max [*phase*_specie_number_min]	float or ‘n’	S0b/S0cb [!o_m] [V: m]	Miner L4	VM	*no*	Maximum total number of this atomic/molecular species with variable or undefined abundance *Condition:* Mandatory when “*mineral*_classification_level” ≠ {unique mineral} *Notes:* - do not fill for well defined unique mineral - only for atomic/molecular species with variable abundance (x,y,z) in the mineral, in solid solutions or in n-hydrated minerals (H2O). Also for mineral groups and subgroups. - For solid solution this maximum value is found by putting all variable composition atomic/molecular species to their maximum. - If there is specific information on a limitation in the maximum number of an atomic/molecular species in variable abundance, then put this number. - For n-hydrated minerals this maximum value for H2O is the maximum value of the fixed structural hydration, thus excluding interlayer (variable) n-hydration in the H2O counts. If undefined then put ‘n’ ***Variable: mineral in Sample and Matters*** *Note:* - maximum number of atomic/molecular species of each type composing the mineral, including replacement, substituted and impurities elements, OH and fixed structural hydration but excluding interlayer

						(variable) n-hydration in the H2O count. *Note xml:* - need to remove any value of '*mineral*_specie_number_max' if molecule number is fixed => put 'NULL'
*mineral*_specie_isotope_mole_fraction [in xml: only in 'variable'] [*phase_specie*_isotope_mole_fraction]	float	U [-] [V: !o_m]	Miner L4	VM	*no*	Mole fraction of the isotopic species in the isotopic mixture of this molecule/atom in the mineral (for non-terrestrial abundance) ➔ Calculated: set to '1' for "*solid*_isotope_mixture_type" = {terrestrial abundance} *Notes:* - it is always set to 1 as fundamental 'Minerals' are only natural terrestrial minerals *Note xml:* - only as 'variable' in the xml ***Variable: mineral in Sample and Matters*** *Condition #1:* mandatory when "*mineral*_specie_uid" ≠ Ø *AND* *Condition #2:* when "*mineral*_isotope_mixture_type" = {pure isotope, partly substituted} AND *Condition #3:* when "*mineral*_specie_uid"/"*molecule*_isotope_mixture_type" = pure isotope, partly substituted} *Note:* - this keyword describes the relative isotopic abundances of a particular species, but not its abundance relative to all species in the solid - value between 0 and 1 - it is set to 1 by default only for the natural terrestrial atomic/molecular species of "*mineral*_specie_uid" *Note xml:* - for a partly substituted mineral, the different isotopes of the specie (pure of substituted) have to be listed with "*mineral*_specie_uid" with their respective "*mineral*_specie_isotope_mole_fraction" while keeping "*mineral*_specie_number_min/_max" at the nominal value for

						the normal species in the mineral (as for the 'terrestrial abundance' mineral). - for a mineral with only one pure isotopomer per specie its abundance need to be set to '1'.
*mineral*_specie_state [*phase*_specie_state]	enum(text)	S1/S1c/ S1 [!_m] [V: !o_m]	Miner L4	VM	--	State of the atomic/molecular species inside the mineral OpenEnum: {constituent element, constituent cation, constituent anion, anionic radical, hydration, interlayer physically adsorbed, pure, clathrate network, clathrate guest, in complex, other, unknown, …} *Definitions:* => See "*constituent*_specie_state" *Note*: - 'pure' can be used for monoatomic minerals - use 'clathrate network, clathrate guest' for clathrate - use 'in complex' for amber, … - use 'other' for included CH4, CO2, … ***Variable: mineral in Sample and Matters*** *Condition:* mandatory when "*mineral*_specie_uid" ≠ Ø
*mineral*_specie_relevance [*phase*_specie_relevance]	enum(text)	S1/S1c/ S1 [!!_m] [V: !!o_m]	Miner L4	VM	--	Relevance of the atomic/molecular species in the mineral Enum: {main, (replacement, substituted, impurity)} *Definitions:* - *'main'*: essential atoms or molecule constituting the nominal elemental formula of the mineral (cf. MinDat). - '*replacement'*: common replacement atom or ion not included in the nominal elemental formula of the mineral but present as replacement elements, mostly in solid solutions. - *'substituted'*: used here only for isotopic atomic species substituting the equivalent "natural element". - '*impuritiy'*: atoms, molecule or ions not contributing to the elemental formula of the mineral and generally not present in such mineral (sometimes it is called in the literature 'atom substitution by impurity',

						but here we will not use ‘substituted’ in such case). *Note:* for all minerals (with fixed and variable composition) all the relevance of their constituting atoms and molecules are ‘main’ as the possible 'replacement atoms' or unexpected ‘atom or molecule impurities’ or substituted isotopes are not included in the nominal elemental formula of the mineral. ***Variable: mineral in Sample and Matters*** Enum: {main, replacement, substituted, impurity} *Condition:* absolute mandatory when “*mineral*_specie_uid” ≠ Ø *Note:* all atoms or molecules not in the mineral formula will be either ‘replacement’, 'impurity', or ‘substituted’ atoms
*mineral*_composition_comments [*phase*_species_comments]	blob	U [m] [V: m]	Miner	VM	--	Any additional information (range of values of ‘x’, ‘y, ‘z’, ‘n’, sum’x+y+z’, …) or comments on the composition and formula of the mineral ***Variable: mineral in Sample and Matters*** Flag ‘replace’: {yes, no} *Definitions*: see “*mineral*_comments” *Note:* the flag ‘replace’ allows to control if the comment replace the original one (‘yes’) or is added to the original one (‘no’).
Mineral oxides composition						
mineral_oxides	***List [L5]***	[!]				£: Description of the oxides composition of the mineral ***Variable: mineral in Sample and Matters*** *Note xml:* need to fully replace the original list of oxides defined in the ‘fundamental mineral phase’, when changed (equivalent to a “*mineral_oxides*_full_definition” = ‘yes’)
*mineral*_oxide_formula [*phase*_oxide_formula]	CS-enum(text)	U [!_m]	Miner L5	VM	--	Formula of the different oxides composing the actual mineral Enum: {Ag2O, Al2O3, As2O3, As2O5, B, B2O3, BaO, BeO, Br, CO2, CaO,

		[V: m]				CdO, CeO2, Ce2O3, Cl, CoO, Co3O4, Cr2O3, Cs2O, CuO, Cu2O, F, Fe, FeO, Fe2O3, Fe3O4, Ga2O3, GeO2, H2O, HfO2, HgO, I, K2O, La2O3, Li2O, MgO, MnO, MnO2, Mn2O3, MoO3, N2O5, Na2O, Nd2O3, Nb2O5, NiO, O2, P2O5, PbO, PbO2, Pt2O3, PtO, Pt, Rb2O, S, SO2, SO3, SO4, Sb2O3, Sb2O5, Sc2O3, SeO2, SiO2, Sm2O3, SnO, SnO2, SrO, Ta2O5, ThO2, TiO2, UO2, U3O8, VO2, V2O3, V2O5, WO3, Y2O3, ZnO, ZrO2} *Note:* cf. http://www.open.ac.uk/earth-research/tindle/AGTWebPages/AGTSoft.html ***Variable: mineral in Sample and Matters*** *Notes:* - include also oxides of substitution and major impurity elements - did not distinguish between isotopic species
*mineral*_oxide_mass_fraction [*phase*_oxide_mass_fraction]	float	U [!o_m] [V: m]	Miner L5	VM	*no*	Mass fraction (in %) of each type of oxide composing the actual mineral *Condition:* mandatory only when "*mineral*_classification_level" = {unique mineral} *Note:* - value between 0 and 1 - variable for generic solid solutions but this fraction will be defined for particular solid solutions at the "solid matter" level. ***Variable: mineral in Sample and Matters*** *Condition:* on all "*mineral*_classification_level" *Note:* cf. http://serc.carleton.edu/research_education/equilibria/mineralformulaerecalculation.html
*mineral*_oxides_comments [*phase*_oxides_comments]	blob	U [m] [V: m]	Miner	VM	--	Any additional information (sum of oxides, typical formula of the analysis, …) or comments on the oxides composition of the mineral *Note:* also additional information on impurities not measured by oxides

Mineral classification: Strunz classification

*mineral*_strunz_class [*phase*_classification_class]	openum(text)	S1/S1c [!!_m]	Miner	F	--	Class of the mineral in the Nickel-Strunz classification (10th ed.) OpenEnum: {01, 02, 03, 04, 05, 06, 07, 08, 09, 10} Label (code): {elements (01), sulfides - sufosalts (02), halides (03), oxides - hydroxides - arsenites (04), carbonates - nitrates (05), borates (06), sulfates - chromates - molybdates - tungstates (07), phosphates - arsenates - vanadates (08), silicates (09), organic compounds (10)} *Note:* glasses and amorphised minerals have the same Strunz class as the crystalline equivalent
*mineral*_strunz_division [*phase*_classification_type]	openum(text)	S1 [!!_m]	Miner	F	--	Sub-class of the mineral in the Nickel-Strunz classification (10th ed.) OpenEnum: {01.A, 01.B, 01.C, …, 10.C} Label (code): {metals and intermetallic alloys (01.A), metallic carbides, silicides, nitrides and phosphides (01.B), metalloids and nonmetals (01.C), nonmetallic carbides and nitrides (01.D), unclassified Strunz elements (01.X), simple sulfides, selenides, etc (02.A), metal sulfides, M:S sup 1:1 (mainly 2:1) (02.B), metal sulfides, M:S = 1:1 (and similar) (02.C), metal sulfides, M:S = 3:4 and 2:3 (02.D), metal sulfides, M:S = 1:2 (02.E), sulfides of arsenic, alkalies; sulfides with halide, oxide, hydroxide, H2O (02.F), sulfarsenites, sulfantimonites, sulfbismuthites (02.G), sulfosalts of SnS archetype (02.H), sulfosalts of PbS archetype (02.J), sulfarsenates, sulfantimonates (02.K), unclassified sulfosalts (02.L), oxysulfosalts of alkalies and alkali earths (02.M), unclassified Strunz sulfides and sulfosalts (02.X), simple halides, without H2O (03.A), simple halides, with H2O (03.B), complex halides (03.C), oxyhalides, hydroxyhalides and related double halides (03.D), unclassified Strunz halogenides (03.X), metal:oxygen = 2.1 and 1:1 (04.A), metal:oxygen = 3:4 and similar (04.B), metal:oxygen = 2:3, 3:5, and similar (04.C), metal:oxygen = 1:2 and similar (04.D), metal:oxygen inf or = 1:2 (04.E), hydroxides (without V or U) (04.F), uranyl hydroxides (04.G), V[5+,6+] vanadates (04.H), arsenites, antimonites, bismuthites, sulfites (04.J),

						iodates (04.K), unclassified Strunz oxides: hydroxides, V[5,6] vanadates, arsenites, antimonites, bismuthites, sulfites, selenites, tellurites, iodates (04.X), carbonates without additional anions, without H2O (05.A), carbonates with additional anions, without H2O (05.B), carbonates without additional anions, with H2O (05.C), carbonates with additional anions, with H2O (05.D), uranyl carbonates (05.E), nitrates (05.N), unclassified Strunz carbonates and nitrates (05.X), monoborates (06.A), diborates (06.B), triborates (06.C), tetraborates (06.D), pentaborates (06.E), hexaborates (06.F), heptaborates and other megaborates (06.G), unclassified borates (06.H), sulfates (selenates, etc.) without additional anions, without H2O (07.A), sulfates (selenates, etc.) with additional anions, without H2O (07.B), sulfates (selenates, etc.) without additional anions, with H2O (07.C), sulfates (selenates, etc.) with additional anions, with H2O (07.D), uranyl sulfates (07.E), chromates (07.F), molybdates, wolframates and niobates (07.G), uranium and uranyl molybdates and wolframates (07.H), thiosulfates (07.J), unclassified Strunz sulfates, selenates, tellurates (07.X), phosphates, etc. without additional anions, without H2O (08.A), phosphates, etc. with additional anions, without H2O (08.B), phosphates without additional anions, with H2O (08.C), phosphates, etc (08.D), uranyl phosphates and arsenates (08.E), polyphosphates, polyarsenates, [4]-polyvanadates (08.F), unclassified Strunz phosphates, arsenates, vanadates (08.X), unclassified Strunz silicates (09.), nesosilicate (09.A), sorosilicate (09.B), cyclosilicate (09.C), inosilicate (09.D), phyllosilicate (09.E), tektosilicate without zeolitic H2O (09.F), tektosilicate with zeolitic H2O (09.G), unclassified silicates (09.H), gemanates (09.J), salts of organic acids (10.A), hydrocarbons (10.B), miscellaneous organic minerals (10.C)} *Note:* glasses and amorphised minerals have the same Strunz division as the crystalline equivalent
*mineral*_strunz_family [*phase*_classification_group]	openum(text)	S2 [!!_m]	Miner	F	--	Family of the mineral in the Nickel-Strunz classification (10th ed.) OpenEnum: {02.BB, 02.CC, 02.EB, …, 09.FA} Label (code): {with Ni, Fe (02.BB), With Ni, Fe, Co, PGE, etc. (02.CC), M:S = 1:2, with Fe, Co, Ni, PGE, etc. (02.EB), with Cl, Br, I (halide-sulfides) (02.FC), M:X = 1:1, 2:3, 3:5, etc. (03.AA), M:X = 1:2 (03.AB), M:X = 1:3

							(03.AC), M:X = 1:1 and 2:3 (03.BA), M:X = 1:2 (03.BB), M:X = 1:3 (03.BC), additional OH (03.BD), M:O = 2:1 (and 1.8:1) (04.AA), M:O = 1:1 (and up to 1:1.25), with small to medium-sized cations only (04.AB), M:O = 1:1 (and up to 1:1.25), with large cations (+/- smaller ones) (04.AC), with small and medium-sized cations (04.BA), with only medium-sized cations (04.BB), with medium-sized and large cations (04.BC), with only large cations (04.BD), with medium-sized cations (04.CB), with large and medium-sized cations (04.CC), with small cations: Silica family (04.DA), with medium-sized cations; chains of edge-sharing octahedra (04.DB), with medium-sized cations; frameworks of edge-sharing octahedra (04.DD) , with large (+/- medium-sized) cations; sheets of edge-sharing octahedra (04.DH), Hydroxides with OH, without H2O; chains of edge-sharing octahedra (04.FD), Hydroxides with OH, without H2O; sheets of edge-sharing octahedral (04.FE), Hydroxides with H2O +/- (OH); sheets of edge-sharing octahedra (04.FL), Alkali-earth (and other M2+) carbonates (05.AB), with medium-sized cations (05.DA), with medium-sized cations (07.AB), with medium-sized and large cations (07.AC), with only large cations (07.AD), with medium-sized cations (07.BB), with medium-sized and large cations (07.BC), with only large cations (07.BD), with small cations (07.CA), with only medium-sized cations (07.CB), with medium-sized and large cations (07.CC), with only large cations (07.CD), Nesosilicates without additional anions; cations in tetrahedral [4] coordination (09.AA), Nesosilicates without additional anions; cations in [4] and greater coordination (09.AB), nesosilicates without additional anions; cations in octahedral [6] coordination (09.AC), Inosilicates with 2-periodic single chains, Si2O6; pyroxene family (09.DA), Single nets of tetrahedra with 4-, 5-, (6-), and 8-membered rings (09.EA), Double nets with 4- and 6-membered rings (09.EB), Phyllosilicates with mica sheets, composed of tetrahedral and octahedral nets (09.EC), Phyllosilicates with kaolinite layers (09.ED), Tektosilicates without additional non-tetrahedral anions, (Al,B):Si = 1:1 (09.FA), … } *Note:* glasses and amorphised minerals have the same Strunz family as the crystalline equivalent
*mineral*_strunz_code [*phase*_classification_code]	varchar(255)	S1/S1c [!!o_mc]	Miner	VM	--	Code of the mineral or group of minerals in the Nickel-Strunz classification (10th ed.)

Condition: Absolute Mandatory when *"mineral*_classification_level" = {solid solution series, variable mineral, unique mineral}.

Constraint: Do not fill when condition is not met.

Notes:

- glasses and amorphised minerals have no Strunz code as the codes of the crystalline chemical equivalents are defined by their crystalline structure.
- However almost all the 31 classified amorphous minerals have a code (opal, allophane, bolivarite, …), but one (amber)

Ex: '09.DA.15', '', …

Variable: mineral in Sample and Matters

Condition: mandatory when *"mineral*_crystal_system" = 'amorphous'

Note xml: for glasses or amorphised minerals of equivalent crystalline mineral: put 'N/A' to remove the Strunz code of the crystalline equivalent.

Mineral classification: Dana classification

*mineral*_dana_major_class [*phase*_classification_class]	openum(text)	S1/S1c [!!_m]	Miner	F	--	Major (old) class of the mineral in the Dana classification (8th ed.) OpenEnum: {I, II, III, IV, V, VI, VII, VIII, IX} Label (code): {native elements (I), sulfides (II), oxides and hydroxides (III), halides (IV), carbonates, nitrates, borates (V), sulfates, chromates, selenates (VI), phosphates, arsenates, vanadates (VII), silicates (VIII), organic minerals (IX)} *Note:* glasses and amorphised minerals have the same Dana major class as the crystalline equivalent
*mineral*_dana_class	openum(text)	S1/S1c [!!_m]	Miner	F	--	Class of the mineral in the Dana classification (78 classes) (8th ed.) OpenEnum: {01, 02, 03, …, 78} Label (code): {native elements (01), sulfides - including selenides and tellurides (02), sulfosalts (03), simple oxides (04), oxides containing uranium

and thorium (05), hydroxides and oxides containing hydroxyl (06), multiple oxides (07), multiple oxides with Nb, Ta, and Ti (08), anhydrous and hydrated halides (09), oxyhalides and hydroxyhalides (10), halide complexes; alumino-fluorides (11), compound halides (12), acid carbonates (13), anhydrous carbonates (14), hydrated carbonates (15), carbonates - hydroxyl or halogen (16), compound carbonates (17), simple nitrates (18), nitrates - hydroxyl or halogen (19), compound nitrates (20), iodates - anhydrous and hydrated (21), iodates - hydroxyl or halogen (22), compound iodates (23), borates - anhydrous (24), anhydrous borates containing hydroxyl or halogen (25), hydrated borates containing hydroxyl or halogen (26), compound borates (27), anhydrous acid and sulfates (28), hydrated acid and sulfates (29), anhydrous sulfates containing hydroxyl or halogen (30), hydrated sulfates containing hydroxyl or halogen (31), compound sulfates (32), selenates and tellurates (33), selenites - tellurites - sulfites (34), anhydrous chromates (35), compound chromates(36), anhydrous acid phosphates (37), anhydrous phosphates (38), hydrated acid phosphates (39), hydrated phosphates (40), anhydrous phosphates containing hydroxyl or halogen (41), hydrated phosphates containing hydroxyl or halogen (42), compound phosphates (43), antimonates (44), acid and normal antimonites, arsenites and phosphites (45), basic or halogen-containing antimonites, arsenites and phosphites (46), vanadium oxysalts (47), anhydrous molybdates and tungstates (48), basic and hydrated molybdates and tungstates (49), salts of organic acids and hydrocarbons (50), nesosilicate insular SiO4 groups only (51), nesosilicate insular SiO4 groups and O, OH, F, and H2O (52), nesosilicate insular SiO4 groups and other anions of complex cations (53), nesosilicate borosilicates and some beryllosilicates (54), sorosilicate Si2O7 groups, generally with no additional anions (55), sorosilicate Si2O7 groups and O, OH, F. and H2O (56), sorosilicate insular Si3O10 and larger noncyclic groups (57), sorosilicate insular, mixed, single, and larger tetrahedral groups (58), cyclosilicate three-membered rings (59), cyclosilicate four-membered rings (60), cyclosilicate six-membered rings (61), cyclosilicate eight-membered rings (62), cyclosilicate condensed rings (63), cyclosilicates (64), inosilicate single-width unbranched chains, w=1 (65), inosilicate double-width unbranched chains, w=2 (66), inosilicate unbranched chains with w sup 2 (67), inosilicate structures with chains of more than one width (68), inosilicate chains with side

						branches or loops (69), inosilicate column or tube structures (70), phyllosilicate sheets of six-membered rings (71), phyllosilicate two-dimensional infinite sheets with other than six-membered rings (72), phyllosilicate condensed tetrahedral sheets (73), phyllosilicate modulated layers (74), tectosilicate Si tetrahedral frameworks (75), tectosilicate Al-Si framework (76), tectosilicate zeolite group (77), unclassified silicates (78)} *Note:* glasses and amorphised minerals have the same Dana class as the crystalline equivalent
*mineral*_dana_type [*phase*_classification_type]	openum(text)	S2 [!!_m]	Miner	F	--	Type of the mineral in the Dana classification (8th ed.) OpenEnum: {01.02, 02.07, 02.08, …, 78.07} Label (code): {native elements with platinum group metals and alloys (01.02), where AmBnXp, with (m+n):p=9:8 (02.07), where AmBnXp, with (m+n):p=1:1 (02.08), where AmBnXp, with (m+n):p=1:2 (02.12), Chlorides (02.15), with a cation charge of 1+ (A+2O) (04.01), with a cation charge of 2+ (A++O) (04.02), with a cation charge of 3+ (A+++2O3) (04.03), with a cation charge of 4+ (A++++O2) (04.04), where X+++O OH (06.01), where X++(OH)2 (06.02), containing multiple cations (06.04), (A+B++)2X4 Spinel group (07.02), where A(B2O6) (08.03), without Dana classification numbers (09.00), where AX (09.01), where A(X)2 (09.02), with simple formula A+CO3 (14.01), with compound formula A+B++(CO3)2 (14.02), -unclassified- (16b.07), (Anhydrous, Acid) (28.01), where (A+)2XO4 (28.02), where (A++)XO4 (28.03), with miscellaneous formulae (28.04), (Hydrated, Acid) (29.01), where (A+)2XO4.x(H2O) (29.02), where (A+)2B(XO4)2.x(H2O) (29.03), where (A+)2Bn(XO4)p.x(H2O) (29.04), where AB(XO4)2.x(H2O) (29.05), where AXO4.x(H2O) (29.06), where A(B)2(XO4)4.x(H2O) (29.07), where (A)2(XO4)3.x(H2O) (29.08), with miscellaneous formulae (29.09), with all cations in octahedral [6] coordination (51.03), with chains P=2 (65.01), with 1:1 layers (71.01), with 2:1 layers (71.02), with 2:1 clays (71.03), interlayered 1:1, 2:1, and octahedra (71.04), with other anions (71.05), SiO2 with [4] coordinated Si (75.01), with Al-Si frameworks (76.01), Feldspathoids and related species (76.02), …} *Note:* glasses and amorphised minerals have the same Dana type as the

						crystalline equivalent.
*mineral*_dana_group [*phase*_classification_group]	openum(text)	S1 [!!_m]	Miner	VM	--	Group of the mineral in the Dana classification (8th ed.) OpenEnum: {02.08.09, 02.07.01, 02.08.10, …, 76.02.01, N/A} Label (code): {Troilite group (02.08.09), Pentlandite group (Isometric: Fm3m) (02.07.01), -Pyrrhotite- group (02.08.10), Pyrite group (Isometric: Pa3) (02.12.01), Djerfisherite group (02.15.02), Gas Hydrate Group (04.01.03), Periclase group (Isometric, Fm3m) (04.02.01), Corundum-Hematite group (Rhombohedral: R-3c) (04.03.01), -Ferrihydrite- group (04.03.02), Perovskite group (04.03.03), Ilmenite group (04.03.05), Rutile group (Tetragonal: P4/mnm) (04.04.01), -Anatase- group (04.04.04), -Brookite- group (04.04.05), Diaspore group (Orthorhombic, Pnma or Pnmd) (06.01.01), Brucite group (Rhombohedral: P-3m1) (06.02.01), -Iowaite- group (06.04.05), Aluminium subgroup (07.02.01), Iron subgroup (07.02.02), Chromium subgroup (07.02.03), Titanium subgroup (07.02.05), Kassite group (08.03.09), -Bromide- group (09.00.00), Halite group (09.01.01), -Hydrohalite- group (09.01.02), Fluorite group (09.02.01), -Lawrencite- group (09.02.03), Bischofite group (09.02.09), Calcite group (Trigonal: R-3c) (14.01.01), Vaterite group (14.01.02), Aragonite group (Orthorhombic: Pmcn) (14.01.03), Natrite group (14.01.06), Dolomite group (Trigonal: R-3) (14.02.01), -Hydromagnesite- group (16b.07.01), -Thenardite- group (28.02.03), -Anhydrite- group (28.03.02), Langbeinite group (28.04.04), -Millosevichite- group (28.04.05), Kieserite Group (Monohydrates) (29.06.02), -Gypsum- group (Dihydrates, monoclinic) (29.06.03), -Sanderite- group (Dihydrates, orthorhombic) (29.06.04), Rozenite Group (Tetrahydrates, monoclinic) (29.06.06), Chalchanthite Group (Pentahydrates, triclinic) (29.06.07), Hexahydrite Group (Hexahydrates, monoclinic) (29.06.08), Melanterite Group (Heptahydrates, monoclinic) (29.06.10), Epsomite Group (Heptahydrates, orthorhombic) (29.06.11), -Meridianiite- group (Undecahydrates, triclinic) (29.06.14), Olivine group (51.03.01), P2/c clinopyroxenes (65.01.01), Orthopyroxenes (65.01.02), C2/c clinopyroxenes (Ca clinopyroxenes) (65.01.03a), C2/c clinopyroxenes (intermediate clinopyroxenes) (65.01.03b), C2/c clinopyroxenes (Na clinopyroxenes) (65.01.03c), Kaolinite group (71.01.01), Serpentine group (71.01.02),

							Serpentine group (-Antigorite- subgroup) (71.01.02a), Serpentine group (Lizardite subgroup) (71.01.02b), Serpentine group (Amesite subgroup) (71.01.02c), Serpentine group (Chrysotile subgroup) (71.01.02d), Allophane group (71.01.04), Pyrophyllite-talc group (71.02.01), Smectite group (Dioctahedral Smectites) (71.03.01a), Smectite group (Trioctahedral Smectites) (71.03.01b), Chlorite group (Tri-Dioctahedral) (71.04.01), Cristobalite group (75.01.01), Quartz group (75.01.03), K (Na,Ba) feldspars (76.01.01), Plagioclase series (76.01.03), Nepheline group (76.02.01), …, N/A} *Notes:* - groups with name between '-': i.e. '-name- group' are not official names (they have no Dana name) but given by us, by extension, from the main mineral of the, generally very short, group. - glasses and amorphised minerals have no Dana group as the group of the crystalline chemical equivalents are defined by their crystalline structure. - However all the 31 classified amorphous minerals have a group *Ex:* '65.01.03a', '75.00.00', 'N/A', … ***Variable: mineral in Sample and Matters*** *Condition:* mandatory when *"mineral*_crystal_system" = 'amorphous' *Note xml:* for glasses or amorphised minerals of equivalent crystalline mineral: put 'N/A' to remove the Dana group of the crystalline equivalent.
*mineral*_dana_code [*phase*_classification_code]	varchar(255)	S1/S1c [!!o_m]	Miner	VM	--	Code of the mineral in the Dana classification (8th ed.) *Condition:* Absolute Mandatory when *"mineral*_classification_level" = {variable mineral, unique mineral}. Do not fill when condition is not met. *Notes:* - glasses and amorphised minerals have no Dana code - However most of the 31 classified amorphous minerals have a code '(opal, allophane, bolivarite, …), but two only a 'fake' non-unique one (amber, lechatelierite)

						Ex: '65.01.03a.03', '', … ***Variable: mineral in Sample and Matters*** *Condition:* mandatory when *"mineral*_crystal_system" = 'amorphous' *Note xml:* for glasses or amorphised minerals of equivalent crystalline mineral: put 'N/A' to remove the Dana code of the crystalline equivalent.
Mineral crystallography						
*mineral*_phase_name [*phase*_phase_name]	varchar(255)	S1S1c/S1 [m] [V: m]	Miner	VM	--	Common name of the mineral phase. *Notes:* – these names are not normalized but mostly a latin numbering or greek alphabet or letter/symbol derived from crystal system – We take the names as defined in the literature. *Ex:* 'alpha-cubic', 'beta-hexagonal', 'orthorhombic', … (mostly for crystalline phase types), 'high density amorphous', Ex:'alpha-quartz', 'beta-quartz'
*mineral*_phase_type [*phase*_phase_type]	enum(text)	S1/S1c/S1 [!_m] [V: £o_m]	Miner	VM	--	Type of phase of the mineral Enum: {crystalline, semicrystalline, paracrystalline, disordered, quasi-amorphous, amorphous, glassy, liquid, mixed, various, unknown} *Definitions:* cf. "*constituent*_phase_type" – 'various': used for groups or sub-groups including minerals with various systems. *Notes:* ***Variable: mineral in Sample and Matters*** *Condition:* compulsory for glasses or amorphised minerals of equivalent crystalline mineral.

*mineral*_crystal_system [*phase*_crystal_system]	enum(text)	S1 [!_m] [V: £o_m]	S1c	Miner Miner	VM F	-- --

Crystal lattice system of the mineral

Enum: {triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, isometric (cubic), amorphous, N/A, various, unknown }

Notes:

- 'isometric': also called 'cubic'
- glasses, solid gels like opals have amorphous crystal system.
- 'various': used for groups or sub-groups including minerals with various systems.
- The crystal system of a given mineral did not change for a solid solution.
- For mineral with variable structural hydration, if crystal structure changes with hydration number 'n', then it is another mineral.
- cf. https://en.wikipedia.org/wiki/Crystal_system

Variable: mineral in Sample and Matters

Condition: compulsory for glasses or amorphised minerals of equivalent crystalline mineral.

Note: mostly modified for "*mineral*_phase_type" = {semicrystalline, paracrystalline, disordered, quasi-amorphous, amorphous, glassy}

*mineral*_crystal_class [*phase*_crystal_class]	enum(text)	S2 [!o_m] [V: m_oc]	S	Miner Miner	VM F	-- --

Crystalline class name of the mineral

Enum: {pedial, pinacoidal, domatic, sphenoidal, prismatic, pyramidal, disphenoidal, dipyramidal, rhombohedral, ditrigonal-pyramidal, trapezohedral, hexagonal-scalenohedral, trigonal-dipyramidal, ditrigonal-dipyramidal, dihexagonal-pyramidal, dihexagonal-dipyramidal, scalenohedral, ditetragonal-pyramidal, ditetragonal-dipyramidal, tetartoidal, diploidal, hextetrahedral, gyroidal, hexoctahedral, N/A, various, unknown}

Condition: mandatory only when "mineral_classification_level" = {unique mineral, variable mineral, solid solution series}

Definitions:

- *'N/A'*: for quasi-amorphous, amorphous, or glassy mineral phase types with 'amorphous' crystal system

- ‘*various*’: used for groups or sub-groups including minerals with various classes.
- ‘*unknown*’: when still unknown and possibly for ‘semicrystalline’, ‘paracrystalline’ (quasi-amorphous) and ‘disordered’ phase types (sample and matters only)

Note:
- see list of crystal classes
  http://webmineral.com/crystall.shtml

Variable: mineral in Sample and Matters

Condition: mandatory when
*“basic_constituent*_mineral_variables_crystal_system” = ‘amorphous’

Notes:
- for glasses or amorphised minerals of equivalent crystalline mineral: ‘N/A’.
- crystal class has no meaning for glasses or amorphized minerals.

*mineral*_crystal_class_symbol [*phase*_crystal_class_symbol]	CS- enum(text)	S2 [!o_m] [V: m_oc]	Miner S	VM F	-- --	Crystalline class (point group) Hermann-Mauguin short symbol (and Schönflies symbol) of the mineral Enum: {1 (C1), -1 (Ci), 2 (C2), m (Cs), 2/m (C2h), 222 (D2), mm2 (C2v), mmm (D2h), 3 (C3), -3 (S6), 32 (D3), 3m (C3v), -3m (D3d), 4 (C4), -4 (S4), 4/m (C4h), 422 (D4), 4mm (C4v), -42m (D2d), 4/mmm (D4h), 6 (C6), -6 (C3h), 6/m (C6h), 622 (D6), 6mm (C6v), -6m2 (D3h), 6/mmm (D6h), 23 (T), m-3 (Th), 432 (O), -43m (Td), m-3m (Oh), N/A, various, unknown} *Condition*: mandatory only when “mineral_classification_level” = {unique mineral, variable mineral, solid solution series} *Definitions:* - ‘N/A’ for ‘amorphous’ system. - ‘unknown’ if unknown (e.g. for ‘hypocrystalline’ and ‘metamict’systems). *Note:* - see list of crystal classes and equivalent full Hermann-Mauguin

symbol:
http://en.wikipedia.org/wiki/Crystallographic_point_group
http://en.wikipedia.org/wiki/Hermann-Mauguin_notation
http://webmineral.com/crystall.shtml
https://fr.wikipedia.org/wiki/Liste_des_groupes_d%27espace

- rotoinversion axis ‘¯1’ for Hermann-Mauguin symbol will be noted: ‘-1’
- true writing of Schönflies symbols is with the number/letter after the capital letter put in underscript. *Ex:* C2v => C_{2v}

Variable: mineral in Sample and Matters

Condition: mandatory when
*“basic_constituent*_mineral_variables_crystal_system” = ‘amorphous’

Notes:

- for glasses or amorphised minerals of equivalent crystalline mineral: ‘N/A’.
- crystal class symbol has no meaning for glasses or amorphized minerals.

*mineral*_crystal_spacegroup [*phase*_crystal_spacegroup]	CS- enum(text)	S2 [!o_m] [V: m_oc]	Miner	VM	--	Crystalline Hermann-Mauguin symbol of symmetry space group in point group of the mineral Enum: {Aba2, Abm2, Ama2, Amm2, C2, C2/c, C2/m, C222, C222(1), Cc, Ccc2, Ccca, Cccm, Cm, Cmc2(1), Cmca, Cmcm, Cmm2, Cmma, Cmmm, F222, F23, F432, F-43c, F-43m, F4(1)32, Fd-3, Fd-3c, Fd-3m, Fdd2, Fddd, Fm-3, Fm-3c, Fm-3m, Fmm2, Fmmm, I222, I23, I2(1)2(1)2(1), I2(1)3, I4, I4/m, I4/mcm, I4/mmm, I41cd, I41md, I422, I432, I4cm, I4mm, I-4, I-42d, I-42m, I-43d, I-43m, I-4c2, I-4m2, I4(1), I4(1)/a, I4(1)/acd, I4(1)/amd, I4(1)22, I4(1)32, Ia-3, Ia-3d, Iba2, Ibam, Ibca, Im-3, Im-3m, Ima2, Imm2, Imma, Immm, P1, P-1, P2, P2/c, P2/m, P222, P222(1), P23, P2(1), P2(1)/c, P2(1)/m, P2(1)2(1)2, P2(1)2(1)2(1), P2(1)3, P3, P312, P31c, P31m, P321, P3c1, P3m1, P-3, P-31c, P-31m, P-3c1, P-3m1, P3(1), P3(1)12, P3(1)21, P3(2), P3(2)12, P3(2)21, P4, P4/m, P4/mbm, P4/mcc, P4/mmm, P4/mnc, P4/n, P4/nbm, P4/ncc, P4/nmm, P4/nnc, P422, P42bc, P42cm, P42mc, P42nm, P42(1)2, P432, P-4, P-42c, P-42m, P-42(1)c, P-42(1)m, P-43m, P-43n, P-4b2, P-4c2, P-

4m2, P-4n2, P4(1), P4(1)22, P4(1)2(1)2, P4(1)32, P4(2), P4(2)/m, P4(2)/mbc, P4(2)/mcm, P4(2)/mmc, P4(2)/mnm, P4(2)/n, P4(2)/nbc, P4(2)/ncm, P4(2)/nmc, P4(2)/nnm, P4(2)22, P4(2)2(1)2, P4(2)32, P4(3), P4(3)22, P4(3)2(1)2, P4(3)32, P4bm, P4cc, P4mm, P4nc, P6, P6/m, P6/mcc, P6/mmm, P622, P6cc, P6mm, P-6, P-62c, P-62m, P-6c2, P-6m2, P6(1), P6(1)22, P6(2), P6(2)22, P6(3), P6(3)/m, P6(3)/mcm, P6(3)/mmc, P6(3)22, P6(3)cm, P6(3)mc, P6(4), P6(4)22, P6(5), P6(5)22, Pa-3, Pba2, Pbam, Pban, Pbca, Pbcm, Pbcn, Pc, Pca2(1), Pcc2, Pcca, Pccm, Pccn, Pm, Pm-3, Pm-3m, Pm-3n, Pma2, Pmc2(1), Pmm2, Pmma, Pmmm, Pmn2(1), Pmmn, Pmna, Pn-3, Pn-3m, Pn-3n, Pna2(1), Pnc2, Pnma, Pnn2, Pnna, Pnnm, Pnnn, R3, R32, R3c, R3m, R-3, R-3c, R-3m, N/A, various, unknown}

Condition: mandatory only when "mineral_classification_level" = {unique mineral, variable mineral, solid solution series}

Definitions:

- 'N/A' for 'amorphous' system.
- 'unknown' if unknown (e.g. for 'microcrystalline', 'nanocrystalline' and 'metamict' systems).

Notes:

- 'indices' are written with '( )' and 'upper bar' with '-' preceding the symbol, as in http://homepage.univie.ac.at/nikos.pinotsis/spacegroup.html
  Ex: $P2_1$ => 'P2(1)'
- for each official space group (in International Tables of Crystallography, Vol. A) there are others equivalent ways to describe the symetries with different associated symbols. A good way to found the standard symbol is to found the space group number (230 groups) and go to the link above and found the standard symbol associated with the space group number.
  Ex: orthorhombic Pbnm = Pnma (62)
- one way to found this space group number is to look at the mineral crystallography on 'webmineral' and view one of the "Additional jPOWD Structure files": you will found there the space group followed by its number.

Ex: Space group: PBNM (62)

See: http://en.wikipedia.org/wiki/Space_group, http://webmineral.com/help/CrystalSystem.shtml http://www.planewave.de/icp/atoms/atoms.sgml-7.html http://homepage.univie.ac.at/nikos.pinotsis/spacegroup.html (list in numerical order (used as reference): one mistake: F4-3m (216) => F-43m) http://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-norm?choose=choose&from=norm&gnum=40&norgens=en (list list in numerical order. 5 are different with previous list!: Aem2=>Abm2 (39), Aea2=>Aba2 (41), Cmce=>Cmca (64), Cmme=>Cmma (67), Ccce=>Ccca (68))

Variable: mineral in Sample and Matters

Condition: mandatory when *"basic_constituent*_mineral_variables_crystal_system" = 'amorphous'

Notes:

- for glasses or amorphised minerals of equivalent crystalline mineral: 'N/A'.
- Crystal Hermann-Mauguin symbol has no meaning for glasses or amorphized minerals.

Mineral crystal sites

mineral_crystal_sites [-xml in precursors]	***List [L6]***	[O] [V Flag: !!o_m]	VM	£: Description of the crystallographic sites of atoms in the mineral structure *Condition:* Optional bloc - Mandatory active below when *"mineral*_crystal_site_label" ≠ 'NULL' ***Variable: mineral in Sample and Matters*** Flag 'full_definition': {yes, no} *Condition:* Flag absolute mandatory when "*mineral*_crystal_site_label" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of crystal sites defined in the

					‘fundamental mineral phase’. Need to fully redefine it. - ‘*no*’: only to add new crystal sites to the original list and modify some already defined (they should have the same “*mineral*_crystal_site_label” than the original site to be modified). *Note:* the flag ‘full_definition’ allows controlling the mode of definition of the crystal sites of the actual mineral.
*mineral*_crystal_site_label [*phase*_crystal_site_label]	varchar(255)	S3 [£od_m] [V: ££o_m]	Miner L6	VM F	--	Label of the crystallographic site of the atom in the mineral structure FreeList: {M1, M2, M3, M4, O1, O2, O3, O4, O5, O6, O7, O8, …} *Default* = ‘NULL’ *Condition:* (option trigger) the filling of this KW is ‘compulsory’ when this optional bloc is used. It triggers the ‘mandatory’ status of several others KW in the optional bloc. *Definition:* ‘M’ (for Metal ion) or ‘O’ (for Oxygen atom) & site order number *Note:* start the list with the sites of the cations, then eventually Oxygen *Ex:* ‘M1’, ‘M2’, ‘O1’, ‘O2’, … *Note:* Determined from “_atom_site_label” of AMCS Database: http://rruff.geo.arizona.edu/AMS ***Variable: mineral in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used *Note:* add labels for replacement and impurities atoms
*mineral*_crystal_site_type [*phase*_crystal_site_type]	enum(text)	S2 [!o_m] [V:!o_m]	Miner L6	VM F	-- --	Type of crystallographic site of the atomic species in the mineral structure Enum: {main, substitutional, isovalent substitutional, aliovalent substitutional, interstitial, split interstitial, topological defect, vacancy, unknown} *Condition:* Mandatory when *“mineral*_crystal_site_label” ≠ ‘NULL’ *Definition:* cf. “*solid*_crystal_site_type” *Ref*: https://en.wikipedia.org/wiki/Crystallographic_defect

						Variable: solid in Sample and Matters *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' *Note:* add site types for impurities atomic species
*mineral*_crystal_site_number [*phase*_crystal_site_number]	int(11)		S [!o_m] [V: !o_m]	Miner L6	VM	*no* Number of equivalent crystallographic sites in the fundamental cell of the mineral structure *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' *Ex:* 'M1' = 1, 'M2' = 2, 'O' = 8 for Albite $Na(Si_3Al)O_8$ ***Variable: mineral in Sample and Matters*** *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' *Note:* should not be modified
*mineral*_crystal_site_wp [*phase*_crystal_site_wp]	varchar 255)		S3 [m] [V: m]	Miner L6	VM	-- Wyckoff position code of the crystallographic sites of the atoms in the mineral structure *Definition:* multiplicity, Wyckoff letter, site symmetry *Note:* cf. http://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-wp-list http://www.cryst.ehu.es/cryst/get_wp.html (calculateur de wp) http://fr.wikipedia.org/wiki/Position_de_Wyckoff (french or German) There is a total of 1731 Wyckoff positions in space groups. *Ex*: '4u1', '2m.2.', '1e222' (space group P222) *Note:* information necessary for the definition of phonon modes (band list) ***Variable: mineral in Sample and Matters*** *Note:* add Wyckoff positions codes for replacement and impurities atoms
mineral_crystal_site_species	***List [L7]***		[!o]			£: specie(s) in the crystallographic site of the mineral structure and their state *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' ***Variable: mineral in Sample and Matters*** *Notes xml*:

						⇨ when the crystal site is changed all species and their related information (coordinence, occupancy, oxidation state) should be listed. ⇨ to change one specie, or its associated information, the whole site should be redefined (with "*mineral_crystal_sites*_full_definition" = 'no')
*mineral*_crystal_site_*specie*_uid [*] [*phase*_crystal_site_specie_uid]	varchar(255)	U [!o_m] [V: !o_m]	Miner Atom L6 L7	VM	--	Link to the existing UID of the specie in the crystallographic site. *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' *Note:* - if a cation has more than one valence, then it is necessary to link to the ion with its valence *Ex:* 'Fe^{2+}', 'Fe^{3+}', 'Mn^{2+}', 'Mn^{3+}', 'Mn^{4+}', 'V^{2+}', 'V^{3+}', 'V^{4+}', 'V^{5+}', 'Cr^{2+}'… - Species can be elements, but may be also molecular species, such as anionic radicals, H_2O of hydratation, H_2O in ice and clathrate, … - the link for mineral is only to the natural species (natural mixture of the isotopologues with terrestrial abundance). ***Variable: mineral in Sample and Matters*** *Condition:* Mandatory when *"mineral*_crystal_site_label" ≠ 'NULL' *Note:* includes the replacement and impurities elements *Note*: this "specie_uid" refers to particular isotopes only for isotopicaly substituted minerals.
*mineral*_crystal_site_*specie*_coordinence [*phase*_crystal_site_specie_coordinence]	enum(text)	S2 [m] [V: m]	Miner Mine L6 L7	VM F	-- --	Coordinences of the species (mostly cations) and associated geometry of the crystallographic sites in the mineral structure Enum: {linear I, linear II, trigonal planar III, tetrahedral IV, square planar IV, trigonal bipyramidal V, square pyramidal V, octahedral VI, trigonal prismatic VI, pentagonal bipyramidal VII, face capped octahedral VII, trigonal prismatic square face monocapped VII, cubic VIII, square antiprismatic VIII, dodecahedral VIII, hexagonal bipyramidal VIII, octahedral trans bicapped VIII, trigonal prismatic triangular face bicapped VIII, trigonal prismatic square face bicapped VIII, tricapped trigonal prismatic IX, monocapped square antiprismatic IX, bicapped square antiprismatic X, trigonal prismatic all faces

					capped XI, icosahedral XII, cuboctahedral XII, anticuboctahedral XII, hexagonal prismatic XII, bicapped hexagonal antiprismatic XIV, no, unknown} *Definition*: number of anions and shape of polyhedra surrounding the cation. But its can also refer to a molecular species such as H_2O or an anionic radical *Note:* 'no' coordinence for O atoms. *Note:* cf. http://en.wikipedia.org/wiki/Coordination_geometry ***Variable: mineral in Sample and Matters*** *Note:* add coordinence for replacement and impurities atoms
*mineral*_crystal_site_*specie*_occupancy [*phase*_crystal_site_specie_occupancy]	float	S [m] [V: m]	Miner L6 L7	VM	*no* specie fractional occupancies of the crystallographic sites of the mineral structure *Note:* Determined from "*mineral_specie*_site_occupancy" of AMCS Database ***Variable: mineral in Sample and Matters*** *Note:* modify occupancy of main atoms and add for replacement and impurities atoms
*mineral*_crystal_site_*specie*_oxidation_state [*phase*_crystal_site_specie_oxidation_state]	int(11)	S [m] [V: m]	Miner L6 L7	VM	-- Oxidation state of the atoms (mostly cations) in the crystallographic sites of the mineral structure. *Note:* no oxidation state for O atoms or molecular species *Reference:* https://en.wikipedia.org/wiki/Oxidation_state https://en.wikipedia.org/wiki/List_of_oxidation_states_of_the_elements ***Variable: mineral in Sample and Matters*** *Note:* add coordinence for replacement and impurities atoms
*mineral*_crystal_composition_order [*phase*_crystal_composition_order]	enum(text)	S [m] [V: m]	Miner	VM	-- Type of compositional order in the crystallographic sites of the mineral structure Enum: {ordered, disordered, partly ordered, unknown}

							Note: for mineral it should be set to ‘ordered’ (TBC) ***Variable: mineral in Sample and Matters*** *Note:* change order if modified in actual mineral, especially by replacement and impurities atoms
*mineral*_crystal_comments [*phase*_crystal_comments]	blob		U [m] [V: m]	Miner	VM	--	Additional information on mineral crystal structure and sites ***Variable: mineral in Sample and Matters*** Flag ‘replace’: {yes, no} *Definitions*: see “*mineral*_comments” *Note:* the flag ‘replace’ allows to control if the comment replace the original one (‘yes’) or is added to the original one (‘no’).
Mineral properties							
*mineral*_molar_mass [*phase*_molar_mass]	varchar(255)		S3 [!o_m] [V: m]	Miner	VM	g/mol	Molar mass (value or range) of the mineral • provided in ‘g/mol’ unit *Condition:* Mandatory when “*mineral*_classification_level” = {unique mineral, variable mineral, solid solution series} *Note:* Molar mass is frequently called ‘molecular weight’ *Note:* range of molar mass for variable mineral, solid solutions and n-hydrated minerals. No requested value for groups and subgroups. *Note:* a mole of mineral is a mole of one ‘chemical formula unit’. Its molar mass is determined from its structural or elemental formula. *ex:* ‘161.7’, ‘160.2 - 162.5’ ***Variable: mineral in Sample and Matters*** *Note:* determined from the actual elemental formula. Different from generic mineral for solid solution, n-hydrated minerals, or minerals with replacement elements. Minor changes with impurities elements.

*mineral*_density [*phase*_density]	varchar(255)	S3 [!o_m] [V: m]	Miner	VM	g/cm3	Density (value or range) of the mineral, or average value when variable • provided in 'g/cm^{3}' unit *Condition:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, solid solution series} *Note:* range of density for variable mineral, solid solutions and n-hydrated minerals. No requested value for groups and subgroups. *ex:* '2.37', '2.45 - 2.58' ***Variable: mineral in Sample and Matters*** *Note:* Different from generic mineral for solid solution, n-hydrated minerals, or minerals with replacement elements. Minor changes with impurities elements.
*mineral*_state_ntp [*phase*_state_ntp]	enum(text)	S1/S1c [!o_m]	Miner	F	--	State of the mineral phase in NTP conditions Enum: {solid, metastable solid - other solid, metastable solid - liquid, other solid, liquid, gas} *Condition:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, mineral solution series} *Definitions: cf. solid*_state_ntp *Note:* NTP conditions (NIST): 293.15K (20°C), 101.325kPa (1 atm) *Ex*: - 'liquid' for 'mercury'as its melting point is 234.32 K - 'liquid ' (+ gas) for CH_4 clathrate, as only liquid H_2O and gaseous CH_4 exist at NTP - 'metastable solid - other solid': for CaCO3 'aragonite' (the other solid phase, stable, is calcite)

Mineral thermodynamic properties

mineral_phase_transitions	***List [L7]***	[!O]				£: Description of the main phase transitions of the mineral *Condition:* Mandatory only when "*mineral*_classification_level" = {unique

						mineral, variable mineral}
*mineral*_phase_transition_type [*phase*_phase_transition_type]	enum(text)	U [!o_m]	Miner L7	F	--	Type of phase transition of the mineral Enum: {solid-solid, solid-liquid, solid-gas, liquid-gas, triple point solid-solid-solid, triple point solid-solid-liquid, triple point solid-liquid-gas, quadruple point, solid decomposition, solid-liquid decomposition } *Notes:* - only the most important transition points need to be given (i.e. solid-solid and solid-liquid at ambient pressure …) - the phase diagram will be given for the mineral polymorphs series with its phase diagram in "*mineral*_figures"
*mineral*_phase_transition_other_phases [*phase*_phase_transition_phases]	varchar(255)	U [!o_m]	Miner L7	F	-	Name(s) of the other phase(s) implied in the phase transition of the mineral *Notes:* - it can be one mineral (solid-solid), one liquid (solid-liquid) or two minerals (triple point solid-solid-solid) or one mineral and one liquid (triple point solid-solid-liquid), or more (quadruple point) - the full name and type of mineral(s) should be given *Ex:* 'Sillimanite, kyanite' (for Andalusite)
*mineral*_phase_transition_temperature [*phase*_phase_transition_temperature]	varchar(255)	U [!o_m]	Miner L7	F	K Pa, bar	Temperature (value(s) or range) of the phase transition of the mineral at defined pressure, or average value when variable • temperature should be provided in 'K' unit, with the unit written after the numbers • pressure should be provided in parenthesis after the temperature and in 'Pa' or 'bar' unit (or their (sub-)multiples), with the unit written after the numbers *Notes:* – range of temperature for variable mineral. – No requested value for groups and subgroups, solid solutions and n-hydrated solids. *Ex:* '35.4 K (100 mbar)', '273.2 - 273.5 K (100 MPa)', '272.3 K (1 bar) –

						275.2 K (100 bar)’
*mineral*_phase_transition_comments [*phase*_phase_transition_comments]	blob	U [m]	Miner	F	--	Additional information on mineral phase transitions (unknown limits of transition, …)
Mineral optical properties						
*mineral*_refringence_type [*phase*_refringence_type]	enum(text)	S2 S2c [!o_m] [V: m]	Miner	VM	--	Type of refringence of the mineral crystal Enum: {isotropic, uniaxial, biaxial, various, unknown} *Condition:* Mandatory only when “*mineral*_classification_level” = {unique mineral, variable mineral, solid solution series} *Note:* depends on the crystalline system of the mineral (“*mineral*_crystal_system”): – ‘*isotropic*’ for ‘isometric’, and ‘amorphous’ – ‘*uniaxial*’ for ‘trigonal’, ‘tetragonal’ and ‘hexagonal’ – ‘*biaxial*’ for ‘monoclinic’, ‘triclinic’ and ‘orthorhombic’ – ‘*various*’ for ‘various’ – ‘*unknown*’ for ‘unknown *Note:* the refringence type did not change for a solid solution because of identical crystal structure *Note:* could be automaticaly determined using “*mineral*_crystal_system” ***Variable: mineral in Sample and Matters*** *Note:* Modified to ‘isotropic’ in case of glasses or amorphised minerals of equivalent uniaxial and biaxial crystalline minerals.
*mineral*_refringence_sign [*phase*_refringence_sign]	enum(text)	U S [!o_m] [V: m]	Miner	VM F	-- --	Sign of birefringence of the mineral crystal *Condition:* Mandatory only when “*mineral*_classification_level” = {unique mineral} AND when “*mineral*_refringence_type”={uniaxial}

							Enum: {positive, negative, positive or negative, no, unknown} *Note:* depends on the type of refringence of the mineral crystal ("*mineral*_refringence_type") and on the difference between refraction indexes ("*mineral*_refraction_index_na" and "_nb") – '*no*': for 'isotropic' crystals – sign of $n_\beta - n_\alpha = n_e - n_o = e - w$ for uniaxial crystals: – '*positif*': for biaxial crystals: (always 'positif' by definition) – '*positif or negatif*'': for 'various' (but can be positif if 'various' only include 'monoclinic', 'triclinic' and 'orthorhombic' systems) – '*unknown*': for 'unknown *Note:* when the birefringence sign can change for a uniaxial solid solution or n-hydrated minerals, especialy when birefringence is low, it is set to 'positif or negatif' ***Variable: mineral in Sample and Matters*** *Notes:* – Do not change for isotropic and biaxial crystals. – Only 'positif' or 'negatif' for uniaxial crystals. – Can be different from generic mineral for solid solution, n-hydrated minerals, or minerals with replacement elements. – Rare changes with impurities elements.
*mineral*_birefringence [*phase*_birefringence]	varchar(255)	U [!o_m] [V: m]	Miner	VM	*no*	Birefringence, Δn, (value or range) of the mineral crystal *Condition:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, solid solution series} AND when "*mineral*_refringence_type"={uniaxial} *Note:* For isotropic crystals: '0' For uniaxial crystals: $\Delta n = abs(n_\alpha - n_\beta) = abs\ (n_o - n_e) = abs\ (w - e)$ For biaxial crystals: $\Delta n = n_\gamma - n_\alpha = n_z - n_x$ *Note:* range of birefringence for variable mineral, solid solutions and n-hydrated minerals

						Ex: '0.026', '0.056-0.083' ***Variable: mineral in Sample and Matters*** *Note:* Not mandatory. Exact value for specific solid solution, n-hydrated minerals, or minerals with replacement elements in actual mineral matter. Minor changes with impurities elements.
*mineral*_refraction_index_na [*phase*_refraction_index_na]	varchar(255)	S2 [!o_m] [V: m]	Miner	VM	*no*	Refraction index, n_α or n_o (*w*) (value or range), of the mineral crystal (isotropic, uniaxial and biaxial crystals) (at 589.3 nm) *Condition:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, solid solution series} *Definition:* Standard refractive index measurements are taken at yellow doublet sodium D line, with a wavelength of 589.29 nm. – For uniaxial crystal (birefringence): ordinary indice, n_o, or *w* (optical axe) – For biaxial crystals (trirefringence): lowest of the three 'n' values *Note:* range of refraction index for variable mineral, solid solutions and n-hydrated minerals *Ex:* '1.326', '1.456 - 1.583' ***Variable: mineral in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated minerals, or minerals with replacement elements in actual mineral matter. Minor changes with impurities elements.
*mineral*_refraction_index_nb [*phase*_refraction_index_nb]	varchar(255)	S3 [!o_m] [V: m]	Miner	VM	*no*	Refraction index, n_β or n_e (*e*) (value or range), of the mineral (at 589.3 nm) (uniaxial and biaxial crystals) *Condition #1:* Mandatory only when "*mineral*_refringence_type" = {uniaxial, biaxial} AND *Condition #2:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, solid solution series}

						– For uniaxial crystals: extraordinary indice, n_e, or *e* (perpendicular to optical axe) – For biaxial crystals: medium of the three 'n' value *Note:* range of refraction index for variable mineral, solid solutions and n-hydrated minerals *Ex:* '1.326', '1.456 - 1.583' ***Variable: mineral in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated minerals, or minerals with replacement elements in actual mineral matter. Minor changes with impurities elements.
*mineral*_refraction_index_ng [*phase*_refraction_index_ng]	varchar(255)	S3 [!o_m] [V: m]	Miner	VM	*no*	Refraction index, n_γ, (value or range) of the mineral (at 589.3 nm) (biaxial crystals only) *Condition #1:* Mandatory only when "*mineral*_refringence_type" = 'biaxial' AND *Condition #2:* Mandatory only when "*mineral*_classification_level" = {unique mineral, variable mineral, solid solution series} – For biaxial crystals: highest of the three 'n' values *Note:* range of refraction index for variable mineral, solid solutions and n-hydrated minerals *Ex:* '1.326', '1.456 - 1.583' ***Variable: mineral in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated minerals, or minerals with replacement elements in actual mineral matter. Minor changes with impurities elements.
*mineral*_dispersion_v [*phase*_dispersion_v]	varchar(255)	U [m] [V: m]	Miner	VM	*no*	Abbe V-number (value, range or qualitative information) expressing the visible dispersion of a transparent mineral crystal (using n_α (TBC)) *Definition:* Called 'constringence'. It is defined as $V = (n_d-1)/(n_F-n_C)$ using the Fraunhofer lines d, F and C at 587.6 nm (d), 486.1 (F) and 656.3 nm (C).

						cf wiki: http://en.wikipedia.org/wiki/Abbe_number *Note:* range of dispersion for variable mineral, solid solutions and n-hydrated minerals *Ex:* '48', '40 - 65' ***Variable: mineral in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated minerals, or minerals with replacement elements in actual mineral matter. Possible significant changes with impurities elements.
Mineral optical aspect						
*mineral*_pure_color [*phase*_pure_color]	enum(text)	S2 [m]	Miner	F	--	Main color of the pure mineral crystals (without any impurity) FreeList: {colorless, white, blue, bluish, azure, green, greenish, emerald, olive, turquoise, yellow, yellowish, orange, pink, pinkish, red, reddish, lilac, violet, indigo, purple, brown, brownish, beige, gray, grayish, black, blackish, bronze, lead, silver, steel, copper, tin, various, …} *Notes*: – The list above contains the main colors in 'WebMineral' website, but there are lot of other nuances (not very homogeneous…). Try to avoid too exotic ones!
*mineral*_true_color [*phase*_true_color]	varchar(255)	S2 [m] [V: m]	Miner	VM	--	Color nuance (pure) and other known colors of the mineral crystals (with impurity) *Ex:* 'pale pinkish - green, pink, blue' ***Variable: mineral in Sample and Matters*** *Note:* actual color of the mineral
*mineral*_diaphaneity [*phase*_diaphaneity]	enum(text)	S2 [!o_m] [V: m]	Miner	VM	--	Capacity of the mineral to transmit light Enum: {transparent, transparent to translucent, transparent to subtranslucent, transparent to opaque, translucent, translucent to subtranslucent, translucent to

							opaque, subtranslucent to opaque, opaque, various, unknown} *Condition:* Mandatory only when "*mineral*_classification_level" = {solid solution series, variable mineral, unique mineral} ***Variable: mineral in Sample and Matters*** *Note:* actual diaphaneity of the mineral
*mineral*_luster [*phase*_luster]	enum(text)	S2 [m] [V: m]	Miner	VM	--	Description of how and how much the surface of a mineral reflects light. Enum: {metallic, submetallic, waxy, vitreous, pearly, silky, greasy, resinous, adamantine, earthy, various, unknown} *Definitions*: - '*metallic*': The mineral is opaque and reflects light as a metal would. - '*submetallic*': The mineral is opaque and dull. The mineral is dark colored. (nonmetallic): The mineral does not reflect light like a metal and are thus qualified of: - '*waxy*': The mineral looks like paraffin or wax. - '*vitreous*': The mineral looks like broken glass. - '*pearly*': The mineral appears iridescent, like a pearl. - '*silky*': The mineral looks fibrous, like silk. - '*greasy*': The mineral looks like oil on water. - '*resinous*': The mineral looks like hardened tree sap (resin). - '*adamantine*': The mineral looks brilliant, like a diamond. - '*earthy*': - '*various*': for (sub)groups and series ***Variable: mineral in Sample and Matters*** *Note:* actual luster of the mineral

Mineral references and comments

mineral_publications	***List [L7a]***	[O]	£: Publications on the mineral phase and its properties.

*mineral*_publication_uid [*] [*phase*_publication_uid]	varchar(255)	U [m]	Miner Publi L7a	F	--	Link to the existing UID of the publications on the mineral *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'phase'
mineral_links *[phase_links]*	***List [L7b]***	[O]				£: Web page(s) describing the mineral and its properties.
*mineral*_link_name [*phase*_link_name]	varchar(255)	U [m]	Miner L7b	F	--	Name of the web page(s) describing the mineral and its properties. *Ex:* 'Wikipedia', 'WebMineral, 'MinDat', 'Handbook of Mineralogy (Min. Soc. Am)', …
*mineral*_link_url [*phase*_link_url]	CS-varchar(255)	U [m]	Miner L7b	F	--	Link(s) to the web page (Webmineral and MinDat database) describing the mineral and its properties => http://webmineral.com => http://www.mindat.org => http://rruff.geo.arizona.edu/AMS/amcsd.php (crystallography) *Ex:* 'http://webmineral.com/data/Wittichenite.shtml' *Ex:* 'http://www.mindat.org/min-1088.html' *Notes*: - you can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
*mineral*_comments [*phase*_comments]	blob	U [m]	Miner	VM Aj	--	Additional information on mineral (possible replacement elements, impurities, …) ***Variable: mineral in Sample and Matters*** Flag 'replace': {yes, no} *Definitions*: see "*mineral*_comments" *Definitions*: – 'yes': the comment replace the original comment of the fundamental mineral

- 'no': the comment is added after the original comment of the fundamental mineral

Note: the flag 'replace' allows to control if the comment replace the original one ('yes') or is added to the original one ('no').

6.4 Solid Phase Table

Root of the table: ***solid***

Data type: 'Fundamental phase'

In "Exp" column 'VS' means a variable key-word of the fundamental solid: when defining a "sample" or a "matter" containing fundamental solid phases (described in "basic constituents") the VS values in "solid phase" can be modified (but will not be changed in the fundamental solid database) to reflect the exact solid properties (for exemple for solid solutions, clathrates, …). See specific notes in ***Variable: solid in Sample and Matters***

Key-word	Type	Level	Table	Exp	Unit	Description
Solid phase import						
*solid*_import_mode [*phase*_import_mode]	enum(text)	P [!!_m]	Solid	(V)	--	Mode of import of the solid data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*solid*_xml_filename [-xml] [*phase*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	Solid	(V)	--	Name of the storage copy of the xml import file of the solid metadata ➔ determined automatically during import (from "*solid*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Solid phase indexes and type						
*solid*_index [**][-xml] [*phase*_index]	int(10)	B [!!_g]	Solid	F	--	Automatic random but unique number (ID) given to new solid
*solid*_uid [**] [*phase*_uid]	varchar(255)	S0/S0c/ S1 [!!_m]	Solid	F	--	Unique identifier code (UID) given to the solid table (to be created) *Nomenclature:* Create this UID with "SOLID_" possibly followed by 'GROUP_' for "*solid*_classification_level" = {solid group, solid subgroup}, or 'SERIES_' for 'solid solution series'

						It should be of the style: ⇨ 'SOLIDGROUP_GroupName' ⇨ 'SOLIDSERIES_SeriesName' or 'SOLIDSERIES_EndmemberName1_EndmemberName2' ⇨ 'SOLID(_Phase)_SolidName' or 'SOLID_SolidFormula' where 'Group/SeriesName' are the group/series names, 'Phase' is the optional phase name of the solid, 'EndmemberName'n'' and 'SolidName' are the "*solid*_official_name" and 'SOLID_SolidFormula' the "solid_chemical_formula" (for small molecules). *Note*: use only lowercase for the solid name *Note*: The fundamental solid phases stored in the database will be, by default, with natural terrestrial abundance. Ex: ⇨ 'SOLID_alpha_Fe', ⇨ 'SOLID_NaCl', ⇨ 'SOLID_CH4_clathrate', …
*solid*_mineral_uid [*] [*phase*_phase_uid]	varchar(255)	S1i [£o_m]	Solid Miner	F	--	Link to the existing UID of the equivalent mineral *Condition:* compulsory if exist *Note:* - mostly for simple solids - this will allow to link the fundamental solid to its equivalent natural mineral and get its classification *Ex:* - 'MINER_halite' for NaCl ionic solid; - 'MINER_ice' for Water ice Ih, - 'MINER_methane-hydrate-I' for CH_4 chathrate hydrate I, - 'MINER_corundum' for alpha-Al_2O_3 aluminum oxide, …
*solid*_liquid_uid [*] [*phase*_phase_uid]	varchar(255)	S1i [£o_m]	Solid Liquid	F	--	Link to the existing UID of the equivalent liquid *Condition:* compulsory if exist *Note:*

- mostly for simple solids. Should have exactly the same molecular or atomic composition
- this will allow to link the fundamental solid to its equivalent liquid

Ex:
- 'LIQUID_H2O' for corresponding liquid of 'Water ice Ih'
- 'LIQUID_Hg' for corresponding liquid of 'Hg metallic solid'

Solid names

*solid*_official_name [*phase*_official_name]	varchar(255)	S0/S0c/ S1 [!!_m] [V: m]	Solid	VS	--	Official name of the solid, series or (sub)group *Notes:* - *As there is no current official classification an naming, we will create these names* - start with the common litteral compound name (starting with a capital letter) including its composition, and followed with the phase name/number. *Ex:* 'Water ice Ih' - for solid solutions series the name should be built with: 'endmember_name-1':'endmember_name-2' followed by the type of solid solution series and with the phase name/number (or in front) *Ex:* 'beta-N2:CH4 solid solution series' *Ex:* 'CH4:C2H6 clathrate hydrate II' - It is used as the title of the solid page on the SSHADE interface ***Variable: solid in Sample and Matters*** *Note:* to provide a more precise name for the actual solid *Ex:* 'beta-N2:CH4 solid solution = 0.97:0.03'
solid_secondary_names [*phase*_secondary_names]	***List [L0]***	[m]				£: List of the alternative names used for the solid
*solid*_secondary_name	varchar(255)	S0/S0c/ S1	Solid	F	--	Alternative name used for the solid

[*phase*_secondary_name]		[m]	L0			*Note:* start with a capital letter
*solid*_cas_number [*phase*_cas_number]	varchar(255)	S1 [m]	Solid	F	--	CAS registry number, unique, of the solid (natural or synthetic) *Note:* the problem is to found them!!! No registry, not systematic! => some (mostly synthetic) in Wikipedia: http://www.chemindustry.com/chemicals/

Solid family, class and type

*solid*_family [*constituent/phase*_family]	enum(text)	S1/S1c/ S1 [!!_m]	Solid	F	--	Phase family (or major class) of the solid Enum: {molecular solid, covalent network solid, ionic solid, metallic solid, molecular and covalent solid, molecular and ionic solid, covalent and ionic solid, complex solid, other, unknown} [to be changed in v0.9.0a] *Definitions:* see in "*constituent*_family" *Notes:* - equivalent to "*constituent*_family"
*solid*_class [*phase*_class]	enum(text)	S1/S1c/ S1 [!!_m]	Solid	F	--	Class of solid Enum: {non polar molecular solid, polar molecular solid, hydrogen bonded molecular solid, mixed molecular solid, chain covalent network solid, sheet covalent network solid, tridimentional covalent network solid, glass, acid salt, alkali salt, normal salt, mixed salt, true metal, pseudometal (semi-conductor)} *Definitions:* - For molecular solids: - 'non polar molecular solid' (01): - 'polar molecular solid' (02): - 'hydrogen bonded molecular solid' (03): - 'mixed molecular solid' (04): - For covalent network solids (synthetic, excluding minerals), - 'chain covalent network solid' (05): - 'sheet covalent network solid' (06):

- ‘tridimentional covalent network solid’ (07):
- ‘glass’: disordered covalent network solid’ (08):

- For ionic solids (synthetic, excluding minerals),
  - ‘acid salt’ (09):
  - ‘alkali salt’ (10):
  - ‘normal salt’ (11):
  - ‘mixed salt’ (12):
- For metallic solids (synthetic, including native metal element minerals),
  - ‘true metal’ (13):
  - ‘pseudometal (semi-conductor)’ (14):

Notes:

- Equivalent to “*constituent*_class”
- similar to “*solid*_classification_class”

*solid*_compound_type [*phase*_compound_type]	openum(text)	S0/S0c/ S0 [!_m]	Solid	F	--	General type of solid compound OpenEnum: {elemental solid, noble gas solid, carbon allotrope, organic molecular solid, inorganic molecular solid, clathrate, clathrate hydrate, hydrate, homopolymer, copolymer, molecular solid solution, solid molecular mixture, oxide, hydroxyde, oxide-hydroxide, non-oxide ceramic, antimonate, antimonite, arsenate, arsenite, borate, bromide, carbonate, chlorate, chloride, chlorite, chromate, cyanate, cyanide, fluoride, fulminate, halide, iodate, iodide, molybdate, nitrate, nitrite, perchlorate, phosphate, phosphite, selenate, selenide, selenite, sulfate, sulfide, sulfite, sulfosalt, tellurate, tellurite, tungstate, vanadate, vanadium oxysalt, organic salt, silicate, cyclosilicate, inosilicate, nesosilicate, phyllosilicate, sorosilicate, tectosilicate, metal, metallic alloy, semi-conductor, other compound, …} - For molecular solids: Homonuclear: - ‘*elemental solid’*: covalent network (ex: , Si…) homonuclear solid (except with C and noble gases atoms) - ‘*noble gas solid’*: - ‘*carbon allotrope’:* molecular (ex: C60, carbon nanotubes) or covalent network (ex: graphite, diamond) homonuclear solid made fully or mostly of C atoms

Polynuclear:
- '*organic molecular solid'*: all molecular solids made of organic molecules (CnHmOpNq)
- '*inorganic molecular solid'*: inorganic molecular solid (without Cn) either homonuclear (ex: N2, S8) or heteronuclear

Polymolecular:
- '*clathrate*': clathrate structure formed with other host molecules
- '*clathrate hydrate'*: clathrate structure formed with H_2O (host)
- '*hydrate*': solid stoichiometric hydrate containing water molecules as an integral part of the crystal and combined in a definite ratio

Polymers:
- '*homopolymer*': mixture of macromolecules composed of the same unique repeating structural unit.
- '*copolymer*': mixture of macromolecules composed of several repeating structural units.

Molecular mixture:
- '*molecular solid solution':* solid-state solution of two or more molecules forming a single homogeneous crystalline phase in thermodynamical equilibrium
- '*solid molecular mixture':* solid-state mixture of two or more molecules forming an homogeneous phase, but generally out of thermodynamical equilibrium (at ow temperature, …)

- For covalent solids:
  - *'elemental solid'*: non-metal elemental solid, except carbon allotropes (*Ex:* Si, Ge, …)
  - *'oxide':* ex: SiO2, TiO_2,
  - *'hydroxide':*
  - *'oxide-hydroxide':*
  - *'non-oxide ceramic':* (ex: SiC, BN, …)
- For ionic solids:
  - antimonate,
  - antimonite,
  - Arsenate (AsO_4^{3-})
  - Borate (BO_3^{3-}, BO_4^{4-})
  - Bromide (Br^-)

- Carbonate (CO_3^{2-})
- Chloride (Cl^-)
- Chlorite (ClO_2^-)
- Chlorate (ClO_3^-)
- Perchlorate (ClO_4^-)
- Chromats (CrO_4^{2-})
- Cyanide (CN^-)
- Cyanate (NCO^-)
- Fluoride (F^-)
- Fulminate (CNO^-)
- Halide
- iodate,
- Iodide (I^-)
- Molybdate (MoO_4^{2-})
- Nitrite (NO_2^-)
- Nitrate (NO_3^-)
- Phosphite (HPO_3^{2-})
- Phosphate (PO_4^{3-})
- phosphite
- Selenide (Se^{2-})
- Selenite (SeO_3^{2-})
- Selenate (SeO_4^{2-})
- Sulfide (S^{2-})
- Sulfite (SO_3^{2-})
- Sulfate (SO_4^{2-})
- tellurate, tellurite
- Tungstate (WO_4^{2-})
- Vanadate (PO_4^{3-})
- Organic salt: (ex: Acetate (CH_3COO^-), Citrate HO-C(COO^-)(CH_2-COO^-)$_2$)...

- For metallic solids:
  - '*metal': Ex:* Fe, Cu, Al, …
  - '*metallic alloy*': *Ex:* Fe-Ni
  - '*semi-conductor*':
- Others compounds:

- '*other compound'*: compounds which cannot be described by one of the above words (describe in "*solid*_comments")

Notes:

- same compound types for "*constituent*_compound_type". It will be used for main search.

*solid*_classification_level [*phase*_classification_level]	enum(text)	S1/S2c/ Solid S2 [!!_m]	F	--	Level of solid classification Enum: {solid group, solid subgroup, solid polymorphs, solid solution series, variable solid, unique solid} *Definitions:* - *' solid group'*: General group of solid, with at least 2 variable molecules or atoms *Ex*: 'mixed clathrates hydrates', 'rare gases solids' … - *' solid subgroup'*: subgroup of a solid group, with one molecule or atom of the group fixed, and at least 1 other variable. *Ex*: 'single clathrate hydrates II', 'Rare gases clathrate hydrates I' - '*solid polymorphs'*: solids with exactly same composition but different crystalline structures - *'solid solution series':* series between 2 endmembers of a group, or subgroup, with one variable between 2 or 3 molecules or atoms *Note:* for solid solutions of *Note:* amorphous multi-molecules/atoms solids will be always classified as 'solid solution series' *Ex:* • 'beta N_2:CH_4 series' (end members are: 'beta-N_2' and 'beta-N_2:$(CH_4)_x$' with x = 0.05 at 40K) • 'CH_4-I:N_2 series' (end members are: 'CH_4-I' and 'CH_4-I:$(N_2)_x$ with x=0.03 at 40K) • '(CH_4,C_2H_6)clathrate hydrate I' (end members are: 'CH_4 clathrate hydrate I' and 'C_2H_6 clathrate hydrate I') - *'variable solid*: solid with at least one molecule or atom in variable amount. *Note*: can be an endmember. *Ex:* 'CH_4 clathrate hydrate', 'NH_3 hydrate'

- *'unique solid*: mineral with a fully defined quantitative formula.
  Note: can be an endmember.
  Ex: 'H_2O ice Ih', 'NH_3 monohydrate'

Solid endmembers and polymorphs

solid_endmembers *[phase_endmembers]*	***List [L1]***	[!o]				£: List of the endmember solids of the series *Condition:* Mandatory when "*solid*_classification_level" = {solid group, solid subgroup, solid solution series}
*solid*_endmember_solid_uid [*] [*phase*_endmembers_phase_uid]	varchar(255)	U [!o_m]	Solid Solid L1	F	--	Link to the existing UID of the endmember solids of the series *Ex:* 'beta N_2·CH_4 series' - 'beta-N_2' - 'CH_4-I'
solid_polymorphs *[phase_polymorph]*	***List [L2a]***	[!o]				£: List of the solid polymorphs *Condition:* Mandatory when "*solid*_classification_level" = {solid polymorphs} *Definition:* polymorphism is the ability of a solid material to exist in more than one form or crystal structure *Ref.:* https://en.wikipedia.org/wiki/Polymorphism_(materials_science) *Note:* For monoatomic solids the polymorphs are called 'allotropes'
*solid*_polymorph_solid_uid [*] [*phase*_polymorph_phase_uid]	varchar(255)	U [!o_m]	Solid Solid L2a	F	--	Link to the existing UID of solid polymorph *Ex:*
*solid*_polymorph_comments [*phase*_polymorph_comments]	varchar(255)	U [m]	Solid L2a	F	--	Additional information on the solid polymorph *Note:* - to tell if it is a true polymorph or a polytype

- to provide some information on the P-T stability domain of the polymorph

solid_polytypes [*phase_polytypes*] | ***List [L2b]*** | [o]

£: List of the polytypes of the solid

Constraint: only when "*solid*_classification_level" = {solid polymorphs, solid solution series, variable solid, unique solid}

Definition: Polytypism is a particular case of polymorphism, the different structures are formed by stacking a module (in most cases a layer or sheet) of almost identical structure and composition. The polytypes differ in how the module is stacked (translation and / or rotation) along one direction: the two lattice parameters in the plane of the module are common to all polytypes, while the third differs. Polytypes are distinguished by specific symbols. The symbols most frequently used are those of Ramsdell, which associate the number of layers in the period of the polytype with the symbol corresponding to the crystalline or reticular system:

- A: anorthic (triclinic)
- M: monoclinic
- O: orthorhombic
- Q: quadratic (tetragonal)
- T: trigonal (with hexagonal Bravais lattice)
- R: trigonal (with rhomboedric Bravais lattice)
- H: hexagonal
- C: cubic (isometric)

Definition: Polytypes can also be used for polymers to describe various types of polymers of a same global formula, i.e. with various monomer numbers (molar mass), various branching, ..

Ex: 'LDPE', 'LLDPE', 'HDPE', 'UHWPE'… for Polyethylene

Variable: solid in Sample and Matters

Note: keep only the actual polytype, if it is known

Note xml: when filled, it will replace the full list of polytypes

*solid*_polytype_name [*phase*_polytype_name]	varchar(255)	S0/S0c/ S1 [o_m] [V: m]	Solid L2b	VS	--	Name of the polytypes of the solid *Note:* - provides a list of the polytypes using their names or names & symbols (follow official nomenclature) whatever they are considered as separate solids or not. - If they are considered as separate solids they need to be also listed in "*solid*_polymorph_solid_uid" *Reference:* http://www.iucr.org/resources/commissions/crystallographic-nomenclature/polytypes
*solid*_polytype_comments [*phase*_polytype_comments]	varchar(255)	U [m] [V: m]	Solid L2b	VS	--	Additional information on the solid polytype *Note:*
*solid*_figures	***List [L2c]***					£: List of the figures on the solid
*solid*_figure_filename [*phase*_figure_filename]	varchar(255)	P/U [m]	Solid L2c	F	--	File name(s) (with extension) of the figure on the solid *Image formats:* .png, .jpg, (.gif) *Notes:* - mostly for polymorphs and series - can be a phase diagram of the polymorphs, or the (end)members diagram of a solid solution series … *Note DB:* this file will be imported in the database
*solid*_figure_caption [*phase*_figure_caption]	varchar(255)	U [m]	Solid L2c	F	--	Caption(s) or comment(s) on the figure(s) on the solid

Solid chemical composition

*solid*_formula [*phase*_formula]	varchar(255)	U [!!_m] [V: m]	Solid	VS	--	Developed structural (empirical) chemical formula of the solid *Syntax:* Latex format *Notations:*

- Small point (.) can separate molecules
- Dot • (\bullet) separates hydration
- LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf
    - *Ex:*
- 'H_2O' for H_2O
- '$(N_2)_x . (CH_4)_{1-x}$' for $(N2)_x.(CH4)_{1-x}$
- '$(CH_4)_{x}.5.75(H_2O)$' for CH4 clathrate I
- '$NH_3 \bullet 2H_2O$' for $NH_3•2H_2O$

Notes:

- For polymers: give the repeating unit with 'n' subscript and add the terminal groupments/functions, if they are generic (fixed) for the polymer.
  Ex: '$H-[O-CH_2-CH_2]_n-OH$' or '$-[O-CH_2-CH_2]_n-$' for polyethylene glycol

Variable: solid in Sample and Matters

Notes:

- Includes replacement atoms and substitution and impurities molecules/atoms, as well as values of x,y,z fractions and n-hydration number
  Ex: '$(CH_4)_{0.92}.5.75H_2O$' for $(CH_4)_{0.92}.5.75H_2O$
- Can contain isotopic information for pure isotopes or when an atom is substituted in a molecule
  Ex: '$^{18}H_2O$ for '$^{18}H_2O$'
- For polymers: give the repeating unit with the value or range of 'n' subscript and add the terminal groupments/functions, if known.
  Ex: '$H-[O-CH_2-CH_2]_{50-75}-OH$'' for polyethylene glycol

*solid*_chemical_formula [*phase*_chemical_formula]	CS-varchar(255)	S0/S0c/S1 [!!_m] [V: m]	Solid	VS	--	Developed global chemical and structural formula of the solid *Ex:* - '(N2,CH4)', or '(N2)·0.03(CH4)' for CH_4 in solid solution in N_2 - '(CH4)(CH4,CO2)3•23H2O' for mixed CH_4-CO_2 clathrate hydrate of type I - 'NH3•n(H2O)' for NH3 hydtrates *Notes:*

- contain ionic information.

Notations:

- solid series are indicated by comma separating the molecules that varies in amount. The more dominant molecule is usually listed first.
- small point '·' separates molecules
- big point '•' (ascii=149) separates hydration in ( )
- 'n' give a variable value for structural hydration.
- a range of hydration number 'n' can be given with 'n1-n2':
  - *Ex:* 'NH3•0.5-2(H2O)'
- For solids with isotopic atomic substitution (non-natural isotopic abundance), substituted atoms will have their atomic mass between square brackets preceding the atom symbol. D can be used for ^{2}H.
  - *Ex:* 'NH3•2(D2[18]O)'
- For polymers: give the repeating unit with 'n' subscript and add the terminal groupments, if known.
  Ex: 'H[OCH2CH2]nOH' or '-[OCH2CH2]n-' for polyethylene glycol

Note: Definition of this type of formula (for minerals):
cf http://webmineral.com/help/ChemicalFormula.shtml

Variable: solid in Sample and Matters

Developed global chemical and structural formula of the actual msolid

*solid*_hydration [*phase*_hydration]	boolean	S0/S0c/ S2 [!!_m]	Solid	F	--	Flag telling if the solid contains structural H_2O BoolEnum: {yes, no} or {true, false}
*solid*_hydration_series [*phase*_hydration_series]	boolean	U [!!o_m]	Solid	F	--	Flag telling if the solid is an isostructural series of n-hydrated solids ('true') BoolEnum: {yes, no} or {true, false} *Condition*: absolute mandatory when "*solid*_hydration" = {true} *Notes:* n-hydrated solids have variable amount of structural H_2O molecules, (limited range of n: min-max, or incremental)

						Ex: $NH_3 \bullet nH_2O$, n = 0.5, 1, 2 (but in this exemple it is not isostructural)
*solid*_hydration_number [*phase*_hydration_number]	varchar(255)	S3/S3c/ S3 [!o_m] [V: m]	Solid	VS	--	Number or range of numbers of structural H_2O in the solid *Condition*: mandatory when "*solid*_hydration" = 'true' *Note:* for hydration series put the current value (if well defined and known), or a range (if not well defined or known) either fixed and continuous ('1 - 3'), or incremental ('0.5, 1, 2') for some groups, or with one limit unknown ('2 - ?', '? – 6'), or open with no upper limit in 'n' ('2 - n'), or 'n' if fully unknown or undefined. *Ex:* '2', '4 - 6', '0 - 2', '0 - n' (if no real limit to 'n'), '0.5, 1, 2' ***Variable: solid in Sample and Matters*** *Note:* It will take into account the level of (de)hydration of the matter. Put the value, but if not well known then put some range.
Solid polymer composition						*Note:* only for polymers
*solid*_polymer_monomer_arrangement [-xml, only in variables]	enum(text)	S1/S1c/ S1 [-] [V: !o_m]	Solid	VS	--	Monomer(s) arrangement in the polymer molecule Enum: {linear homopolymer, branched homopolymer, sequence-controlled copolymer, alternating copolymer, periodic copolymer, statistical copolymer, random copolymer, block copolymer, stereoblock copolymer, branched Graft copolymer, branched star copolymer, other, unknown} *Note:* not for fundamental solids (not in xml "phase_solids', only in "solid_varialbles" ***Variable: solid in Sample and Matters*** *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} *Definitions*: - '*linear homopolymer*': linear polymer with only a single A unit - '*branched homopolymer*': polymer with only a single A unit but with several polymer chains connected to a central core - '*sequence-controlled copolymer'*: macromolecule, in which the

						sequence of monomers is controlled to some degree - '*periodic copolymer'*: linear polymer with A and B units arranged in a repeating sequence (e.g. $(A\text{-}B\text{-}A\text{-}B\text{-}B\text{-}A\text{-}A\text{-}A\text{-}A\text{-}B\text{-}B\text{-}B)_n$) - '*alternating copolymer'*: periodic copolymer with regular alternating A and B units with formula: -A-B-A-B-A-B-A-B-A-B-, or $-(\text{-}A\text{-}B\text{-})_n-$ - '*statistical copolymer'*: copolymers in which the sequence of monomers follows a statistical rule - '*random copolymer'*: purely random arrangement of chemically distinct monomers - '*block copolymer'*: comprise two or more homopolymer subunits (the blocks) linked by covalent bonds - '*stereoblock copolymer'*: in which the blocks differ only in the tacticity of the monomers (relative stereochemistry of adjacent chiral centers within a macromolecule) - '*branched Graft copolymer'*: in which the main chain is formed from one type of monomer (A) and branches are formed from another monomer (B) - '*branched star copolymer'*: with several polymer chains connected to a central core - '*other*': any other monomer(s) arrangement not listed above (provide the information in "*solid*_polymer_comments") - '*unknown*': unknown arrangement *Note:* there is a lot of other types or subdivisions of polymer arrangements *Ex:* A biopolymer (for example a protein) with a perfectly-defined primary structure is a sequence-controlled polymer.
*solid*_polymer_terminal_function	varchar(255)	U [!o_m] [V: !o_m]	Solid	VS	--	Terminal chemical function(s) of the polymer *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} *Syntax:* Latex format *Note:* - Generally one type of function, but sometimes two - the terminal functions can also be given in "*solid*_formula" and

						"*solid*_chemical_formula" - This function and number should be listed in the "*solid_chemical_functions"* bloc - Ex: '$-CH_3, -C(=O)OH$' ***Variable: solid in Sample and Matters*** *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} *Note:*
*solid*_polymer_monomer_number	varchar(255)	U [!o_m] [V: !o_m]	Solid	VS	--	Average number or range of numbers of monomers in the solid polymer molecules *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} and when "*solid*_polymer_molar_mass" = Ø *Note:* put 'n' if undefined *Ex:* '50', '30 - 45', 'n' ***Variable: solid in Sample and Matters*** *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} and when "*solid*_polymer_molar_mass" = Ø *Note:* average or range of numbers of monomers of the actual polymer *Note:* put 'unknown' if unknown
*solid*_polymer_molar_mass	varchar(255)	S3 [!o_m] [V: !o_m]	Solid	VS	*g/mol*	Average molar mass or range of molar masses of the polymer molecules *Condition*: mandatory when "*solid*_compound_type" = {homopolymer, copolymer} and when "*solid*_polymer_monomer_number" = Ø • provided in 'g/mol' unit *Ex:* '320', '300 - 450' ***Variable: solid in Sample and Matters*** *Condition*: mandatory when "*solid*_compound_type" = {homopolymer,

						copolymer} and when "*solid*_polymer_monomer_number" = Ø *Note:* average molar mass or range of molar masses of the actual polymer *Note:* put 'unknown' if unknown
*solid*_polymer_polymolecularity_index	varchar(255)	U [m] [V: m]	Solid	VS	--	Polymolecularity index (or polydispersity index) of the numbers of monomers or molar masses of the polymer molecules *Constraint*: only when "*solid*_compound_type" = {homopolymer, copolymer} *Ex:* '2.6', '2.3 – 3.1' *Definition*: measure of the heterogeneity of sizes of molecules in a mixture. It is calculated using the equation ĐM = Mw/Mn, where Mw is the weight-average molar mass and Mn is the number-average molar mass. It can also be calculated according to degree of polymerization, where ĐX = Xw/Xn, where Xw is the weight-average degree of polymerization and Xn is the number-average degree of polymerization. Note: $Đ = 4 * \Sigma (Mi)^2 / (\Sigma Mi)^2$ with Mi the molecular mass of the monomer ***Variable: solid in Sample and Matters*** *Note:* polymolecularity index of the actual polymer
*solid*_polymer_crystallinity_degree	varchar(255)	U [m] [V: m]	Solid	VS	--	Crystallinity degree of the solid polymer *Constraint*: only when "*solid*_compound_type" = {homopolymer, copolymer} *Note:* the degree of crystallinity may be expressed in terms of a weight fraction or volume fraction of crystalline material: number between 0 and 1 ***Variable: solid in Sample and Matters*** *Note:* crystallinity degree of the actual polymer
*solid*_polymer_comments [*phase*_species_comments]	blob	U [m] [V: m]	Solid	VS	--	Any additional information or comments on the polymer *Note:* for exemple any information on polymer branching ***Variable: solid in Sample and Matters***

						Flag 'replace': {yes, no} *Definitions*: see "*mineral*_comments" *Note:* the flag 'replace' allows to control if the comment replace the original one ('yes') or is added to the original one ('no').
Solid chemical functions and bonds						
solid_chemical_functions	***List [L3a]***	[O] [V: £_m] [V Flag: !!o_m]		VS		£: List of different chemical functions present in the solid, except those already in the molecular species and anionic radicals described as 'species' of the solid ***Variable: solid in Sample and Matters*** *Condition:* compulsory to list the new chemical functions and those with changing 'number' Flag 'full_definition': {yes, no} *Condition:* Flag absolute mandatory when "*solid*_chemical_function_uid" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of chemical functions defined in the 'fundamental solid phase'. Need to fully redefine it. - '*no*': only to add new chemical functions to the original list and modify some already defined (they should have the same "*solid*_chemical_function_uid" than the original chemical function to be modified). *Note:* the flag 'full_definition' allows to control the mode of definition of the chemical functions of the actual solid.
*solid*_chemical_function_uid [*] [*phase*_chemical_function_uid]	varchar(255)	S2/S2c [!o_m] [V: ££o_m]	Solid ChemF L3a	VS	--	Link to the existing UID of the chemical function present in the solid *Condition*: mandatory when *"solid*_chemical_function_number" ≠ Ø (i.e. the bloc is used) *Note*: - If the solid is described in terms of molecular species with

						"*solid*_species_uid" their chemical functions (already implicitely taken into account) should not be listed here - it is mostly used to describe chemical functions when a molecular solid is described in terms of atoms (such as in covalent or ionic solids), or when it cannot be fully described in terms of molecules, as for exemple for the terminal functions of polymers ***Variable: solid in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used
*solid*_chemical_function_number [+] [*phase*_chemical_function_number]	varchar(255)	S3/S3c [m] [V: m]	Solid L3a	VS	--	Number, minimum number, of this chemical function present in the solid ➔ Calculation for display: ➔ For solids described with molecular species ("*solid*_specie_family"={molecule, chemical function}): for each 'function_i' of all 'molecule_j' or ''function_j' of "*solid*_specie_uid" it is: – n_min(function_i) = *solid*_chemical_function_number(function_i) + $\sum_{molecule_j}$ (*solid*_specie_number_min(molecule_j) * *specie*_chemical_function_number(molecule_j,function_i) + *solid*_specie_number_min(function_i) – if "*solid*_specie_number_min/_max(molecule_j)" or "*solid*_specie_number_min(function_i)" = 'n' then: n_min(function_i) = n ***Variable: solid in Sample and Matters*** Actual number of the chemical functions
solid_chemical_bonds *[phase_chemical_bonds]*	***List [L3b]***	[!O]				£: List of the intermolecular bonds and ionic bonds of the solid *Condition:* mandatory when "*solid*_class" = 'hydrogen bonded molecular solid, acid salt, alkali salt, normal salt, mixed salt' OR *"solid*_compound_type" = {homopolymer, copolymer} *Note*: These bonds are only the inter-molecular bonds (hydrogen bonds, bond between 'mer'…) and ionic bonds between molecules or atoms. All the other

						intra-molecular chemical bonds are already described in the isolated molecules (or anionic radical).
*solid*_chemical_bond_uid [*] [*phase*_chemical_bond_uid]	varchar(255)	S2/S2c [!o_m]	Solid ChemB L3b	F	--	Link to the existing UID of the intermolecular bonds and ionic bonds of the solid *Note*: – These bonds are only the hydrogen bonds between molecules. All the other chemical bonds are already described in the isolated molecules. – The chemical bonds used for solids are only 'generic mixture' with terrestrial abundance *Ex:* for H_2O ice Ih: 2 x 'BOND_HhO' – For isotopic substituted solid made of at least one molecule with a purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope of the others
*solid*_chemical_bond_number [+] [*phase*_chemical_bond_number]	varchar(255)	S3/S3c [!o_m]	Solid L3b	F	--	Number, or minimum number, of intermolecular bonds and ionic bonds of each type composing the solid ➔ Calculation of 'n_max(bond_i)' for display: ➔ For solids described with molecular species ("*solid*_specie_family"={molecule, chemical function}): for each 'bond_i' of all 'molecule_j' of "*solid*_specie_uid" it is: – n_min(bond_i) = *solid*_chemical_bond_number(bond_i) + $\sum_{specie_j}$ (*solid*_specie_number_min(specie_j) * *specie*_chemical_bond_number(specie_j,bond_i)) – if "*solid*_specie_number_min(specie_j)" = 'n' then: n_min(bond_i) = n *Notes*: - determined relative to a formula unit *Ex:* '2' hydrogen bonds per H_2O molecule for H_2O ice Ih ***Variable: solid in Sample and Matters*** Actual number of the chemical bonds

Solid molecular and atomic composition

*solid*_elemental_formula [-xml] [*phase*_elemental_formula]	CS-varchar(255)	S0/S0c/S1 [!_c] [V: c]	Solid	VS	--	Empirical elemental formula of the solid ➔ Calculated: ⇨ see "*constituent*_elemental_formula" *Notations:* see "*constituent*_elemental_formula" *Ex:* 'C4 O23 H62' for CH_4 clathrate hydrate I ***Variable: solid in Sample and Matters*** ➔ Calculated for each 'atom_i' excepted those with "*solid*_specie_relevance" = {impurity} when one or more "*solid*_specie_uid" is added or changed ⇨ see "*constituent*_elemental_formula" This formula includes substitution molecules or elements plus replacement elements in the actual solid.
*solid*_isotope_mixture_type [*phase*_isotope_mixture_type]	enum(text)	S1/S1c/S1 [!!_m] [V: £o_m]	Solid	VS	--	Type of isotopic mixture of the solid Enum: {pure isotope, partly substituted, terrestrial abundance} *Definitions: cf "constituent*_isotope_mixture_type" *Notes:* – the fundamental solid phases stored in the database will be either with natural terrestrial abundance or with molecules/atoms as pure isotopes (but limited to simple solids). – Some of the partly isotopically substituted (molecular) solids (the most important/simple/commercially available ones) may be also entered as fundamental phases in the database. ***Variable: solid in Sample and Matters*** Enum: {pure isotope, partly substituted, terrestrial abundance, specific abundance, unknown} *Condition:* Compulsory when "*solid*_isotope_mixture_type" ≠ 'terrestrial abundance'

Notes:

- isotopic mixtures in solids with some molecules/atoms not in natural isotopic abundance will be set to 'specific abundance' or to 'partly substituted' (one or more molecule with an atom as a pure isotopic species).
- their abundance will be defined in "*solid*_specie_isotope_mole_fraction" using pure or partly substituted isotopologue molecules

Note: define the effectif type of isotopic mixture

solid_species *[phase_species]*	***List [L4]***	[!!o] [V: £_m] [VFlag: !!o_m]

£: Description of the molecular and/or atomic composition of the solid

Condition: absolute mandatory when "*solid*_classification_level" = {solid subgroup, solid solution series, variable solid, unique solid}

Variable: solid in Sample and Matters

Condition: compulsory to list the replacement, impurity, or substituted molecules/atoms, as well as the main molecules/atoms of the solid (defined in the fundamental solid) with better defined or changing 'number_min/_max'

Notes:

- for isotopic substitution of one or more molecules/atoms, or for solids with specific abundance (i.e. non-terrestrial), all or at least the main isotopic species present will be listed with same nominal values of "*solid*_specie_number_min/_max" but with their isotopic fractional abundance given in "*solid*_specie_isotope_mole_fraction"

Note xml: You have the choice either to fully redefine the solid composition, or only to add new species and modify some already defined

Flag 'full_definition': {yes, no} or {true, false}

Condition: flag absolute mandatory when "so*lid*_specie_uid" ≠ Ø

Definitions:

- '*yes*': fully replace the original list of species defined in the 'fundamental solid phase'. Need to fully redefine it.
- '*no*': only to add new species to the original definition of composition

						and modify some already defined (they should have both the same "*solid*_specie_uid" and "*solid*_specie_relevance" than the original species to be modified). *Note:* the flag 'full_definition' allows to control the mode of definition of the atomic and molecular composition of the actual solid.
*solid*_specie_family [*phase*_specie_family] [-xml]	enum(text)	U [!!_c] [V: !_c]	Solid L4	VS	--	Family of the species composing the solid Enum: {element, molecule, chemical function} *Note:* - equivalent to "*constituent*_specie_family" - "chemical functions"='anionic radical' in synthetic minerals (or other solids) will be described directly instead by their atoms *Note xml:* determined automatically from the type of the species ***Variable: solid in Sample and Matters*** *Notes*:
*solid*_specie_uid [*] [*phase*_specie_uid]	varchar(255)	S0/S0c/ S1 [!!_m] [V: ££_m]	Solid Molec Atom L4	VS	--	Link to the existing UID of the molecular species (molecule or molecular ion) the element (atom or ion), or the chemical function (anionic radical) composing the solid. *Notes:* - it is possible to mix elements, molecular species and anionic radicals for mixed molecular/atomic solids - for polymers use the 'radical' species and add the terminating functions. - the links are either to natural molecules/atoms (for solids made of natural molecular/atomic mixtures of the isotopologues in terrestrial abundance), or to pure isotopes (for pure isotopic, or partly substituted solids) - In some limited cases (simple partly substituted solids) it can be also to partly isotopically substituted molecules. *Note xml:* the same species (same "*solid*_specie_uid") can occurs several times only if its relevance ("*solid*_specie_relevance") is different. They are

						considered as different species. ***Variable: solid in Sample and Matters*** *Condition:* absolute compulsory when the bloc is used *Notes*: - includes the replacement, substituted and impurities molecules/atoms - For solids as 'pure isotope', and in 'specific abundance' this "specie_uid" should refer only to pure isotopes. - only in specific cases it can refer to partly substituted molecules. - for 'partly substituted' solids "specie_uid" will refer to both 'terrestrial abundance' and 'pure isotope' molecules
*solid*_specie_number_min [*phase*_specie_number_min]	float or 'n'	S0b/S0 cb [!_m] [V:!o_m]	Solid L4	VS	*no*	Nominal or minimum total number of this molecular/atomic species composing the solid *Definitions:* - It is the nominal value when "*solid*_classification_level" = {unique solid} - It is the nominal or minimum value when "*solid*_classification_level" ≠ {unique solid} *Notes:* For 'unique solid': - Total number of this molecular/atomic species, but considering all isotopic species. - The mole fraction a specific isotope (i.e. not a species with terrestrial mixture) will be given by "*solid*_specie_isotope_mole_fraction" For all other solids: - Minimum value only for molecules/atoms with variable abundance (x,y,z) in the solid (solid solutions, clathrate hydrates, n-hydrated solids (H_2O), …). Also for solid groups and subgroups. - For solid solution the minimum number is found by putting all variable composition of molecules/atoms to their minimum. - If there is specific information on a limitation in the minimum number of a molecule/atom in variable abundance, then put this number. - For n-hydrated solids the minimum number of H_2O is found by putting

						'n' of H_2O to its minimum structural hydration value. ***Variable: solid in Sample and Matters*** *Condition:* absolute mandatory when "*solid*_specie_uid" ≠ Ø *Notes:* For 'unique solid': - total number of molecules/atoms of each type composing the solid, including replacement atoms, substituted and impurities molecules/atoms. - when an essential (main) molecule of a variable solid, or of a solid (sub-)group is not present, its number has to be set to '0'. For all other solids: - minimum number of molecules/atoms of each type composing the solid, including replacement atoms, substituted and impurities molecules/atoms.
*solid*_specie_number_max [*phase*_specie_number_max]	float or 'n'	S0b/S0cb [!o_m] [V: m]	Solid L4	VS	*no*	Maximum total number of this molecular/atomic species with variable or undefined abundance *Condition:* mandatory when "*solid*_classification_level" ≠ {unique solid} *Notes:* - do not fill for well defined unique solid - only for molecules/atoms with variable abundance (x,y,z) in the solid (solid solutions, clathrate hydrates, n-hydrated solids (H_2O), …). Also for solid groups and subgroups. - For solid solution this maximum value is found by putting all variable composition molecules/atoms to their maximum. - If there is specific information on a limitation in the maximum number of a molecule/atom in variable abundance, then put this number. - For n-hydrated solids the maximum number of H_2O is found by putting 'n' of H_2O to its maximum structural hydration value. If undefined then put 'n' ***Variable: solid in Sample and Matters*** *Note:* maximum number of molecules/atoms of each type composing the solid,

						including replacement, substituted and impurities molecules/atoms. *Note xml:* need to remove any value of '*solid*_specie_number_max' if the molecule/atom number is fixed => put 'N/A'
*solid*_specie_mole_fraction [-xml] [*phase*_specie_mole_fraction]	float	U [o_c] [V:c]	Solid L4	VS	*no*	Mole fraction of the molecular species composing the molecular solid *Condition*: only for "*solid*_family" = {molecular solid} ➔ Calculated from *"solid*_specie_number_max/_min" ⇨ 'specie_mole_fraction' = 'specie_isotope_mole_fraction' * ('specie_number_min' + 'specie_number_max') / $\sum_{(Solid)}$ ['specie_isotope_mole_fraction' * ('specie_number_min' + 'specie_number_max')] ⇨ when "specie_isotope_mole_fraction" is void => "*solid*_specie_mole_fraction" = 1 ⇨ when "specie_number_min" or "specie_number_max" = 'n' => "*solid*_specie_mole_fraction" has no value *Note*: 'specie_isotope_mole_fraction' is set to '1' when it is not defined (species with terrestrial abundance) *Definitions:* - It is an 'element' or a 'molecule' mole fraction depending on "*solid*_specie_family" - It is the nominal value (from "specie_number_min") when "*solid*_classification_level" = {unique solid} - It is the nominal or average value when "*solid*_classification_level" ≠ {unique solid} - For a purely or partly isotopic solid the mole fraction of each pure isotopic specie constituting the solid is its partial abundance relative to the whole solid, not only relative to its own specie (where it should be '1'). Ex: N_2 = '0.3', $^{13}CH_4$ = '0.70' for a mixture with 30% N_2 + 70% $^{13}CH_4$ ***Variable: solid in Sample and Matters*** *Notes:*

					Ex: N_2 = '0.3', $^{12}CH_4$ = '0.35', $^{13}CH_4$ = '0.35' for a mixture with 30% N_2 + 70% CH_4 with $^{13}CH_4/^{12}CH_4$ = 1
*solid*_specie_mole_fraction_error [- float xml] [*phase*_specie_mole_fraction_error]	U [o_c] [V:o_c]	Solid L4	VS	*no*	Mole fraction error of the molecular species composing the molecular solid *Condition*: only for "*solid*_family" = {molecular solid} ➔ Calculated from *"solid*_specie_number_max/_min" ⇨ 'specie_mole_fraction_error' = 0.5 * specie_isotope_mole_fraction * ('specie_number_max' -'specie_number_min') / $\sum_{(Solid)}$ ['specie_isotope_mole_fraction' * ('specie_number_max' + 'specie_number_min')] *Note*: 'specie_isotope_mole_fraction' is set to '1' when it is not defined (species with terrestrial abundance) *Notes:* - It is '0' when "*solid*_classification_level" = {unique solid} - It is '0' or half the range when "*solid*_classification_level" ≠ {unique solid} ***Variable: solid in Sample and Matters*** *Notes:*
*solid*_specie_isotope_mole_fraction float [*phase*_specie_isotope_mole_fraction]	U [!o_mc] [V: !o_m]	Solid L4	VS	*no*	Mole fraction of the isotopic species in the isotopic mixture of this molecule/atom in the solid (for non-terrestrial abundance) *Condition #1:* mandatory when "*solid*_isotope_mixture_type" = {pure isotope, partly substituted} AND *Condition #2:* when "*solid*_specie_uid"/" *molecule*_isotope_mixture_type" = {pure isotope, partly substituted} *Notes:* - All values should be '1' as we will only include in the fundamental database partly substituted solids with only one type of isotopic species. Ex: - D2O:NH3, H2O:ND2H, HDO:ND3

    - But not (D2O,H2O):NH3, H2O:(ND2H,NH3)
- this keyword describes the relative isotopic abundances of a particular species,
- but not its abundance relative to all species in the solid

Note xml:

- for a partly substituted solid, the different isotopes of the specie (pure or substituted) have to be listed with "*solid*_species_uid" with their respective "*solid*_species_isotope_mole_fraction" set to '1' while keeping "*solid*_specie_number_min/_max" at the nominal value for the solid (as for the 'terrestrial abundance' solid).

Ex: N_2 = '1', $^{13}CH_4$ = '1' for a mixture with 30% N_2 + 70% $^{13}CH_4$

Variable: solid in Sample and Matters

➔ Calculated: set to '1' for "*solid*_isotope_mixture_type" = {terrestrial abundance}

Condition #3: mandatory when "*solid*_specie_uid" ≠ Ø
AND
Condition #1: when "*solid*_isotope_mixture_type" = {pure isotope, partly substituted, specific abundance}
AND
Condition #2: when "*solid*_specie_uid"/" *molecule*_isotope_mixture_type" = {pure isotope, partly substituted}

Notes:

- value between 0 and 1
- for solids with a specific isotopic composition (for isotopic substitution of one or more molecule/atom, or for liquids with specific abundance, i.e. non-terrestrial, …), it is the partial abundance of each isotope relative to its species in the solid.
- all, or at least the main isotopic species present should be listed.

Note xml:

- for a solid with specific abundance, the different isotopes of the specie (pure or substituted) have to be listed with "*solid*_species_uid" with their respective "*solid*_species_isotope_mole_fraction" while keeping

						"*solid*_specie_number_min/_max" at the nominal value for the solid (as for the 'terrestrial abundance' solid). Ex: N_2 = '1', $^{12}CH_4$ = '0.5', $^{13}CH_4$ = '0.5' for a mixture with 30% N_2 + 70% CH_4 with $^{13}CH_4/^{12}CH_4$ = 1
*solid*_specie_state [*phase*_specie_state]	enum(text)	S1/S1c/ S1 [!_m] [V: !o_m]	Solid L4	VS	--	State of the molecular/atomic species inside the solid OpenEnum: {constituent element, constituent cation, constituent anion, constituent mer, constituent molecular, anionic radical, pure, mixed, matrix, monomers, dimers, multimers, solute, solvent, solid solution, clathrate network, clathrate guest, hydration, hydrated, interlayer physically adsorbed, other, unknown, …} *Definitions:* => See "*constituent*_specie_state" *Note:* This state depends on "*solid*_compound_type" which gives the type of solid and tells how the molecular/atomic species are organized at the molecular/atomic level ***Variable: solid in Sample and Matters*** *Condition:* mandatory when "*solid*_specie_uid" ≠ Ø *Notes*:
*solid*_specie_relevance [*phase*_specie_relevance]	enum(text)	S1/S1c/ S1 [!!_m] [V: !!o_m]	Solid L4	VS	--	Relevance of the molecular/atomic species in the solid phase Enum: {main, (replacement), substituted, (impurity)} *Definitions:* - *'main'*: essential molecules/atoms constituting the nominal molecular/atomic formula of the solid, - '*replacement'*: common replacement atom not included in the nominal elemental formula of the solid but present as replacement atoms, mostly in solid solutions, - *'substituted'*: used only for isotopic molecular/atomic species substituting the equivalent "natural molecule/atom" - '*impuritiy'*: molecules not contributing to the molecular formula of the

solid but accidentally present

Notes:

- for all fundamental solid phases (with fixed and variable composition) their species relevance are ‘main’ as the possible 'replacement molecules' or unexpected ‘molecule/atom impurities’ are not included in the nominal molecular/elemental formula of the solid.
- substituted will be used only when purely isotopic or substituted isotopic solids are described.

Variable: solid in Sample and Matters

Enum: {main, replacement, substituted, impurity}

Condition: absolute mandatory when “*solid*_specie_uid” ≠ Ø

Note: all molecules not in the solid formula will be either ‘replacement’, 'impurity', or ‘substituted’ molecules

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*solid*_composition_comments [*phase*_species_comments]	blob	U [m] [V: m]	Solid	VS	--	Any additional information (range of values of ‘x’, ‘y, ‘z’, ‘n’, sum’x+y+z’, …) or comments on the composition and formula of the solid ***Variable: solid in Sample and Matters*** Flag ‘replace’: {yes, no} *Definitions*: see “*mineral*_comments” *Note:* the flag ‘replace’ allows to control if the comment replace the original one (‘yes’) or is added to the original one (‘no’).

Solid oxides composition

solid_oxides	***List [L4b]***	[O]				£: Description of the oxides composition of the solid ***Variable: solid in Sample and Matters*** *Note xml:* need to fully replace the original list of oxides defined in the ‘fundamental solid phase’, when changed (equivalent to a

						"*solid_oxides*_full_definition" = 'yes')
*solid*_oxide_formula [*phase*_oxide_formula]	CS- enum(text)	U [m] [V: m]	Solid L4b	VS	--	Formula of the different oxides composing the actual solid Enum: *see mineral*_oxide_formula ***Variable: solid in Sample and Matters*** *Notes:* - include also oxides of substitution and major impurity elements did not distinguish between isotopic species
*solid*_oxide_mass_fraction [*phase*_oxide_mass_fraction]	float	U [m] [V: m]	Solid L4b	VS	*no*	Mass fraction (in %) of each type of oxide composing the actual solid *Note:* - value between 0 and 1 - variable for generic solid solutions but this fraction will be defined for particular solid solutions at the "solid matter" level. ***Variable: solid in Sample and Matters*** *Note:* cf. http://serc.carleton.edu/research_education/equilibria/mineralformulaerecalculation.html
*solid*_oxides_comments [*phase*_oxides_comments]	blob	U [m] [V: m]	Solid	VS	--	Any additional information or comments on the oxides composition of the solid ***Variable: solid in Sample and Matters***
Solid classification						Simple classification (class, type, group, code) of solids (under development)
*solid*_classification_class [*phase*_classification_class]	openum(text)	S1/S1c [!!_m]	Solid	F	--	Class of the solid in the classification (14 classes) OpenEnum: {01, 02, 03, 04, 05, 06, 07, 08, 09, 10, 11, 12, 13, 14} Label (code): {molecular solids with apolar molecules (01), molecular solids with polar molecules (02), molecular solids with hydrogen bonded molecules (03), molecular solids with mixed molecules (04), acid salts (05), alkali salts

						(06), normal salts (07), mixed salts (08), chain covalent networks (09), sheet covalent networks (10), tridimensional covalent networks (11), glasses (12), true metals (13), pseudometals (14)} *Note:* glasses and amorphised solids have the same class as the crystalline equivalent
*solid*_classification_type [*phase*_classification_type]	openum(text)	S1/S1c [!_m]	Solid	F	--	Type of the solid in the classification OpenEnum: {01.01, 01.02, 01.03, 01.04, …, 04.01, 04.02, …, 14.04} Label (code): {with monoatomic apolar molecules (A) (01.01), with diatomic homonuclear apolar molecules (A2) (01.02), with tetratomic homonuclear apolar molecules (A4) (01.03), with octatomic homonuclear apolar molecules (A8) (01.04), with polyatomic homonuclear apolar molecules (An) (01.05), with polyatomic organic apolar molecules (CnHm…) (01.06), with polyatomic inorganic apolar molecules (01.07), with polyatomic organic polar molecules (CnHm…) (02.01), with polyatomic inorganic polar molecules (02.02), homomolecular H-bonded solids (03.01), polymolecular H-bonded solids with H2O (hydrates) (03.02), polymolecular mixed solids with H2O network (clathrate hydrates) (04.01), polymers (04.02), Dianin's compounds (04.03), binary molecular solid solutions (04.04), simple acid salts (05.01), double acid salts (05.02), complex acid salts (05.03), hydrated acid salts (05.04), simple alkali salts (06.01), double alkali salts (06.02), complex alkali salts (06.03), hydrated alkali salts (06.04), simple normal salts (07.01), double normal salts (07.02), complex normal salts (07.03), hydrated normal salts (07.04), simple mixed salts (08.01), double mixed salts (08.02), complex mixed salts (08.03), hydrated mixed salts (08.04), homonuclear chain networks (09.01), two non-metal atoms chain networks (09.02), homonuclear sheet networks (10.01), two non-metal atoms sheet networks (10.02), homonuclear tridimensional networks (11.01), two non-metal atoms tridimensional networks (11.02), multi non-metal atoms tridimensional networks (11.03), homonuclear glasses (12.01), two non-metal atoms glasses (12.02), multi non-metal atoms glasses (12.03), homovalent monolayer metals (13.01), homovalent bilayer metals (13.02), mixed-valent monolayer metals (13.03), mixed-valent bilayer metals (13.04), homovalent monolayer pseudometals (14.01), homovalent bilayer pseudometals (14.02), mixed-valent monolayer pseudometals (14.03), mixed-

						valent bilayer pseudometals (14.04), ... } *Note:* glasses and amorphised solids have the same type as the crystalline equivalent.
*solid*_classification_group [*phase*_classification_group]	openum(text)	S2/S2c [!_m] [V: m]	Solid	VS	--	Group of the solid in the classification OpenEnum: {01.01.01, …, 04.01.01, …, N/A} Label (code): {..., H2O polymorphes (03.01.01), …single clathrate hydrates, non polar guest (04.01.01), double clathrate hydrates, non polar guest (04.01.02), mixed clathrate hydrates, non polar guest (04.01.03), single clathrate hydrates, polar guest (04.01.04), double clathrate hydrates, polar guest (04.01.05), mixed clathrate hydrates, polar guest (04.01.06), single clathrate hydrates, hydrogen bonded guest (04.01.07), double clathrate hydrates, hydrogen bonded guest (04.01.08), mixed clathrate hydrates, hydrogen bonded guest (04.01.09),..., N/A} *Notes:* - Groups (defined by their crystalline structure) will be created for the most common glasses and amorphised solids. ***Variable: solid in Sample and Matters*** *Condition:* mandatory when *"solid*_crystal_system" = 'amorphous' *Note xml:* for glasses or amorphised solids of equivalent crystalline solid: put 'N/A' to remove the group of the crystalline equivalent.
*solid*_classification_code [*phase*_classification_code]	varchar(255)	S2/S2c [!o_m] [V: m]	Solid	VS	--	Code of the solid in the classification *Condition:* Absolute mandatory when *"solid*_classification_level" = {variable solid, unique solid}. Do not fill when condition is not met. *Notes:* - Codes will be created for the most common glasses and amorphised solids. *Ex:* '04.01.01.05', … ***Variable: solid in Sample and Matters***

						Condition: mandatory when *"solid*_crystal_system" = 'amorphous' *Note xml:* for glasses or amorphised solids of equivalent crystalline solid: put 'N/A' to remove the code of the crystalline equivalent.
Solid crystallography						
*solid*_phase_name [*phase*_phase_name]	varchar(255)	S1/S1c/ S1 [!o_m] [V: m]	Solid	VS	--	Common name of the solid phase. *Condition:* Mandatory only when *"solid*_classification_level" = {solid solution series, variable solid, unique solid}. *Notes:* – these names are not normalized but mostly a latin numbering or greek alphabet or letter/symbol derived from crystal system – We take the names as defined in the literature. *Ex:* 'alpha-cubic', 'beta-hexagonal', 'orthorhombic', … (mostly for crystalline phase types), 'high density amorphous', *Ex:* H_2O ices: 'H2O ice Ia (LDA)', 'H2O ice Ia (HDA)', 'H2O ice Ia (VHDA)', 'H2O ice Ic', 'H2O ice Ih', 'H2O ice II', 'H2O ice III', …, 'H2O ice IX', … 'H2O ice XVI'
*solid*_phase_type [*phase*_phase_type]	enum(text)	S1/S1c/ S1 [!!_m] [V: £o_m]	Solid Matter	VS	--	Type of phase of the solid Enum: {crystalline, semicrystalline, paracrystalline, disordered, quasi-amorphous, amorphous, glassy, mesophase, mixed, various, unknown} *Definitions:* cf. "*constituent*_phase_type" – 'various': used for groups or sub-groups including solids with various systems. *Notes:* ***Variable: solid in Sample and Matters*** *Condition:* compulsory for glasses or amorphised solids of equivalent crystalline solid.

*solid*_crystal_system [*phase*_crystal_system]	enum(text)	S1/S1c [!_m] [V: £o_m]	Solid Miner F	VS	--	Crystal lattice system of the solid Enum: {triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, isometric (cubic), amorphous, N/A, various, unknown } *Notes:* see "*mineral*_crystal_system" (change 'mineral' by 'solid') ***Variable: solid in Sample and Matters*** *Condition:* compulsory for glasses or amorphised solids of equivalent crystalline solid. *Note:* mostly modified for "*solid*_phase_type" = {hypocrystalline, metamict, quasi-amorphous, amorphous, glassy}
*solid*_crystal_class [*phase*_crystal_class]	enum(text)	S2 [!o_m] [V: m_oc]	Solid Miner F	VS	--	Crystalline class name of the solid Enum: see "*mineral*_crystal_class" *Condition*: mandatory only when "solid_classification_level" = {unique solid, variable solid, solid solution series} *Definitions:* see "*mineral*_crystal_class" ***Variable: solid in Sample and Matters*** *Condition:* mandatory when *"basic_constituent*_solid_variables_crystal_system" = 'amorphous' *Notes:* see "*mineral*_crystal_class" (change 'mineral' by 'solid')
*solid*_crystal_class_symbol [*phase*_crystal_class_symbol]	CS- enum(text)	S2 [!o_m] [V: m_oc]	Solid Miner F	VS	--	Crystalline class (point group) Hermann-Mauguin short symbol (and Schönflies symbol) of the solid Enum: see "*mineral*_crystal_class_symbol" *Condition*: mandatory only when "solid_classification_level" = {unique solid, variable solid, solid solution series} *Definitions:* see "*mineral*_crystal_class_symbol" *Note:* see "*mineral*_crystal_class_symbol" ***Variable: solid in Sample and Matters***

						Condition: mandatory when *"basic_constituent*_solid_variables_crystal_system" = 'amorphous' *Notes:* see "*mineral*_crystal_class_symbol"
*solid*_crystal_spacegroup [*phase*_crystal_spacegroup]	CS- enum(text)	S2 [!o_m] [V: m_oc]	Solid Miner	VS	--	Crystalline Hermann-Mauguin symbol of symmetry space group in point group of the solid Enum: see "*mineral*_crystal_spacegroup" *Condition*: mandatory only when "solid_classification_level" = {unique solid, variable solid, solid solution series} *Definitions:* see "*mineral*_crystal_spacegroup" *Notes:* see "*mineral*_crystal_spacegroup" ***Variable: solid in Sample and Matters*** *Condition:* mandatory when *"basic_constituent*_solid_variables_crystal_system" = 'amorphous' *Notes:* see "*mineral*_crystal_spacegroup"

Solid crystal sites

solid_crystal_sites [-xml in precursors]	***List [L5]***	[O] [VFlag: !!o_m]	£: Description of the crystallographic sites of molecular/atomic species in the solid structure *Condition:* Optional bloc - Mandatory active below when *"solid*_crystal_site_label" ≠ 'NULL' ***Variable: solid in Sample and Matters*** Flag 'full_definition': {yes, no} *Condition:* Flag absolute mandatory when "so*lid*_crystal_site_label" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of crystal sites defined in the 'fundamental solid phase'. Need to fully redefine it. - '*no*': only to add new crystal sites to the original list and modify some

already defined (they should have the same "so*lid*_crystal_site_label" than the original site to be modified).

Note: the flag 'full_definition' allows to control the mode of definition of the crystal sites of the actual solid.

*solid*_crystal_site_label [*phase*_crystal_site_label]	varchar(255)	S3 [£od_m] [V:£o_m]	Solid Miner L5	F	VS	--

Label of the crystallographic site of the molecular/atomic species in the solid structure

FreeList: {M1, M2, M3, M4, O1, O2, O3, O4, O5, O6, O7, O8, …}

Default = 'NULL'

Condition: (option trigger) the filling of this KW is 'compulsory' when this optional bloc is used. It triggers the 'mandatory' status of several others KW in the optional bloc.

Definitions:

- 'M1', 'M2', 'M3', 'M4': used for main sites of metals ions (main, substitutional, vacancy), or the metal can be specified when unique in the site: Fe1, Ag2, …
- 'O1', 'O2', 'O3', …: used for main sites of Oxygen
- …

Variable: solid in Sample and Matters

Note: add site labels for impurities atomic species

*solid*_crystal_site_type [*phase*_crystal_site_type]	enum(text)	S2 [!o_m] [V:!o_m]	Solid Miner L5	F	VS	--

Type of crystallographic site of the atomic species in the molecular solid structure

Enum: {main, substitutional, isovalent substitutional, aliovalent substitutional, interstitial, split interstitial, topological defect, vacancy, unknown}

Condition: Mandatory when "*solid*_crystal_site_label" ≠ 'NULL'

Definition:

- '*main*': normal sites of the atoms in the solid structure
- *'substitutional'*: main site used by another main atomic species, an impurity or an isotopic species (neutral)

  Note: sometimes its occurs as a Antisite defect, an exchange of

positions between A and B: A substitutes B and B substitutes A

- *'isovalent substitutional'*: main site used by a ionic impurity of the same oxidation state as the ion it is substituting
- '*aliovalent substitutional*': main site used by an impurity or an isotopic species of a different oxidation state than the ion it is substituting
- '*interstitial*': interstitial site (where usually there is not an atom) occupied by an impurity or a main atomic specie.
  Note: sometimes its occurs as a Frenkel pair: interstitial + vacancy
- '*split interstitial*': interstitial site (where usually there is not an atom) shared by two impurities or main atomic species.
  Note: generally neither atoms actually occupy the site
- '*topological defect'*: normal sites of the atoms in the solid structure but with a different chemical bonding environment than the surrounding sites
- '*vacancy*': site normally occupied, but vacant.
- '*unknown*': …

Ref: https://en.wikipedia.org/wiki/Crystallographic_defect

Variable: solid in Sample and Matters

Condition: Mandatory when *"solid*_crystal_site_label" ≠ 'NULL'

Note: add site types for impurities atomic species

*solid*_crystal_site_number [*phase*_crystal_site_number]	int	11)	SU [!o_m] [V: !o_m]	Solid L5	IVS	~~no~~	Number of equivalent crystallographic sites in the fundamental cell of the solid structure *Condition:* Mandatory when *"solid*_crystal_site_label" ≠ 'NULL' ***Variable: solid in Sample and Matters*** *Condition:* Mandatory when *"solid*_crystal_site_label" ≠ 'NULL' *Note:* add site numbers for impurities atomic species
*solid*_crystal_site_wp [*phase*_crystal_site_wp]	varchar(255)		S3 [m]	Solid Miller	IVS ou	--	Wyckoff position code of the crystallographic sites of the atoms in the solid structure

		[V: m]	L5	F?		*Definition:* multiplicity, Wyckoff letter, site symmetry *Note:* - only for ionic, covalent network and metallic solids - see "*mineral*_crystal_site" ***Variable: solid in Sample and Matters*** *Note:* add Wyckoff positions codes for replacement and impurities atoms
solid_crystal_site_species	***List [L6]***	[!]				£: Atomic species in the crystallographic site of the solid structure and their state ***Variable: solid in Sample and Matters*** *Notes xml*: ⇨ when the crystal site is changed all aspecies and their related information (coordinence, occupancy, oxidation state) should be listed. ⇨ to change one specie, or one of its associated information, the whole site should be redefined (with "*solid_crystal_sites*_full_definition" = 'no')
*solid*_crystal_site_specie_uid [*] [*phase*_crystal_site_specie_uid]	varchar(255)	S1i [!_m] [V: !o_m]	Solid Molec L5 L6	VS	--	Link to the existing UID of the atomic species in the crystallographic site. *Condition:* Mandatory when *"solid*_crystal_site_label" ≠ 'NULL' *Notes:* - the links are either to natural atomic species (for solids made of natural mixtures of the isotopologues in terrestrial abundance), or to pure isotopes (for pure isotopic, or partly substituted solids) ***Variable: solid in Sample and Matters*** *Condition:* Mandatory when *"solid*_crystal_site_label" ≠ 'NULL' *Notes:* - includes the impurities and substitution atomic species - this "*solid*_crystal_site_specie_uid" refers to particular isotopes only for isotopicaly substituted solids.

*solid*_crystal_site_specie_coordinence [*phase*_crystal_site_species_coordinence]	enum(text)	S2 [m] [V: m]	Solid Miner L5 L6	VS F	-- -	Coordinences of the atomic species and associated geometry of the crystallographic sites in the solid structure Enum: {linear I, linear II, trigonal planar III, tetrahedral IV, square planar IV, trigonal bipyramidal V, square pyramidal V, octahedral VI, trigonal prismatic VI, pentagonal bipyramidal VII, face capped octahedral VII, trigonal prismatic square face monocapped VII, cubic VIII, square antiprismatic VIII, dodecahedral VIII, hexagonal bipyramidal VIII, octahedral trans bicapped VIII, trigonal prismatic triangular face bicapped VIII, trigonal prismatic square face bicapped VIII, tricapped trigonal prismatic IX, monocapped square antiprismatic IX, bicapped square antiprismatic X, trigonal prismatic all faces capped XI, icosahedral XII, cuboctahedral XII, anticuboctahedral XII, hexagonal prismatic XII, bicapped hexagonal antiprismatic XIV, no, unknown} *Definition*: number of other atomic species and shape of polyhedra surrounding the atomic specie in the site. *Note:* 'no' coordinence for ?? *Reference:* cf. http://en.wikipedia.org/wiki/Coordination_geometry ***Variable: solid in Sample and Matters*** *Note:* add coordinence for substitution and impurities atomic species and replacement atoms
*solid*_crystal_site_specie_occupancy [*phase*_crystal_site_specie_occupancy]	float	SU [m] [V: m]	Solid Miner L5 L6	VS F	~~no~~	Atomic species fractional occupancies of the crystallographic sites of the solid structure *Note:* For atoms determined from "*solid*_atom_site_occupancy" of AMCS Database ***Variable: solid in Sample and Matters*** *Note:* modify occupancy of main atomic species and add for substitution and impurities atomic species and replacement atoms
*solid*_crystal_site_specie_oxidation_state	int(11)	SU [m]	Solid Miner L5	VS F	--	Oxidation state of the atoms (mostly cations) in the crystallographic sites of the solid structure.

[*phase*_crystal_site_specie_oxidation_state]		[V: m]	L6	*Note:* - no oxidation state for O atoms. - only for ionic, covalent network and metallic solids *Reference*: see in "*mineral*_crystal_site_atom_oxidation_state" ***Variable: solid in Sample and Matters*** *Note:* add oxidation state for replacement and impurities atomic species

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Solid crystal molecule sites

solid_crystal_molecule_sites [-xml in precursors]	***List [L5b]***	[O] [VFlag: !!o_m]		£: Description of the crystallographic sites of molecular species in the solid structure *Condition:* Optional bloc - Mandatory active below when *"solid*_crystal_molecule_site_label" ≠ 'NULL' ***Variable: solid in Sample and Matters*** Flag 'full_definition': {yes, no} *Condition:* Flag absolute mandatory when "so*lid*_crystal_molecule_site_label" ≠ Ø *Definitions*: - '*yes*': fully replace the original list of crystal sites defined in the 'fundamental solid phase'. Need to fully redefine it. - '*no*': only to add new crystal sites to the original list and modify some already defined (they should have the same "so*lid*_crystal_molecule_site_label" than the original site to be modified). *Note:* the flag 'full_definition' allows to control the mode of definition of the crystal sites of the actual solid.
*solid*_crystal_molecule_site_label [*phase*_crystal_site_label]	varchar(255)	S3 [£od_m] [V:£o_m]	Solid Miner L5b	IVS -- Label of the crystallographic site of the molecular species in the molecular solid structure FreeList: {A, B, C…, I, I1, I2…, cage 5-12, cage 5-12_6-4, cage 5-12_6-4, cage 4-3_5-6_6-3, cage 5-12_6-8, …}

Default = 'NULL'

Condition: (option trigger) the filling of this KW is 'compulsory' when this optional bloc is used. It triggers the 'mandatory' status of several others KW in the optional bloc.

Definitions:

- 'A', 'B', 'C': used for main site (main, substitutional, vacancy)
- 'I', 'I1', 'I2', …: used for interstitial site
- 'cage 5-12', 'cage 5-12_6-4', …: used for clathrate cages

Note: some labels are specific to molecules in molecular solids, and some to specific type of molecular solids (such as clathrates)

Ex:

- 'cage 5-12', 'cage 5-12_6-2' for the 2 cage types of type I clathrate hydrate
- 'cage 5-12', 'cage 5-12_6-4' for the 2 cage types of type II clathrate hydrate
- 'cage 5-12', 'cage 4-3_5-6_6-3', 'cage 5-12_6-8' for the 3 cage types of type H clathrate hydrate

Variable: solid in Sample and Matters

Note: add site labels for impurities molecular species

*solid*_crystal_molecule_site_type [*phase*_crystal_site_type]	enum(text)	S2 S [!o_m] [V:!o_m]	Solid Miner L5b	F	VS	-- --

Type of crystallographic site of the molecular species in the molecular solid structure

Enum: {main, substitutional, interstitial, split interstitial, topological defect, vacancy, unknown}

Condition: Mandatory when "*solid*_crystal_molecule_site_label" ≠ 'NULL'

Definition:

- '*main*': normal sites of the molecules in the solid structure
- *'substitutional*': main site of a molecule of the molecular solid used by another main molecular species of the molecular solid, or by an impurity or an isotopic species

  Note: sometimes its occurs as a Antisite defect, an exchange of

positions between A and B: A substitutes B and B substitutes A

- '*interstitial*': interstitial site (where there is normaly no molecule) occupied by a molecule of the molecular solid, or by an impurity
  Note: sometimes its occurs as a Frenkel pair: interstitial + vacancy
- '*split interstitial*': interstitial site (where usually there is no molecule) shared by two impurities or main atomic species.
  Note: generally neither molecule actually occupy the site
- '*topological defect'*: normal sites of the atoms in the solid structure but with a different chemical bonding environment than the surrounding sites
- '*vacancy*': site normally occupied by a molecule, but vacant.
- '*unknown*': …

Note: the cages of clathrate hydrates are 'main' sites

Variable: solid in Sample and Matters

Condition: Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL'

Note: add site types for impurities molecular species

*solid*_crystal_molecule_site_number [*phase*_crystal_site_number]	int(11)	SU [!o_m] [V: !o_m]	Solid Number L5b	VS	~~no~~	Number of equivalent crystallographic sites in the fundamental cell of the solid structure *Condition:* Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Ex:* 2x '5-12', + 6x '5-12_6-2' for type I clathrate 16x '5-12', + 12x '5-12_6-4' for type II clathrate 3x '5-12', + 2x '4-3_5-6_6-3', + 1x '5-12_6-8' for type H clathrate ***Variable: solid in Sample and Matters*** *Condition:* Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Note:* add site numbers for impurities molecular species
*solid_crystal*_molecule_*site_species*	***List [L6b]***	[!]				£: Molecular species in the crystallographic site of the solid structure and their state ***Variable: solid in Sample and Matters***

						Notes xml: ⇨ when the crystal site is changed all aspecies and their related information (coordinence, occupancy, oxidation state) should be listed. ⇨ to change one specie, or one of its associated information, the whole site should be redefined (with "*solid_crystal_molecule_sites*_full_definition" = 'no')
*solid*_crystal_molecule_site_specie_uid [*] [*phase*_crystal_site_species_uid]	varchar(255)	U [!o_m] [V: !o_m]	Solid Molec L5b L6b	VS	--	Link to the existing UID of the molecular species in the crystallographic site. *Condition:* Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Notes:* - the links are either to natural molecular species (for solids made of natural molecular mixtures of the isotopologues in terrestrial abundance), or to pure isotopes (for pure isotopic, or partly substituted solids) - In some limited cases (simple partly substituted solids) it can be also to partly isotopically substituted molecules. ***Variable: solid in Sample and Matters*** *Condition:* Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Notes:* - includes the impurities and substitution molecular species - this "*solid*_crystal_molecule_site_specie_uid" refers to particular isotopes only for isotopicaly substituted solids.
*solid*_crystal_molecule_site_specie_coordinence [*phase*_crystal_site_species_coordinence]	enum(text)	S2 [m] [V: m]	Solid Mole L5b L6b	VS F	-- -	Coordinences of the molecular species and associated geometry of the crystallographic sites in the solid structure Enum: {linear I, linear II, trigonal planar III, tetrahedral IV, square planar IV, trigonal bipyramidal V, square pyramidal V, octahedral VI, trigonal prismatic VI, pentagonal bipyramidal VII, face capped octahedral VII, trigonal prismatic square face monocapped VII, cubic VIII, square antiprismatic VIII, dodecahedral VIII, hexagonal bipyramidal VIII, octahedral trans bicapped VIII, trigonal prismatic triangular face bicapped VIII, trigonal prismatic square face bicapped VIII, tricapped trigonal prismatic IX, monocapped square antiprismatic IX, bicapped square antiprismatic X, trigonal prismatic all faces

						capped XI, icosahedral XII, cuboctahedral XII, anticuboctahedral XII, hexagonal prismatic XII, bicapped hexagonal antiprismatic XIV, pentagonal dodecahedron XX, hexagonal truncated trapezohedron XXIV, hexadecahedron XXVIII, no, unknown} *Definition*: number of other molecular species and shape of polyhedra surrounding the molecular specie in the site. *Ex*: For clathrate hydrates: - tetrahedral IV (H2O), - pentagonal dodecahedron XX (5-12 cage), for type I, II & H clathrates - tetradecahedron/hexagonal truncated trapezohedron XXIV (5-12_6-2 cage), for type I clathrate - hexadecahedron XXVIII (5-12_6-4 cage), for type II clathrate *Reference:* cf. http://en.wikipedia.org/wiki/Coordination_geometry ***Variable: solid in Sample and Matters*** *Note:* add coordinence for substitution and impurities molecular species
*solid*_crystal_molecule_site_specie_occupancy [*phase*_crystal_site_specie_occupancy]	float	SU [m] [V: m]	Solid Miner L5b L6b	VS	~~no~~	Molecular species fractional occupancies of the crystallographic sites of the solid structure ***Variable: solid in Sample and Matters*** *Note:* modify occupancy of main molecular species and add for substitution and impurities molecular species
*solid*_crystal_molecule_site_specie_order [*phase*_crystal_site_specie_order]	enum(text)	U [!o_m] [V: !o_m]	Solid L5b L6b	VS	--	Order of the molecular species in the crystallographic site. Enum: {fixed position, orientationaly disordered, rotating, unknown} *Condition:* mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Notes:* ***Variable: solid in Sample and Matters*** *Condition:* Mandatory when *"solid*_crystal_molecule_site_label" ≠ 'NULL' *Note:* includes the impurities and substitution molecular species

*solid*_crystal_composition_order [*phase*_crystal_composition_order]	enum(text)	SU [m] [V: m]	Solid Miner	VS	--	Type of compositional order in the crystallographic sites of the solid structure Enum: {ordered, disordered, partly ordered, unknown} *Note:* for fundamental solid phases it should be set to 'disordered' ***Variable: solid in Sample and Matters*** *Note:* change order if modified in actual solid, especially by for substitution and impurities molecular/atomic species and replacement atoms
*solid*_crystal_comments [*phase*_crystal_comments]	blob	U [m] [V: m]	Solid	VS	--	Additional information on solid crystal structure and sites ***Variable: solid in Sample and Matters*** Flag 'replace': {yes, no} *Definitions*: see "*mineral*_comments" *Note:* the flag 'replace' allows to control if the comment replace the original one ('yes') or is added to the original one ('no').

Solid properties

*solid*_molar_mass [*phase*_molar_mass]	varchar(255)	S3 [!o_m] [V: m]	Solid	VS	g/mol	Molar mass (value or range) of the solid • provided in 'g/mol' unit *Condition:* Mandatory when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} *Notes:* ⇨ Molar mass is frequently called 'molecular weight' ⇨ range of molar mass for variable solid, solid solutions and n-hydrated solids. No requested value for groups and subgroups. ⇨ a mole of solid is a mole of one 'chemical formula unit'. Its molar mass is determined from its structural or molecular formula. *ex:* '161.7', '160.2 - 162.5' ***Variable: solid in Sample and Matters***

						Note: determined from the actual molecular formula. Different from generic solid species for solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.
*solid*_density [*phase*_density]	varchar(255)	S3 [!o_m] [V: m]	Solid	VS	g/cm3	Density (value or range) of the solid, or average value when variable • provided in 'g/cm^3' unit *Condition:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} *Note:* range of density for variable solid, solid solutions and n-hydrated solids. No requested value for groups and subgroups. *ex:* '2.37', '2.45 - 2.58' ***Variable: solid in Sample and Matters*** *Note:* Different from generic solid species for solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.
Solid thermodynamic properties						
*solid*_state_ntp [*phase*_state_ntp]	enum(text)	S1/S1c [!o_m]	Solid	F	--	State of the solid phase in NTP conditions Enum: {solid, metastable solid - other solid, metastable solid - liquid, other solid, liquid, gas} *Condition:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} *Definitions:* - *'solid':* this solid phase is stable at NTP conditions - *'metastable solid - other solid':* this solid phase can exist at NTP conditions under some conditions but it is outside its thermodynamic stability zone. Another solid phase is stable at NTP conditions. - *'metastable solid - liquid':* this solid phase can exist at NTP conditions under some conditions but it is outside its thermodynamic stability

zone. The liquid phase is stable at NTP conditions.

- *'other solid':* this solid phase cannot exist at NTP conditions but all or some of its constituting species form at least another stable solid phase at NTP conditions
- *'liquid':* this solid phase cannot exist at NTP conditions but all or some of its constituting species are stable in liquid phase at NTP conditions, the other species being stable only in gaseous state.
- *'gas':* neither this solid phase nor any other solid or liquid phases can exist at NTP conditions. The gas is the only stable phase at NTP conditions.

Note: NTP conditions (NIST): 293.15K (20°C), 101.325kPa (1 atm)

Ex:

- 'liquid' for H_2O ice Ih as its melting point is 273.15 K
- 'gas' for solid beta-N_2
- 'liquid' (+gas) for CH_4 clathrate, as only liquid H_2O and gaseous CH_4 exist at NTP
- 'metastable solid - other solid': for CaCO3 'aragonite' (the other solid is calcite)

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solid_phase_transitions	***List [L7]***	[!O]				£: Description of the main phase transitions of the solid *Condition:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid}
*solid*_phase_transition_type [*phase*_phase_transition_type]	enum(text)	U [!o_m]	Solid L7	F	--	Type of phase transition of the solid Enum: {solid-solid, solid-liquid, solid-gas, triple point solid-solid-solid, triple point solid-solid-liquid, triple point solid-liquid-gas, quadruple point, solid decomposition, solid-liquid decomposition} *Notes:* - only the most important transition points need to be given (i.e. triple points, solid-solid and solid-liquid at ambient pressure …) - the phase diagram will be given for the solid polymorphs series with its phase diagram in "*solid*_figures"

*solid*_phase_transition_other_phases [*phase*_phase_transition_phases]	varchar(255)	U [!o_m]	Solid L7	F	-	Name(s) of the other phase(s) implied in the phase transition of the solid *Notes:* - it can be one solid (solid-solid), one liquid (solid-liquid) or two solids (triple point solid-solid-solid) or one solid and one liquid (triple point solid-solid-liquid), or more (quadruple point) - the full name and type of phase should be given *Ex:* 'amorphous Water ice Ia' for Water ice Ic, 'water ice Ih, liquid, gas' for triple point of water
*solid*_phase_transition_temperature [*phase*_phase_transition_temperature]	varchar(255)	U [!o_m]	Solid L7	F	K Pa, bar	Temperature (value(s) or range) of the phase transition of the solid at defined pressure, or average value when variable • temperature should be provided in 'K' unit, with the unit written after the numbers • pressure should be provided in parenthesis after the temperature and in 'Pa' or 'bar' unit (or their (sub-)multiples), with the unit written after the numbers *Notes:* – range of temperature for variable solid. – No requested value for groups and subgroups, solid solutions and n-hydrated solids. *Ex:* '35.4 K (100 mbar)', '273.2 - 273.5 K (100 MPa)', '272.3 K (1 bar) – 275.2 K (100 bar)'
*solid*_phase_transition_comments [*phase*_phase_transition_comments]	blob	U [m]	Solid	F	--	Additional information on solid phase transitions (unknown limits of transition, …)

Solid optical properties

*solid*_refringence_type [*phase*_refringence_type]	enum(text)	S3/S2c [!o_m] [V: m]	Solid Miner	F VS	--	Type of refringence of the solid crystal Enum: {isotropic, uniaxial, biaxial, various, unknown}

Condition: Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series}

Note: depends on the crystalline system of the solid ("*solid*_crystal_system"):

- '*isotropic*' for 'isometric', and 'amorphous'
- '*uniaxial*' for 'trigonal', 'tetragonal' and 'hexagonal'
- '*biaxial*' for 'monoclinic', 'triclinic' and 'orthorhombic'
- '*various*' for 'various'
- '*unknown*' for 'unknown

Note: the refringence type did not change for a solid solution because of identical crystal structure

Note: could be automaticaly determined using "*solid*_crystal_system"

Variable: solid in Sample and Matters

Note: Modified to 'isotropic' in case of glasses or amorphised solids of equivalent uniaxial and biaxial crystalline solids.

*solid*_refringence_sign [*phase*_refringence_sign]	enum(text)	U S [!0_m] [V: m]	Solid Miner	VS F	-- --	Sign of birefringence of the solid crystal

Condition: Mandatory only when "*solid*_classification_level" = {unique solid} AND when "*solid*_refringence_type"={uniaxial}

Enum: {positive, negative, positive or negative, no, unknown}

Note: depends on the type of refringence of the solid crystal ("*solid*_refringence_type") and on the difference between refraction indexes ("*solid*_refraction_index_na" and "_nb")

- '*no*': for 'isotropic' crystals
- sign of $n_\alpha - n_\beta = n_o - n_e$ for uniaxial crystals:
- '*positif*': for biaxial crystals: (always 'positif' by definition)
- '*positif or negatif*': for 'various' (but can be positif if 'various' only include 'monoclinic', 'triclinic' and 'orthorhombic' systems)
- '*unknown*': for unknown sign

Note: when the birefringence sign can change for a uniaxial solid solution or n-hydrated solids, especialy when birefringence is low, it is set to 'positif or

						negatif' ***Variable: solid in Sample and Matters*** *Note:* Do not change for isotropic and biaxial crystals. Only 'positif' or 'negatif' for uniaxial crystals. Can be different from generic solid species for solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Rare changes with impurities molecular/atomic species.
*solid*_birefringence [*phase*_refringence_birefringence]	varchar(255)	U [!o_m] [V: m]	Solid	VS	*no*	Birefringence, Δn, (value or range) of the solid crystal *Condition:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} AND when "*solid*_refringence_type"={uniaxial} *Note:* For isotropic crystals: '0' For uniaxial crystals: $\Delta n = abs(n_\alpha - n_\beta) = abs\ (n_o - n_e)$ For biaxial crystals: $\Delta n = n_\gamma - n_\alpha = n_z - n_x$ *Note:* range of birefringence for variable solid, solid solutions and n-hydrated solids *Ex:* '0.026', '0.056 - 0.083' ***Variable: solid in Sample and Matters*** *Note:* Not mandatory. Exact value for specific solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.
*solid*_refraction_index_na [*phase*_refraction_index_na]	varchar(255)	S3 [!o_m] [V: m]	Solid	VS	*no*	Refraction index, n_α, (value or range) of the solid crystal (isotropic, uniaxial and biaxial crystals) (at 589.3 nm) *Condition:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} *Definition:* Standard refractive index measurements are taken at yellow doublet sodium D line, with a wavelength of 589.29 nm. For uniaxial crystal (birefringence): ordinary indice, n_o, or *w* (optical axe) if

						positive (or positive/negative, or unknown); n_e, or *e* (perpendicular to optical axe) if negative For biaxial crystals (trirefringence): lowest of the 3 ‘n’ values *Note:* range of refraction index for variable solid, solid solutions and n-hydrated solids *Ex:* ‘1.326’, ‘1.456 - 1.583’ ***Variable: solid in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.
*solid*_refraction_index_nb [*phase*_refraction_index_nb]	varchar(255)	S3 [!o_m] [V: m]	Solid	VS	*no*	Refraction index, n_β, (value or range) of the solid (at 589.3 nm) (uniaxial and biaxial crystals) *Condition #1:* Mandatory only when “*solid*_refringence_type” = ‘uniaxial’ or ‘biaxial’ AND *Condition #2:* Mandatory only when “*solid*_classification_level” = {unique solid, variable solid, solid solution series} For uniaxial crystals: extraordinary indice, n_e, or *e* (perpendicular to optical axe) if positive (or positive/negative, or unknown; n_o, or *w* (optical axe) if negative For biaxial crystals: medium ‘n’ value *Note:* range of refraction index for variable solid, solid solutions and n-hydrated solids *Ex:* ‘1.326’, ‘1.456 - 1.583’ ***Variable: solid in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.

*solid*_refraction_index_ng [*phase*_refraction_index_ng]	varchar(255)	S3 [!o_m] [V: m]	Solid	VS	*no*	Refraction index, n_γ, (value or range) of the solid (at 589.3 nm) (biaxial crystals only) *Condition #1:* Mandatory only when "*solid*_refringence_type" = 'biaxial' AND *Condition #2:* Mandatory only when "*solid*_classification_level" = {unique solid, variable solid, solid solution series} For biaxial crystals: highest of the 3 'n' values *Note:* range of refraction index for variable solid, solid solutions and n-hydrated solids *Ex:* '1.326', '1.456 - 1.583' ***Variable: solid in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Minor changes with impurities molecular/atomic species.
*solid*_dispersion_v [*phase*_dispersion_v]	varchar(255)	U [m] [V: m]	Solid	VS	*no*	Abbe V-number (value, range or qualitative information) expressing the visible dispersion of a transparent solid crystal (using n_α) *Definition:* Called 'constringence'. It is defined as $V_D = (n_d-1)/(n_F-n_C)$ using the Fraunhofer lines D, F and C at 587.6 nm (D), 486.1 (F) and 656.3 nm (C). cf wiki: http://en.wikipedia.org/wiki/Abbe_number *Note:* range of dispersion for variable solid, solid solutions and n-hydrated solids *Ex:* '48', '40 - 65' ***Variable: solid in Sample and Matters*** *Note:* Exact value for specific solid solution, n-hydrated solids, or solids with replacement atoms and substitution molecules or atoms. Possible significant changes with impurities molecular/atomic species.

Solid optical aspect

*solid*_pure_color [*phase*_pure_color]	enum(text)	S2 [m]	Solid	F	--	Main color of the pure solid crystals (without any impurity) FreeList: {colorless, white, blue, bluish, azure, green, greenish, emerald, olive, turquoise, yellow, yellowish, orange, pink, pinkish, red, reddish, lilac, violet, indigo, purple, brown, brownish, beige, gray, grayish, black, blackish, bronze, lead, silver, steel, copper, tin, various, …}
*solid*_true_color [*phase*_true_color]	varchar(255)	S2 [m] [V: m]	Solid	VS	--	Color of the solid ***Variable: solid in Sample and Matters*** Actual color of the solid *Note:* *Ex:* 'pale pinkish - green'
*solid*_diaphaneity [*phase*_diaphaneity]	enum(text)	S2 [m] [V: m]	Solid	VS	--	Capacity of the solid to transmit light ***Variable: solid in Sample and Matters*** Capacity of the actual solid to transmit light Enum: {transparent, transparent to translucent, transparent to subtranslucent, transparent to opaque, translucent, translucent to subtranslucent, translucent to opaque, subtranslucent to opaque, opaque, various, unknown} *Definitions*: see "*mineral*_diaphaneity"
*solid*_luster [*phase*_luster]	enum(text)	S2 [m] [V: m]	Solid	VS	--	Description of how and how much the surface of the solid reflects light. ***Variable: solid in Sample and Matters*** Description of how and how much the surface of the actual solid reflects light. Enum: {metallic, submetallic, waxy, vitreous, pearly, silky, greasy, resinous, adamantine, earthy, various, unknown} *Definitions*: see "*mineral*_luster"

Solid references and comments

solid_publications	***List [L7a]***	[O]				£: Publications on the fundamental solid phase and its properties.
*solid*_publication_uid [*] [*phase*_publication_uid]	varchar(255)	U [m]	Solid Publi L7a	F	--	Link to the existing UID of the publications on the solid *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'phase'
solid_links *[phase_links]*	***List [L7b]***	[O]				£: Web page(s) describing the solid species and its properties.
*solid*_link_name [*phase*_link_name]	varchar(255)	U [m]	Solid L7b	F	--	Name of the web page(s) describing the solid and its properties. *Ex:* 'Wikipedia', ('WebMineral, 'MinDat'), …
*solid*_link_url [*phase*_link_url]	CS-varchar(255)	U [m]	Solid L7b	F	--	Link(s) to the web page describing the solid and its properties For those classified as minerals: => http://webmineral.com (Webmineral database) => http://www.mindat.org (MinDat database) => http://rruff.geo.arizona.edu/AMS/amcsd.php (crystallography) *Ex:* 'https://en.wikipedia.org/wiki/Ice#Phases' *Ex:* 'https://en.wikipedia.org/wiki/Dry_ice' *Notes*: - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
*solid*_comments [*phase*_comments]	blob	U [m]	Solid	VS Aj	--	Additional information on solid (possible substitution molecules/atoms, impurities, replacement atoms, …). Occuring in nature (equivalent mineral exists), … ***Variable: solid in Sample and Matters*** Flag 'replace': {yes, no} *Definitions*: see "*mineral*_comments"

Note: the flag ‘replace’ allows to control if the comment replace the original one (‘yes’) or is added to the original one (‘no’).

7. Matters (minerals, rocks, meteorites, natural organics, ...)

7.1 Definition

The ***natural matters*** include all types of solids matters, terrestrials or extraterrestrials, which are collected in natural environments. They can be simple, with a single material composed of a single constituent made of a single mineral phase (pure mineral), or with several materials (collected mixture of minerals or with some impurities from other minerals), or with several simple constituents (rocks made of several mineral phases). But these matters can be more complex mixtures of more or less well defined and numerous constituting materials and constituents (natural organics, meteorites, ...). We also consider here matters being extracts of natural matters, such as organic extracts from meteorites, ...

We distinguish several types of natural matters which have their own keywords table but with, as much as possible, some common keywords [*matter*_xxx_keyword]:

- ☐ Terrestrials
  - Mineral matters
  - Rocks
  - Organics matters (coals, kerogen, ...)
  - Snows and ices
- ☐ Extraterrestrials
  - Meteorites and their Organic extracts
  - Micrometeorites
  - IDPs
- ☐ Planetary
  - Lunar mineral matters
  - …

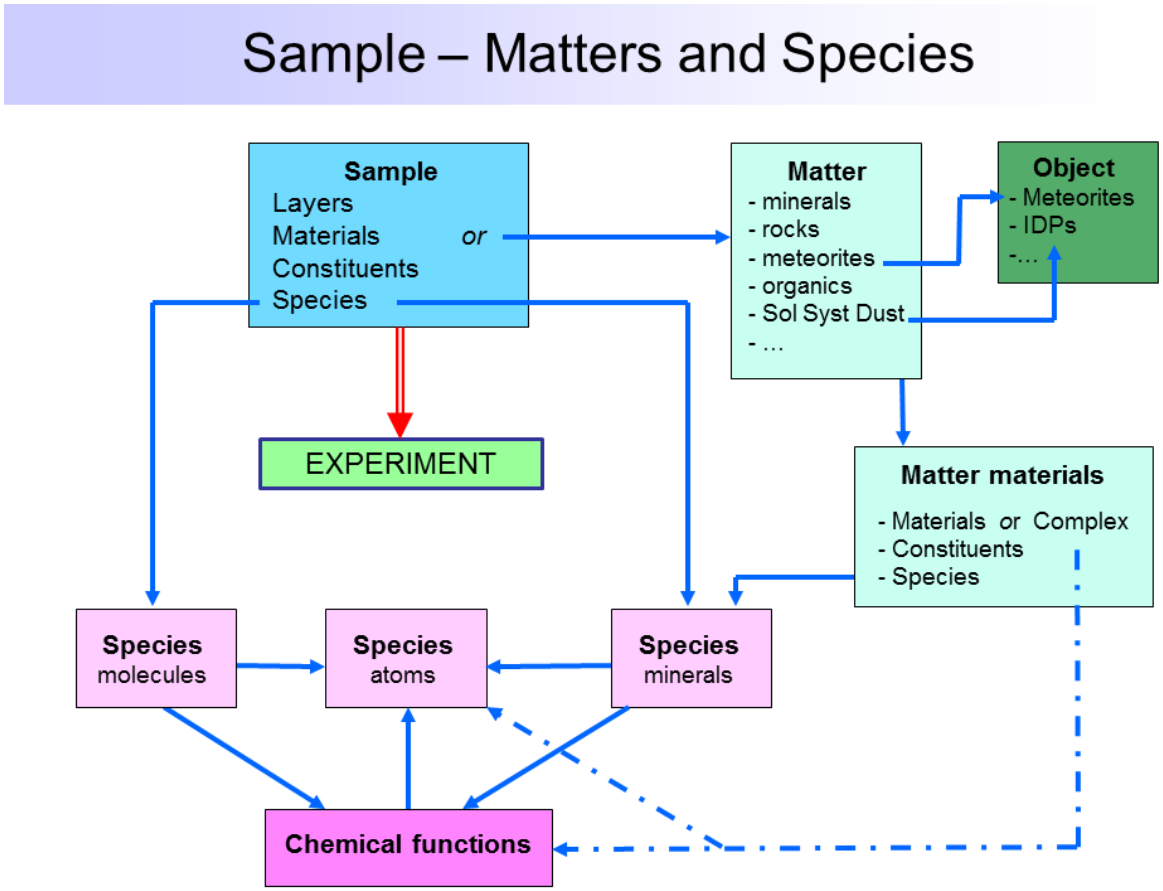
* We define as **Matters** the "***materials***" (or mixtures of materials) that have either a **natural origin** (terrestrial or extraterrestrial) or are produced in a systematic way (**synthetic materials** from laboratory or industry).

They can be ***complex solids*** (organic matters, coal, meteorites, …) natural and synthetics, or ***simple natural materials*** (snow, collected minerals, rocks, …) that have their own origin and "nature controlled" composition and properties.

In most cases (except some rare natural micro-materials such as meteorite particles) they are “basic materials” that can be provided in quantities such that they can be used several times as ***materials*** in various samples. They thus need to have their composition, properties and origin described once and independently of the “experimental samples”.

Synthetic matters are those produced either by chemical or physical processing (by any way) of 'precursor' materials (synthetics or naturals) or of species (molecular, atomic, minerals). These processings create either new species (chemical), or new constituents (physical phases) in the material.

- **Simple synthetic matters** are produced as grains or films (ices, "minerals", coated minerals, ...) that can be fully described in terms of assemblage of individual ***constituents*** made of simple ***species*** (molecules, ions or minerals).
- **Complex synthetic matters** (tholins, ...) are composed of solid pieces (grains, film, ...) of homogeneous composition (same complex constituent(s)) but which can only be characterized by global elemental/chemical composition + other global physical information. They are difficult to characterize at the individual constituent level.
- "**Infamous" synthetic inhomogeneous mixtures** of several grain types (with different complex constituent(s)) or some continuous distribution of them) are similar to a layer made of a mixture of several complex materials. They are difficult to characterize at the matter level by another way than their production method, and by global atomic composition.



Figures 5:Relations between Sample, Matters ans Species

Natural matters are those of terrestrial or extraterrestrial origins.

- **Simple natural matters** are those that are homogeneous and can be described in term of simple ***materials, constituents*** and ***species*** (molecular or minerals). Collected minerals, many rocks (simple assemblage of minerals) and collected natural ices/snows are of such type. Each type of these matters needs some specific description key-words.
- **Complex natural matters** and their extracts (organic extracts, …) cannot be described in term of simple assemblage of constituents and species (molecular or minerals). We also classify here the matters that cannot be described in terms of a simple mixture (more than a few different grains) of simple materials. They need specific classification and description, plus some information on origin. They need their own description key-words (meteorites matter, or natural organic matter in particular).

Several of these matters are linked with geologic ***"objects"*** (e.g. ***extraterrestrial matter*** from a ***meteorite object***).

- Each ***matter*** is defined by *"name and identifiers"*, *"origin", "description and preparation"*, *"composition"* and some *"physical properties"*. The full description of the *composition* of the matters use the "sample" description structure from "materials" to "species".

7.1.1 Fluids (TBD)

7.1.2 Solids, Minerals and rocks

A natural ***mineral matter*** (sample coming from a particular place on Earth) is made either of a single or of multiple major fundamental mineral phases (mineral classification) plus possible additional impurity species mostly mixed at grain level (material) or inside grains (constituents). It is also characterized by its geologic origin, the precise composition of each of its major mineral phases (fully defined mineral, solid solution, n-hydrated mineral, replacement elements, impurities) as well as their crystals shape, size and organization of the crystals (constituents) within the material grains (if multi constituents: hetero polycrystals, coating, crystal inclusions, …).

A ***rock matter*** is considered as a material with several simple constituents which are mostly mineral phases (but there can be some organic inclusion). It is also characterized by its geologic origin, the precise composition of each of its major mineral phases (solid solution, replacement elements, impurities) as well as their crystals shape, size and organization within the rock material (if multi constituents).

Both mineral matter and rock matter can also have an official provider and some unique reference name or code.

Composition and properties of the actual minerals in a mineral or rock matter (for each mineral with composition different from the fundamental mineral phases)

A simplified "sample" structure (linked with its "sample_uid" and with "sample_is_matter" key-word set to 'true') provides the compostion, texture and properties of simple mineral matters and rocks trough possible mixing of mineral phases (plus eventually some organic matter) at the materials (granular mixture) and constituents (polycrystal grains) levels.

The chemical composition of a mineral matter made of one or more "mineral phases" with *variable composition* (mostly solid solution and n-hydrated minerals, but also any other mineral phases including isotopic substitution, replacement elements or important impurities, …) is given by linking to their generic mineral phases and by providing their actual composition ('x' fractions, 'n' hydration number, non-natural isotopic abundances, replacement and impurities atoms) and properties (crystallographic site occupancy, molar mass, density, refraction indexes, color, …) that will override the corresponding 'mean' or 'min' values given in the fundamental 'mineral phases' table (these variable properties are taged 'VM'). But no change is needed for the "fixed composition" mineral phases. In addition the "oxides composition' analysis can be provided, when available (given in "mineral phases" only for fixed composition mineral phases).

Note: (almost) all the variable parameters have to be redefined when "*mineral*_classification_level" = {variable mineral, unique mineral} or "*mineral*_hydration_series" = 'true' (solid solutions and n-hydrated minerals).

Note: For "fixed composition minerals" some properties (color, …) can strongly change without significant composition change (very minor impurities). Only this (and possibly others) property may be changed in such a case and some information of these minor impurities may be given in "*matter_solid*_composition_comments" (but better to describe these impurities by modifying the "atomic composition" of the mineral phases).

Note: Minerals with inserted molecules (H_2O (except n-hydration of minerals), CH_4, NH_3, CO_2, …), such as zeolites, will be described in the "matter_solid_sample" structure as a mineral matter with a constituent composed of a mineral phase and of molecules inserted in cages or in interlayer using "constituent_species_sorption"='insertion' or 'interlayer'**.**

7.1.3 Carbonaceous matters

7.1.4 Extraterrestrial (Meteorites, IDPs, …)

A ***extraterrestrial matter*** will be:

- All raw meteorite pieces, or already prepared sample, received at the lab
  => This will allow to link them with their meteorite object, meteorite piece provider, … and to describe their composition, texture, …
- Any extraterrestrial matter prepared or extracted from one of these raw pieces.
  => They will be linked with its parent 'raw piece' and will have all its preparation procedure described as well as its final composition, texture, …

However a piece of meteorite, or some amount of extraterrestrial matter specifically prepared for a measurement will be described as a "sample". If it is used another time for another experiment then it will be refered either by the same sample (if no change) or as a parent sample if some additional processing is applied to it prior measurement.

A ***extraterrestrial matter*** can be a piece of a meteorite with a quite heterogeneous composition. It is the "global characteristic" of this piece of matter that needs to be described in the Matter table. It is then necessary to describe its constituents (mineral, organics) plus some quantitative information on composition, and then the species that constitute the complex organic constituents (chemical functions and atomic composition). The preparation mode of the piece (before reception and storage: section, coating, …) should be specified here too, but not the preparation of this piece of meteorite (or a smaller piece) during the process of making it a "sample". This needs to be described in the "sample" table (mostly at "material" level). The specific composition of the piece used as a sample should also be described in the sample/material/constituent/matterspecies tables (in particular for microscopic analysis: cf 3.8.3).

A general practice being to ***extract*** some constituents (soluble and insoluble organics, …) from this piece of meteorite (or from a smaller piece) and then to store it for one or more spectroscopic measurements (or other analysis) it is thus necessary also to describe this "extracted matter" in the matter table and give reference to the parent from which it is extracted. So information on the extraction process should be also available here.

There is also the case of very small matter pieces, such as IDPS or Stardust grains, that will make a unique sample. Although they cannot be considered as "a reservoir of matter" (as, e.g. a box of 1 kg of olivine) they must be described in the matter because they are unique and have associated references on their origin, NASA number, …

7.1.5 Matters Tables (fluid matter, solid matter, carbonaceous matter, extraterrestrial matter, planetary matter)

The different types of matter are stored in different DB tables and are imported within <matter_xxx></matter_xxx> tags defined below:

Definitions:

- '*fluid matter'*: natural (from Earth or planetary bodies) or synthetic matter made of molecular liquid or gas, excluding extraterrestrial fluids from meteorite, micrometeorites, IDPs or cosmic dust (asteroidal and cometary dust, …).
- '*solid matter'*: natural (from Earth or planetary bodies) or synthetic matter made of inorganic solids or minerals, including rocks: natural matter made of assemblage of minerals, excluding extraterrestrial minerals from meteorite, micrometeorites, IDPs or cosmic dust.
- '*carbonaceous matter'*: complex natural (from Earth or planetary bodies) or synthetic matter made of organic species or of a carbonaceous macromolecular structure, excluding extraterrestrial carbonaceous materials from meteorite, micrometeorites, IDPs or cosmic dust.
- '*extraterrestrial matter'*: complex extraterrestrial matter made of organics and/or minerals found either on Earth (meteorite, micrometeorites), or collected in Earth atmosphere or in orbit (IDPs), or in interplanetary space (Cosmic dust, …), but excluding planetary bodies (planets, satellites, asteroids, comets, …)
- '*planetary matter'*:

Notes:

- Extraterrestrial minerals, carbonaceous matters, or fluids (when it will be!) extracted from meteorite, micrometeorites, IDPs or cosmic dust will be entrered as "*extraterrestrial matters*"
- Extraterrestrial minerals/rocks, carbonaceous matters, or fluids collected at the surface or in the atmosphere of planetary bodies (planets, satellites, asteroids, comets, TNO, …) will be entered as "*fluid, solid or carbonaceous matters*"
-

7.2 Fluid Matters Table

Root of the table: ***matter_fluid***

Data type: 'Matter'

> *Definition: 'fluid matter'* is any natural (from Earth or planetary bodies) or synthetic matter made of molecular liquid or gas, excluding extraterrestrial fluids from meteorite, micrometeorites, IDPs or cosmic dust (asteroidal and cometary dust, …).

Notes:

- Simple synthetic organic gases and liquids, such as C2H2, C3H8, …, will be entrered as "fluid matters"
- Natural terrestrial organic fluids, such as petroleum and derivatives, will be also preferentiably entrered as "carbonaceous matters"
- Extraterrestrial fluids extracted from meteorite, micrometeorites, IDPs or cosmic dust will be entrered as "extraterrestrial matters"
- Any fluids collected at the surface or in the atmosphere of planetary bodies (planets, satellites, asteroids, comets, TNO, …) will be entered as "Fluid matters"

Key-word	Type	Level	Table	Exp	Unit	Description
Fluid matter import						
*matter_fluid*_import_mode [*matter*_import_mode]	enum(text)	P [!!_m]	MatFluid	(V)	--	Mode of import of the "fluid matter" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*matter_fluid*_xml_filename [-xml] [*matter*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	MatFluid	(V)	--	Name of the storage copy of the xml import file of the "*matter_fluid*" metadata ➔ determined automatically during import (from "*matter_fluid*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Fluid matter indexes						
*matter_fluid*_index [**][-xml] [*matter*_index]	int(10)	B [!!_g]	MatFluid	F	--	Automatic random but unique number (ID) given to new fluid matter

*matter_fluid*_uid [**] [*matter*_uid]	varchar(255)	S0 [!!_m]	MatFluid	F	--	Unique identifier code (UID) given to the fluid matter table (to be created) *Nomenclature:* Create this UID with 'MATFLUID_' and be very accurately formatted in order to be simple and unique • It could be of the style 'MATFLUID_Species_Code_Provider(_AB_yyyymmdd)' (or something similar) where 'Species' is the formula or name of the main species of the fluid, 'Code' some provider or local code (typicaly giving purity), and 'Provider' the provider name or acronym (synthetized commercial) or the lab acronym (synthetized laboratory), and, if relevant, 'AB' are the initials of the person preparing the import, or of the experimentalist, and 'yyyymmdd' is full date of creation of the matter (from *matter_fluid*_date) or the date of the day. *Note*: if several matters are created the same day with the same fluid material(s) then add some distinguishing property after 'Species_Code_Provider'. *Ex:* - MATFLUID_C2H4_N35_AIRLIQUIDE_20081002 - MATFLUID_CH3OH_N25_FISHER_20160205 - MATFLUID_air_atm_dry - MATFLUID_vacuum_ultrahigh *Note:* the Nxy code mean purity of 99.9(x)y% with 'x' the number of '9' and 'y' as the last digit. *Ex:* N28 = 99.8%, N45= 99.995%
matter_fluid_owner_databases	***List [L0]***	[!!]				£: databases which manage this matter
*matter_fluid*_owner_database_uid [*] [*matter*_owner_database_uid]	varchar(255)	S1 [!!o_m]	MatFluid DatBas L0	F	--	Link(s) to the existing UID(s) of the database which owns and manages this matter information *Condition:* at least one database *Note:* For common 'reference' matters and for matters from external laboratories (not managed by a database), it should be 'DB_SSHADE'

Fluid matter experimentalist

matter_fluid_experimentalists	***List [L1]***	[O]				£: experimentalists which prepared the matter
*matter_fluid*_experimentalist_uid [*] [*matter*_experimentalist_uid]	varchar(255)	S1 [m]	MatFluid Exper L1	F	--	Link to the existing UID of the experimentalist(s) which prepared the matter *Condition:* should be no experimentalist when the matter is stored as it is delivered

Fluid matter description

*matter_fluid*_family [-xml] [*matter*_family]	enum(text)	S0 [!!_g]	MatFluid	F	--	Family of the fluid matter Enum: {fluid} *Default* = 'fluid' *Definitions:* - '*fluid'*: matters primarily made of fluid materials
*matter_fluid*_name [*matter*_name]	varchar(255)	S0 [!!_m]	MatFluid	F	--	Common or given name of the fluid matter *Notes:* – It should contain explicit info on the matter and constituting materials/constituent/species: name(s) and some typical properties of the matter (phase type, components, …). – It maybe for exemple the name of the main species in the fluid (if pure, almost pure, or the major component) or a name describing the main species if mixed – It is used as the title of the matter page on the SSHADE interface *Ex:* 'CO2 gas', 'Sulfuric acid', 'Air with 350ppm CO2', *Note DB*: In SSHADE it will be an 'air' with various CO2 and H2O fractions, as well as several 'vacuum' with various molecules impurities, or for different vacuum levels (primary, secondary, ultra-high) but with unknown species.

*matter_fluid*_date [*matter*_date]	date	S1 [!_m]	MatFluid	F	YYYY-MM-DD	Date of creation of the matter *Note:* This date can be the date of collection for natural matters, or of delivery for commercial ones, or of creation for synthetic ones, or of end of processing(s) in the case of a matter generated by processing another one (parent matter). *Note:* general matters such as air or vacuum will have no date.
*matter_fluid*_parent_matter_uid [*] [*matter*_parent_matter_uid]	varchar(255)	S2/S1i [$o_m]	MatFluid MatXxx	F	--	Link to the existing UID of the parent matter (if present in the database) used to create this one by some processing (e.g. thermal cycle, irradiation, sieving, …) *Recommendation:* Strongly recommended when already exist in the database
*matter_fluid*_first_parent_matter_uid [*] [-xml] [*matter*_first_parent_matter_uid]	varchar(255)	S2/S1i [!o_c]	MatFluid MatXxx	F	--	Link to the existing UID of the first parent of the generation of matters (present in the database) that has been initially used to create this one by a series of processes. *Condition:* when "*matter_fluid*_parent_matter_uid" ≠ Φ ➔ calculated recursively using "*matter_fluid*_parent_matter_uid", when it exist
Fluid matter origin						
*matter_fluid*_level [*matter*_level]	enum(text)	S2 [!_m]	MatFluid Matter	F	--	-- Level of the fluid matter Enum: {from sample return mission, from international repository, from laboratory repository, from commercial supplier, local matter, other} *Definitions:* cf. *"matter_solid*_level"
*matter_fluid*_origins	***List [L2]***	[!!]				£: Origins of the fluid matter
*matter_fluid*_origin [*matter*_origin]	enum(text)	S0 [!!_m]	MatFluid Matter L2	F	--	-- Origin of the fluid matter Enum: {natural terrestrial, extraterrestrial, planetary, laboratory, commercial,

simulated}

Definitions: cf. *"matter_solid_*origin"

Note:

- a fluid matter should be predominantly synthetic (laboratory or commercial)
- it may also be mixed with some natural material as long as this material is not the main focus of the matter (e.g. darkening material, dilution material, …)
- it may also be simulated (numerical simulation)

Fluid matter provider

*matter_fluid*_provider [*matter*_provider]	varchar(255)	S2 [!_m]	MatFluid	F	--	--	Provider name of the fluid matter *Note:* industrial/commercial company, individual + laboratory name, ... *Ex:* 'Air Liquide' (Gas factory), 'Catania Observatory, INAF', 'IPAG'
*matter_fluid*_provider_reference_code [*matter*_provider_reference_code]	varchar(255)	S1bs [m]	MatFluid	F	--	--	Reference number or name given by the provider of the fluid matter *Ex: '*CO2 N95 B20'
*matter_fluid*_igsn_code [*matter*_igssn_code]	varchar(255)	S1bs [m]	MatFluid	F	--	--	'International Geo Sample Number'code (*IGSN*) of the fluid matter *Constraint:* only when *"matter_fluid_*origin" = {natural terrestrial, extraterrestrial} *Definition*: The IGSN is an alphanumeric code that uniquely identifies samples from our natural environment and related sampling features (http://www.geosamples.org) *Ex:* 'IEJEN00CH'
*matter_fluid*_igsn_url [-xml] [*matter*_igssn_url]	varchar(255)	SU [!o_c]	MatFluid	F	--	--	url address of the information page for fluid matters with an IGSN code *Condition:* mandatory when "*matter_fluid*_igsn_code" ≠ Ø

							➔ *Calculated* with https://app.geosamples.org/sample/igsn/"*matter_fluid*_igsn_code" *Ex*: 'https://app.geosamples.org/sample/igsn/IEJEN00CH' for IGSN='IEJEN00CH'
*matter_fluid*_local_reference_code [*matter*_local_reference_code]	varchar(255)	S1/S1bs [m]	MatterFluid	F	--	--	Local reference number or name given by local experimentalists to the fluid matter *Ex:* 'CO2-N95-B20_AirLiq'

Natural fluid matter: planetary body

*matter_fluid*_body_uid [*] [-xml] [*matter*_body_uid]	varchar(255)	S1/S1s [!!o_c]	MatterFluid Body	F	--	--	Link to the existing UID of the planetary body from which the natural matter originates *Condition:* absolute mandatory when "*matter_fluid*_origin" = {natural terrestrial, extraterrestrial} ➔ Calculated: ⇨ = 'BODY_planet_Earth' when "*matter_fluid*_origin" = {natural terrestrial} ⇨ = "*matter_fluid*_body_object_uid" / "*object_planetary_body*_uid" when "*matter_fluid*_origin" = {planetary} *Note:* - added in order to be able to set "body" automatically to 'Earth' for 'natural terrestrial' matters who did not have a mandatory 'planetary object') - not used for laboratory, commercial and simulated matters
*matter_fluid*_body_object_uid [*] [*matter*_body_object_uid]	varchar(255)	S1/S1s [!!o_m]	MatterFluid Object	F	--	--	Link to the existing UID of the planetary object from which the natural matter originates *Condition:* absolute mandatory when "*matter_fluid*_origin" = {planetary} *Notes:* see "*matter_solid*_body_object_uid"

*matter_fluid*_body_terrain_type [*matter*_body_terrain_type]	openum(text)	S2 [!o_m]	MatFluid	F	--	--	Type of geological/geophysical terrain on the planetary body where the natural matter is/was situated. OpenEnum: {mineral surface, icy surface, organic surface, liquid surface, mixed surface types, mineral subsurface, icy subsurface, organic subsurface, liquid subsurface, mixed subsurface types, atmosphere, other, unknown} *Condition:* mandatory when *"matter_fluid*_origin" = {natural terrestrial, extraterrestrial} *Definitions:* see *"matter_solid*_body_terrain_type" *Note:* the precise type and location on the planetary body is described in "*matter_fluid*_geolocation_xxx"
*matter_fluid*_body_coordinate_system [*matter*_body_coordinate_system]	openum(text)	U [!o_m]	MatFluid	F	--		Coordinate system on the planetary body of the geographic location of the natural matter OpenEnum: {WGS84, Mars 2000, Moon 2000, Pluto 2015, …} *Condition:* mandatory when "*matter_fluid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Definitions*: see "*experiment*_body_coordinate_system" *Notes*: - Prefer 'Planetocentric latitude with east longitude' coordinate systems approved by the International Astronomical Union - currently only 'WGS84' system for Earth

Natural fluid matter: geolocation

*matter_fluid*_geolocation_place [*matter*_geolocation_place]	varchar(255)	S1b [!o_m]	MatFluid	F	--	--	Geologic source and geographic location on the planetary body of the natural matter (geologic type, place and area names) *Condition:* mandatory when *"matter_fluid*_origin" = {natural terrestrial, extraterrestrial} *Ex:*

						-
*matter_fluid*_geolocation_region [*matter*_geolocation_region]	varchar(255)	S1b [!o_m]	MatFluid	F	--	Region, state, province or county (administrative location) on Earth of the natural matter *Condition:* mandatory and only when "*matter_fluid_body*_uid" = 'BODY_planet_Earth' *Ex:* - 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi' (Earth)
*matter_fluid*_geolocation_country_code [*matter*_geolocation_country_code]	enum(text)	S1b [!o_m]	MatFluid	F	--	2-digit code of the country of the geographic location on Earth of the natural matter Enum: {CH, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory and only when "*matter_fluid*_body_uid" = 'BODY_planet_Earth' *Definitions:* see "*laboratory*_address_country_code"
*matter_fluid*_geolocation_type [*matter*_geolocation_type]	enum(text)	U [!!o_m]	MatFluid	F	--	Type of geographic location the natural matter Enum: {point, line, box, polygon} *Condition:* mandatory when "*matter_fluid*_body_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_fluid*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_geolocation_type"
matter_fluid_geolocation_coordinates [*matter_geolocation_coordinates*]	**List [L3]**	[!O]				£: Geolocation on the planetary body of the natural matter *Condition:* mandatory when "*matter_fluid*_body_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_fluid*_geolocation_type" ≠ Ø

						Conditions: on the number of long/lat couple: see *"experiment*_geolocation_coordinates" *Note*: *Note DB*: will be stored in shapefile format ?
*matter_fluid*_geolocation_coordinate_latitude [*matter*_geolocation_coordinate_latitude]	float	S3 [!o_m]	MatFluid L3	F	deg	Latitude of the geographic location on the planetary body of the natural matter *Format*: in N 'decimal degrees' in "*matter_fluid*_body_coordinate_system" *Condition:* mandatory when "*matter_fluid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_fluid*_geolocation_coordinate_longitude [*matter*_geolocation_coordinate_longitude]	float	S3 [!o_m]	MatFluid L3	F	deg	Longitude of the geographic location on the planetary body of the natural matter *Format*: in E 'decimal degrees' (in the E direction only) in "*matter_fluid*_body_coordinate_system" *Condition:* mandatory when "*matter_fluid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_fluid*_geolocation_coordinate_altitude [*matter*_geolocation_coordinate_altitude]	float	S3 [m]	MatFluid L3	F	m	Altitude of the geographic location on the planetary body of the natural matter *Format*: in 'meter' in "*matter_fluid*_body_coordinate_system" *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*matter_fluid*_geolocation_comments [*matter*_geolocation_comments]	blob	U [m]	MatFluid	F	--	Any additional information or comments about the geolocation of this matter *Ex:* 'matter was collected within 100m of this point', 'very approximate coordinates (+/- 0.1°)'…

Fluid matter images

matter_fluid_images	***List [L4]***	[O]				£: Pictures of the fluid matter

*matter_fluid*_image_filename [*matter*_image]	varchar(255)	U [m]	MatFluid L4	F	--	File name(s) (with extension) of the picture(s) of the fluid matter *Image formats:* .png, .jpg, (.gif) *Note:* could be used to put picture(s) of fluid cylinder or flask, or of the matter from which the fluid has been extracted (natural fluids) *Note:* this file will be imported in the database
*matter_fluid*_image_caption [*matter*_image_caption]	varchar(255)	U [m]	MatFluid L4	F	--	Caption(s) or comment(s) on the picture(s) of the fluid matter

Fluid matter preparation and component types

*matter_fluid*_method [*matter*_method]	varchar(255)	S2 [m]	MatFluid L4	F	--	Method of extraction (natural) or synthesis of the fluid matter *Ex:* 'gas extracted by crushing volcanic glasses', 'isotope enrichment by centrifugation', 'CO2 gas produced by natural coal combustion and separated by filters'
*matter_fluid*_storage_condition [*matter*_storage_condition]	varchar(255)	SU [m]	MatFluid L4	F	--	Storage condition of the fluid matter *Ex:* 'stored at 20°C in 1 bar of pure and dry Ar gas since formation', … *Notes*: see "*matter_solid*_storage_condition"
*matter_fluid*_phase_type [*matter*_phase_type]	enum(text)	S0/S2s [!_m]	MatFluid	F	--	Type of phase of the fluid matter Enum: {liquid, gas} *Note:* if there are several phase types, then give the main here and add a comment in "*matter_fluid*_comments"
matter_fluid_components [*matter_components*]	***List [L5]***	[!]				£: Components type and group of the fluid matter
*matter_fluid*_component_type [*matter*_component_type]	enum(text)	S1 [!_m]	MatFluid L5	F	--	Type of fluid matter Enum: {molecular, ionic, covalent, metallic} *Definitions:*

- ‘*molecular*’: made up of atoms or molecules held together by London dispersion forces, dipole-dipole forces, or hydrogen bonds (ex: N_2, CH_4)
- ‘*ionic*’: made up of positive and negative ions and held together by electrostatic attractions
- ‘*covalent*’: made up of atoms connected by covalent bonds
- ‘*metallic*’: made up of metal atoms that are held together by metallic bonds (ex: mercury)

*matter_fluid*_component_group [*matter*_component_group]	openum(text)	S1 [!_m]	MatFluid L5	F	--	Group of fluid matter (type of ‘mixture’) OpenEnum: {pure, mixture, solution, alloy, emulsion, suspension, colloid, …} *Definitions:* – ‘*pure*’: one single type of atom, molecule, … (all) – ‘*mixture*’: simple homogeneous mixture without any special interactions between components (gas, liquid) – ‘*solution*’: homogeneous mixture (1 phase) of a solvent and a solute (liquid) – ’*alloy*’: mixture or metallic solid solution composed of two or more elements (liquid metal) – ‘*emulsion*’: heterogenous mixture (several phases) of two or more liquids that are normally immiscible (liquid) – ‘*suspension*’: heterogenous mixture (several phases) containing solid or liquid particles that are sufficiently large for sedimentation (gas, liquid). Particles have diameters > 1 µm (note: for gas it is called an aerosol) – ‘*colloid*’: substance (phase) microscopically dispersed throughout another substance (phase). Particles have diameters ~1 - 1000 nm
*matter_fluid*_components_comments [*matter*_components_comments]	blob	U [m]	MatFluid	F	--	Additional comments on the component(s) of the fluid matter

Fluid matter global density

*matter_fluid*_density [*layer/matter*_density]	float	U [m]	MatFluid	F	g/cm3	Density of the fluid matter • stored in the database and provided to user in 'g/cm^3' unit *Note:* value of the raw matter before any preparation for sample
*matter_fluid*_density_error [*layer/matter*_density_error]	float	U [m]	MatFluid	F	g/cm3	Absolute uncertainty on the density of the fluid matter • stored in the database and provided to user in 'g/cm^3' unit
*matter_fluid*_texture_comments [*matter*_texture_comments]	blob	U [m]	MatFluid	F	--	Any information or comments about the texture of the fluid matter *Note:* this replace the « global texture » block presents in all the other solid matter tables (grain_size/_texture, …) *Ex:* viscous fluid with micron sized iron particles, non-newtonian fluid, …

Fluid matter composition

Note: Whatever are the materials, gas or liquid, that constitute the matter they will be always defined from the "material" level (link(s) with "*matter_fluid*_material_index") through their "constituents" and "species", or through other matter(s). Only their type of mixing is described here.

*matter_fluid*_materials_mixing [+] enum(text) [*matter*_materials_mixing]		S2 [!_m]	MatFluid	F	--	How the different materials are mixed in the fluid matter Enum: {single material, homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, spatial distribution...} *Definitions:* cf. "*layer*_materials_mixing" *Note:* for fluid it will be generally one 'single material' and one constituent
*matter_fluid*_materials_number [+][-xml] [*matter*_materials_number]	int(10)	U [!_c]	MatFluid	F	*no*	Number of different materials mixed in the fluid matter ➔ calculated from " *matter_fluid*_materials" list
matter_fluid_matters	***List [L6a]***	[!]				£: matters constituting this fluid matter
*matter_fluid*_matter_index [*][-xml] [*matter*_matter_index]	int(10) [Internal link]	B/S1 [!_g]	Matfluid MatXxx	F	--	ID of the matters(s) constituting the 'fluid matter' *Note xml:* in practice the description of the material(s) is done directly under

			L6a			"*matter_fluid*" without providing the ID link

➢ Same structure as "*sample*"

matter_fluid_materials	***List [L6b]***	[!]				£: materials constituting this fluid matter
*matter_fluid*_material_index [*][-xml] [*matter*_material_index]	varchar(255) [Internal link]	B/S1 [!_g]	MatFluid Mater L6b	F	--	ID of the material(s) constituting the 'fluid matter' *Notes:* – for fluids there is generally one material and one constituent (except when there are particles in suspension in the fluid: colloids). The different fundamental liquid phases composing the fluid matter are linked inside this matter-materials structure at the basic constituent level. – the modifications of the liquid parameters (VL in 'liquid' phases) (composition and properties) are also described at the constituent level *Note:* ID determined automatically during import *Note xml:* in practice the description of the matter- material(s) is done directly under "matter" without providing the ID link

➢ Same structure as "*sample*"

*matter_fluid*_comments [*matter*_comments]	blob	U [m]	MatFluid	F	--	Additional information on the fluid matter (minor impurities, …) or comments on the composition and formula of the species composing the fluid matter

Precursor materials

Note: "*material*_is_precursor" = 'true'

Note: refer to the same table as "*materials*" in the sample structure but without the "material arrangement and abundance" bloc

See definitions and notes in "*Mineral matter*"

matter_fluid_precursor_materials *[matter_precursor_materials]*	***List [L7]***	S2 [O]	Mater PreMater L7			£: Precursor materials used to create the fluid matter *Condition:* description of precursor materials is optional.

➢ Use exactly the same structure as for "*Mineral matter*"

Fluid matter processings:

matter_fluid_processings [*matter_processings*]	***List [L8]***	[O]	MatFluid L8			£: Processing steps of the precursor materials/matters *Condition:* only when there is processing of materials or parent matter/sample

- Use exactly the same structure as for "*Mineral matter*"

Fluid matter documentation and references

matter_fluid_documentations	***List [L9]***	[O]				£: Documentations about the fluid matter
*matter_fluid*_documentation_name [*matter*_documentation_name]	varchar(255)	U [m]	MatFluid L9	F	--	Name of the documentation describing the fluid matter *Note:* this name will appear as the documentation title in the interface *Ex:* 'Specifications of liquid C3H4 purity'
*matter_fluid*_documentation_filename [*matter*_documentation_filename]	varchar(255)	U [m]	MatFluid L9	F	--	File name (with extension) of the documentation describing the fluid matter *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database
matter_fluid_links	***List [L10]***	[O]				£: Web pages describing the fluid matter and its properties
*matter_fluid*_link_name [*matter*_link_name]	varchar(255)	U [m]	MatFluid L10	F	--	Name of the web page(s) describing the fluid matter and its properties. *Ex:* 'Air Liquide', 'Sigma Aldrich', …
*matter_fluid*_link_url [*matter*_link_url]	CS-varchar(255)	U [m]	MatFluid L10	F	--	URL address(es) of web page(s) describing the fluid matter and its properties *Note:* usefull only when the fluid matter comes from a stable commercial supplier, or an individual/laboratory providing information on a web page (gas extracts, synthesis method, …) *Notes*: - can also link to various types of measurements made on this matter - you can link to a publication by giving its url address, preferably through its DOI.

						Ex: https://doi.org/10.1002/ejic.200700067
matter_fluid_publications	***List [L11]***	[O]				£: Publications describing the fluid matter and its properties.
*matter_fluid*_publication_uid [*] [*matter*_publication_uid]	varchar(255)	S2 [m]	MatFluid Publi L11	F	--	Link to the existing UID of the publications describing the fluid matter and its properties. *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

7.3 Solid Matters Table

Root of the table: ***matter_solid***

Data type: 'Matter'

Definition: 'solid matter' is any natural (from Earth or planetary bodies) or synthetic matter made of inorganic solids or minerals, including rocks: natural matter made of assemblage of minerals , excluding extraterrestrial minerals from meteorite, micrometeorites, IDPs or cosmic dust (asteroidal and cometary dust, …).

Notes:

- Mineral, rocks and synthetic inorganic solids will be entered as "solid matters"
- Natural and synthetic snows and ices will be entered as "solid matters"
- Carbonaceous mineral matters (carbon, anthracite, lignite, …) will be preferentiably entrered as "carbonaceous matters" as the KW are more adapted.
- Organic minerals (such as amber) and organic molecular solids, will be also preferentiably entrered as "carbonaceous matters"
- Extraterrestrial minerals extracted from meteorite, micrometeorites, IDPs or cosmic dust will be entrered as "extraterrestrial matters"
- Any minerals/rocks collected at the surface or in the atmosphere of planetary bodies (planets, satellites, asteroids, comets, TNO, …) will be entered as "Solid matters"

Key-word	Type	Level	Table	Exp	Unit	Description
Solid matter import						
*matter_solid*_import_mode [*matter*_import_mode]	enum(text)	P [!!_m]	MatSol	F	--	Mode of import of the "solid matter" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*matter_solid*_xml_filename [-xml] [*matter*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	MatSol	(V)	--	Name of the storage copy of the xml import file of the "*matter_solid*" metadata ➔ determined automatically during import (from "*matter_solid*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction

Solid matter indexes

*matter_solid*_index [**][-xml] [*matter*_index]	int(10)	B [!!_g]	MatSol	F	no	Automatic random but unique number (ID) given to new solid matter
*matter_solid*_uid [**] [*matter*_uid]	varchar(255)	S0/S1 [!!_m]	MatSol	F	--	Unique identifier code (UID) given to the solid matter table (to be created) *Nomenclature:* Create this UID with 'MATSOL_' for synthetic solids or 'MATMIN_' for minerals It should be of the style: - 'MATSOL_SolidMatter_AB_yyyymmdd' where 'SolidlMatter' is the matter name (part of "*matter*_solid_name") or main solid name, - 'MATMIN_MineralMatter_AB_yyyymmdd' where 'MineralMatter' is the matter name (part of "*matter*_solid_name") or main mineral name, - and where 'AB' are the initials of the person preparing the import, or of the experimentalist preparing the matter (*experimentalist*_acronym of *matter_solid*_experimentalist), 'yyyymmdd' is full date of creation of the matter (from "*matter_solid*_date") or the date of the day. *Note*: if several matters are created the same day with the same solid material(s) then add some distinguishing property after 'Mineral/SolidMatter'. *Ex:* - MATSOL_Snow-Chamrousse_BS_20170105 - MATMIN_SWy2_25-50_BS_20131003, - MATMIN_Portlandite_96_AG_20130828 - MATMIN_Basalt-Moon_BS_20130828
matter_solid_owner_databases	***List [L0]***	[!!]				£: databases which manage this matter
*matter_solid*_owner_database_uid [*] [*matter*_owner_database_uid]	varchar(255)	S1 [!!o_m]	MatSol DatBas L0	F	--	Link(s) to the existing UID(s) of the database which owns and manages this matter information *Condition:* at least one database *Note:* For common 'reference' matters and for matters from external

						laboratories (not managed by a database), it should be ‘DB_SSHADE’
Solid matter experimentalist						
matter_solid_experimentalists	***List [L1]***	[O]				£: experimentalists who prepared the matter
*matter_solid*_experimentalist_uid [*] [*matter*_experimentalist_uid]	varchar(255)	S1 [m]	MatSol Exper L1	F	--	Link to the existing UID of the experimentalist(s) which prepared the matter *Condition:* can be no experimentalist when the matter is stored as it is delivered
Solid matter description						
*matter_solid*_family [*matter*_family]	enum(text)	S0/S1s [!!_m]	MatSol	F	--	Family of the solid matter Enum: {solid, mineral} *Definitions:* - ‘*solid’*: matters made of different types of synthetic solids - ‘*mineral’*: matters made primarily with natural minerals
*matter_solid*_name [*matter*_name]	varchar(255)	S0/S1 [!!_m]	MatSol	F	--	Common or given name of the solid matter *Notes:* – It should contain explicit info on the matter and constituting materials/constituent/species: name(s) and some typical properties of the matter (phase type, components, …). – It may be the name of the main solid (if pure, almost pure, or the major component) or a name describing the main solid components if mixed – the names of glasses will be that of the equivalent solid followed by 'glass' – It is used as the title of the matter page on the SSHADE interface *Ex:* ‘Olivine’, Smectite SWy-2’, ‘Smectite with Quartz and Feldspar’, … *Ex:* 'forsterite glass'

*matter_solid*_date [*matter*_date]	date	S1 [!_m]	MatSol	F	YYYY-MM-DD	Date of creation of the matter *Note:* This date can be the date of collection or delivery for natural matters, or of creation for synthetic ones, or of end of processing(s) in the case of a matter generated by processing another one (parent matter).
*matter_solid*_parent_matter_uid [*] [*matter*_parent_matter_uid]	varchar(255)	S2/S1i [$o_m]	MatSol MatXxx	F	--	Link to the existing UID of the parent matter (if present in the database) used to create this one by some processing (e.g. thermal cycle, irradiation, sieving, …) *Recommendation:* Strongly recommended when already exist in the database *Ex:* a granular matter sieved to a specific grain size range gives a daughter matter from the parent unsieved matter.
*matter_solid*_first_parent_matter_uid [*] [-xml] [*matter*_first_parent_matter_uid]	varchar(255)	S2/S1i [!o_c]	MatSol MatXxx	F	--	Link to the existing UID of the first parent of the generation of matters (present in the database) that has been initially used to create this one by a series of processes. *Condition:* when "*matter_solid*_parent_matter_uid" ≠ Φ ➔ calculated recursively using "*matter_solid*_parent_matter_uid", when it exist
Solid matter origin						
*matter_solid*_level [*matter*_level]	enum(text)	S2 [!_m]	MatSol	F	--	Level of the solid matter Enum: {from sample return mission, from international repository, from laboratory repository, from commercial supplier, local matter, other} *Definitions:* - '*from sample return mission*': extraterrestrial matter collected during a space mission, returned to Earth and stored in an official repository and distributed. *Ex*: 'Apollo 15, 15040 soil at Johnson Space Center /NASA' - '*from international repository'*: natural terrestrial matter collected in large amount and stored in an official repository and widely

distributed.

Ex: 'Johnson Space Center JSC Mars-1 simulant', 'Coals repository at Pittsburgh Mining Technology Center', 'source clays of Clay Mineral Society repository', 'meteorite from MNHM', …

- '*from laboratory repository'*: natural or synthetic matter collected or synthesized in substantial amount by a laboratory and stored in a local repository and distributed more or less widely.

  Ex: '2% CH4 tholins at LATMOS'
- '*from commercial suppliers'*: mostly synthetic matter provided by a commercial supplier,

  Ex: 'CH4 gas bottle', 'Natrite, Merck Co'
- *'local matter':* natural or synthetic matter collected or synthesized for local use only (not shared with other laboratories). Includes matters measured on the field.
- '*other*': any other types of matter

Note: for the 4 first cases the repository or supplier should be given in "*matter_solid*_provider"

---

*matter_solid*_origins	***List [L2]***	[!!]						£: Origins of the solid matter
*matter_solid*_origin [*matter*_origin]	enum(text)	S0/S1s [!!_m]	MatSol L2	F	F	--	--	Synthetic origin of the solid matter Enum: {natural terrestrial, extraterrestrial, planetary, laboratory, commercial, simulated} *Definitions:* - *'natural terrestrial'*: natural matter (mineral, rock, snow-ice, organic, …) colleted on Earth - *'extraterrestrial'*: extraterrestrial matter collected on Earth (meteorite, micrometeorite, IDP). - *'planetary'* extraterrestrial matter (planetary soil, rock or grains, …) collected on or around planetary bodies (planets, satellites, comets, asteroids, …) and in the interplanetary space. - *'laboratory'*: non-natural solid matter experimentally synthesized in a laboratory (well or relatively well-known synthesis process) - *'commercial'*: non-natural solid matter synthesized by a chemical

company (less or no knowledge on the synthesis process)
- *'simulated'*: fictive matter defined for a numerical simulation

Note:
- a solid matter should be predominantly synthetic (laboratory or commercial),
- it may also be mixed with some natural material as long as this material is not the main focus of the matter (e.g. darkening material, dilution/matrix material, …)
- it may also be simulated (numerical simulation)

Solid matter provider

*matter_solid*_provider [*matter*_provider]	varchar(255)	S2 [!_m]	MatSol Miner	F	F	--	--	Name, address, … of the provider of the solid matter *Note:* Mineral repository, commercial company, individual + laboratory name, ... *Ex:* 'Clay Mineral Society' (Mineral repository)
*matter_solid*_provider_reference_code [*matter*_provider_reference_code]	varchar(255)	S1/S1bs [m]	MatSol Miner	F	F	--	--	Reference number or name given by the provider of the solid matter *Ex:* 'SWy-2'
*matter_solid*_igsn_code [*matter*_igssn_code]	varchar(255)	S1/S1bs [m]	MatSol Miner	F	F	--	--	'International Geo Sample Number'code (*IGSN*) of the solid matter *Constraint:* only when *"matter_solid*_origin" = {natural terrestrial, extraterrestrial} *Definition*: The IGSN is an alphanumeric code that uniquely identifies samples from our natural environment and related sampling features (http://www.geosamples.org) *Ex:* 'IEJEN00CH'
*matter_solid*_igsn_url [-xml] [*matter*_igssn_url]	varchar(255)	SU [!o_c]	MatSol Miner	F	F	--	--	url address of the information page for solid matters with an IGSN code *Condition:* mandatory when "*matter_solid*_igsn_code" ≠ Ø

							➔ *Calculated* with https://app.geosamples.org/sample/igsn/"*matter_solid*_igsn_code" *Ex*: 'https://app.geosamples.org/sample/igsn/IEJEN00CH' for IGSN='IEJEN00CH'
*matter_solid*_local_reference_code [*matter*_local_reference_code]	varchar(255)	S1/S1bs [m]	MatSol Miner	F	F	--	--	Local reference number or name given by local experimentalists to the solid matter *Ex:* 'Smectite SWy-2 - CMS'

Natural solid matter: planetary body

*matter_solid*_body_uid [*] [-xml] [*matter*_body_uid]	varchar(255)	S1/S1s [!!o_c]	MatSol Miner Body	F	F	--	--	Link to the existing UID of the planetary body from which the natural matter originates *Condition:* absolute mandatory when *"matter_solid*_origin" = {natural terrestrial, extraterrestrial} ➔ Calculated: ⇨ = 'BODY_planet_Earth' when "*matter_solid*_origin" = {natural terrestrial} ⇨ = *"matter_solid*_body_object_uid" / "*object_planetary*_body_uid" when *"matter_solid*_origin" = {planetary} *Note:* - added in order to be able to set "body" automatically to 'Earth' for 'natural terrestrial' matters who did not have a mandatory 'planetary object') - not used for laboratory, commercial and simulated matters
*matter_solid*_body_object_uid [*] [*matter*_body_object_uid]	varchar(255)	S1/S1s [!!o_m]	MatSol Miner Object	F	F	--	--	Link to the existing UID of the planetary object from which the natural matter originates *Condition:* absolute mandatory when *"matter_solid*_origin" = {planetary} *Notes:* - it is the "*object_planetary*_uid"

- the use of "*object_planetary*" to describe the collection on the planetary body is absolute mandatory for extraterrestrial matters collected on another planetary body than Earth.
- extraterrestrial matters collected on Earth (meteorites, micrometeorites, IDPs) should use "*matter_extraterrestrial*"
- natural terrestrial matters collected on Earth generally do not use an "*object_planetary*" to describe the collection, but it can.

*matter_solid*_body_terrain_type [*matter*_body_terrain_type]	openum(text)	S2 [!o_m]	MatSol	F	F	--	--

Type of geological/geophysical terrain on the planetary body where the natural matter is/was situated.

OpenEnum: {mineral surface, icy surface, organic surface, liquid surface, mixed surface types, mineral subsurface, icy subsurface, organic subsurface, liquid subsurface, mixed subsurface types, atmosphere, other, unknown}

Condition: mandatory when *"matter_solid*_origin" = {natural terrestrial, extraterrestrial}

Definitions:

- '*mineral surface'*: situated at a predominantly mineral surface or close surface (sand desert, salty lake, everywhere on Mars and Moon, …)
- '*icy surface'*: situated a predominantly icy surface or close surface (e.g. snow covered surface, icy satellite surfaces, …)
- '*organic surface'*: situated a predominantly organic surface or close surface (e.g. tholins surface, comet surface, vegetation surface, …)
- '*liquid surface'*: situated a predominantly liquid surface or close surface (e.g. lake surface, river, Titan lakes, …)
- lake bottom, ocean, …)
- '*mixed surface types'*: mix of the above surface types
- '*mineral subsurface'*: situated in a predominantly mineral subsurface
- '*icy subsurface'*: situated in a predominantly icy subsurface (e.g. in polar cap, …)
- '*organic subsurface'*: situated in a predominantly organic subsurface (e.g. coal mine, hydrocarbon reservoir, …)
- '*liquid subsurface'*: situated in a predominantly liquid subsurface (e.g.
- '*mixed subsurface types'*: mix of the above subsurface types
- '*atmosphere'*: situated in the atmosphere

						- ‘*other*’: any other terrain type - ‘*unknown*’: unknown terrain type! *Note:* the precise type and location on the planetary body is described in “*matter_solid*_geolocation_xxx”
*matter_solid*_body_coordinate_system [*matter*_body_coordinate_system]	openum(text)	U [!o_m]	MatSol	F	--	Coordinate system on the planetary body of the geographic location of the natural matter OpenEnum: {WGS84, Mars 2000, Moon 2000, Pluto 2015, …} *Condition:* mandatory when “*matter_solid*_body_uid” / “*body*_family” = {planet, dwarf planet, satellite} *Definitions*: see “*experiment*_body_coordinate_system“ *Notes*: - Prefer 'Planetocentric latitude with east longitude’ coordinate systems approved by the International Astronomical Union - currently only ‘WGS84’ system for Earth

Natural solid matter: geolocation

*matter_solid*_geolocation_place [*matter*_geolocation_place]	varchar(255)	S1b [!o_m]	MatSol	F	--	--	Geologic source and geographic location on the planetary body of the natural matter (geologic type, place and area names) *Condition:* mandatory when *“matter_solid*_origin” = {natural terrestrial, extraterrestrial} *Ex:* - ‘Center of a convection cell, South part of Sputnik Planitia’ (Pluto) - ‘Armstrong crater, Mare Tranquilitatis’ (Moon), - ‘east side of Ploskaya Mt, Western Keivy Massif, Kola Peninsula’ (Earth) - ‘volcanic flow 1 km SW from crater rim, Etna volcano’ (Earth)
*matter_solid*_geolocation_region [*matter*_geolocation_region]	varchar(255)	S1b	MatSol	F	--		Region, state, province or county (administrative location) on Earth of the natural matter

		[!o_m]				*Condition:* mandatory and only when "*matter_solid_body*_uid" = 'BODY_planet_Earth' *Ex:* - 'Murmanskaja Oblast', 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi' (Earth)
*matter_solid*_geolocation_country_code [*matter*_geolocation_country_code]	enum(text)	S1b [!o_m]	MatSol	F	--	2-digit code of the country of the geographic location on Earth of the natural matter Enum: {CH, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory and only when "*matter_solid_body*_uid" = 'BODY_planet_Earth' *Definitions:* see "*laboratory*_address_country_code"
*matter_solid*_geolocation_type [*matter*_geolocation_type]	enum(text)	U [!!o_m]	MatSol	F	--	Type of geographic location of the natural matter Enum: {point, line, box, polygon} *Condition:* mandatory when "*matter_solid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_solid*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_geolocation_type"
matter_solid_geolocation_coordinates [*matter_geolocation_coordinates*]	**List [L3]**	[!o]				£: Geolocation on the planetary body of the natural matter *Condition:* mandatory when "*matter_solid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_solid*_geolocation_type" ≠ Ø *Conditions:* on the number of long/lat couple: see *"experiment*_geolocation_coordinates"

						Note DB: will be stored in shapefile format ?
*matter_solid*_geolocation_coordinate_latitude [*matter*_geolocation_coordinate_latitude]	float	S3 [!o_m]	MatSol L3	F	deg	Latitude of the geographic location on the planetary body of the natural matter *Format*: in N 'decimal degrees' in "*matter_solid*_body_coordinate_system" *Condition:* mandatory when "*matter_solid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_solid*_geolocation_coordinate_longitude [*matter*_geolocation_coordinate_longitude]	float	S3 [!o_m]	MatSol L3	F	deg	Longitude of the geographic location on the planetary body of the natural matter *Format*: in E 'decimal degrees' (in the E direction only) in "*matter_solid*_body_coordinate_system" *Condition:* mandatory when "*matter_solid_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_solid*_geolocation_coordinate_altitude [*matter*_geolocation_coordinate_altitude]	float	S3 [m]	MatSol L3	F	m	Altitude of the geographic location on the body of the natural matter *Format*: in 'meter' in "*matter_solid*_body_coordinate_system" *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*matter_solid*_geolocation_comments [*matter*_geolocation_comments]	blob	U [m]	MatSol	F	--	Any additional information or comments about the geolocation of this matter *Ex:* 'matter was collected within 100m of this point', 'very approximate coordinates (+/- 0.1°)'…

Solid matter images

matter_solid_images	***List [L4]***	[O]				£: Pictures of the solid matter
*matter_solid*_image_filename [*matter*_image]	varchar(255)	U [m]	MatSol L4	F	--	File name(s) (with extension) of the picture(s) of the solid matter *Image formats:* .png, .jpg, (.gif)

						Note: this file will be imported in the database
*matter_solid*_image_caption [*matter*_image_caption]	varchar(255)	U [m]	MatSol L4	F	--	Caption(s) or comment(s) on the picture(s) of the solid matter
Solid matter preparation and component types						
*matter_solid*_preparation [*matter*_preparation]	enum(text)	S1 [!_m]	MatSol	F	--	Type of preparation of the solid matter Enum: {raw, section, polished section, selected components, sieved fraction, extracted components} *Definitions:* - '*raw'*: piece of rock or without chemical treatment nor selection of a particular component nor other type of preparation (cutting, polishing, …) - '*section*': raw solid/rock (or mineral grain) cut and potentially polished by different ways - '*selected components'*: peculiar petrologic entity (specific mineral, ...) selected mechanically without any chemical treatment - '*sieved fraction'*: size fraction separated by sieving - '*extracted components'*: mineral/solid phase(s) extracted using a chemical or physical treatment
*matter_solid*_method [*matter*_method]	varchar(255)	S2 [m]	MatSol Miner	F	--	-- Method of extraction of this (natural) mineral matter or synthesis of this solid matter *Ex:* 'mineral mixture extracted by crushing and sieving granite rock extracted with geologic hammer', 'rock collected at foot of cliff', …
*matter_solid*_storage_condition [*matter*_storage_condition]	varchar(255)	SU [m]	MatSol Miner	F	--	-- Storage condition of this solid matter *Ex:* 'stored at 20°C in 1 bar of pure and dry Ar gas since formation', … *Notes*: – avoid to use for common 'international matters' as each laboratory may store their matter differently. – you can use "*matter*_comments" in sample to provide this information

						or to alter it.
*matter_solid*_phase_type [*matter*_phase_type]	enum(text)	S0/S2s [!_m]	MatSol	F	--	Type of phase of the solid matter Enum: {solid, liquid, gas} *Note:* if there are several phase types, then give the main here and add a comment in "*matter_solid*_comments"
matter_solid_components [*matter_components*]	***List [L5]***	[!]				£: Components type and group of the mineral matter
*matter_solid*_component_type [*matter*_component_type]	enum(text)	S1 [!o_m]	MatSol L5	F	--	Type of the component in the mineral matter Enum: {mineral, igneous rock, metamorphic rock, sedimentary rock, superficial deposit, magmatic ice, sedimentary ice, metamorphic ice} *Condition:* Mandatory and only when "*matter_solid*_origin" = {natural terrestrial, planetary} *Definitions:* – '*mineral*': – '*igneous rock'*: – '*metamorphic rock'*: – '*sedimentary rock'*: – '*superficial deposits'*: – '*magmatic ice'*: ice formed by direct cristallization of large bodies of liquid water. Includes sea ice, lake and river ice, ... – '*sedimentary ice'*: ice formed in the atmosphere and sedimenting on the surface, or formed by direct condensation on the surface. Includes, snow, hail ice, rime ice, frost – '*metamorphic ice'*: magmatic or sedimentary ice that was subjected to high pressure or temperature. Includes mantle ice, glacier ice, firn ice
*matter_solid*_component_group [*matter*_component_group]	openum(text)	S1 [!o_m]	MatSol L5	F	--	Group of the component in the mineral matter OpenEnum: {native element, non-silicate mineral, silicate mineral, organic

mineral, carbonatite, melilitic rock, kalsilitic rock, kimberlite, lamproite, leucitic rock, lamprophyre, plutonic rock (coarse-grained crystalline rock), volcanic rock (fine-grained crystalline rock), pyroclastic rock or sediment, tuffite, volcaniclastic sedimentary rock or sediment, sedimentary protolith, volcaniclastic protolith, igneous protolith, unknown protolith, brocken and reconstituted rock, metasomatic and hydrothermal rock, siliciclastic sediment, carbonate sediment, phosphate-sediment or phosphorite, iron-sediment or ironstone, organic-rich sediment, non-carbonate salt, non-clastic siliceous sediment, miscellaneous oxide and hydroxide and silicate sediment, hybrid sediment, sediment with volcaniclastic debris, mass movement deposit, residual deposit, aeolian deposit, organic deposit, biological deposit, chemical deposit, alluvial deposit, lacustrine deposit, coastal deposit, marine deposit, proglacial deposit, glacigenic deposit, lunar basaltic regolith sediment, lunar anorthositic regolith sediment, asteroidal regolith, organic-rich cometary regolith, sea ice, lake and river ice, ground ice, icicle, snow, atmospheric ice, rime ice, frost, mantle ice, glacier ice, firn ice, complex mix, other, unknown}

Condition: Mandatory and only when "*matter_solid_*origin" = {natural terrestrial, planetary}

Definitions:

For 'mineral':

- 'native element': Dana major class: I, Strunz class: 1
- 'non-silicate mineral': Dana major class: II to VII, Strunz class: 2 to 8
- 'silicate mineral': Dana major class: IX, Strunz class: 9
- 'organic mineral': Dana major class: VIII, Strunz class: 10

For 'igneous rock':

- 'carbonatite': contains more than 50% modal primary carbonate
- 'melilitic rock': contains more than 10% modal melilite
- 'kalsilitic rock': contains more than 10% modal kalsilite
- 'kimberlite': volatile-rich (dominantly CO_2), potassic, ultrabasic rock with common distinctive inequigranular texture.
- 'lamproite': presence of widely variable amounts (5-90 vol.%) of Al_2O_3-poor titanian phlogopite, titanian tetraferriphlogopite, titanian potassic richterite, forsteritic olivine, Al_2O_3-poor Na_2O-poor

diopside, Fe-rich leucite, Fe-rich sanidine (TBD)
- ‘leucitic rock’: see QAPF diagram
- ‘lamprophyre’:
- ‘plutonic rock (coarse-grained crystalline rock)’: plutonic rock (IUGS)
- ‘volcanic rock (fine-grained crystalline rock)’: volcanic rock (IUGS)
- ‘pyroclastic rock or sediment’:
- ‘tuffite’:
- ‘volcaniclastic sedimentary rock or sediment’:

For ‘metamorphic rock’:
- sedimentary protolith,
- volcaniclastic protolith,
- igneous protolith,
- unknown protolith,
- brocken and reconstituted rock,
- metasomatic and hydrothermal rock

For ‘sedimentary rock’:
- siliciclastic sediment,
- carbonate sediment,
- phosphate-sediment or phosphorite,
- iron-sediment or ironstone,
- organic-rich sediment,
- non-carbonate salt,
- non-clastic siliceous sediment,
- miscellaneous oxide and hydroxide and silicate sediment,
- …,
- hybrid sediment,
- sediment with volcaniclastic debris
- lunar basaltic regolith sediment
- lunar anorthositic regolith sediment
- asteroidal regolith

For ‘superficial deposit’:
- ‘*mass movement deposit*’:

- ‘*residual deposit’*:
- ‘*aeolian deposit’*:
- ‘*organic deposit’*:
- ‘*biological deposit’*:
- ‘*chemical deposit’*:
- ‘*alluvial deposit’*:
- ‘*lacustrine deposit’*:
- ‘*coastal deposit’*:
- ‘*marine deposit’*:
- ‘*proglacial deposit’*:
- ‘*glacigenic deposit’*:
- ‘*organic-rich cometary regolith’*:

For ‘magmatic ice’:

- ‘sea ice’: ice formed by solidification of salty sea water
- ‘lake and river ice’: ice formed by solidification of stagnant or flowing water. Includes ‘aufeis’ (sheet-like mass of layered ice that forms from successive flows of ground water during freezing temperatures.)
- ‘ground ice’: ice formed inside the ground. Inludes permafrost.
- ‘icicle’: spike of ice formed when water dripping or falling from an object freezes. Include ice stalactites

For ‘sedimentary ice’:

- ‘snow’: ice formed by water vapor condensation in the atmosphere and subsequent sedimentation
- ‘atmospheric ice’: ice formed by liquid water solidification in the atmosphere and subsequent sedimentation. Includes hail, sleet and ice pellets.
- ‘rime ice’: ice formed by direct liquid water solidification on a surface
- ‘frost’: ice formed by direct water vapor condensation on a surface

For ‘metamorphic ice’:

- ‘*mantle ice’*: ice constituting the mantle inside several planets and satellite
- ‘*glacier ice’*: ice from ice sheets, ice caps and glaciers formed by

compression of snow and flowing
  - '*firn ice'*: ice formed only by compression of snow

For 'other' component group:
  - '*complex mix'*:
  - '*other*':
  - '*unknown*':

Note: for rocks the major mineral group(s) composing the rock can be also specified in addition to the rock group.

Note: classification defined by British Geological Survey (except planetary components): http://www.bgs.ac.uk/bgsrcs/
Ref: BGS Rock Classification Scheme, British Geological Survey Research Report, Volumes 1 to 4:
  - igneous rocks (RR 99-01) M.R. Gillespie and M.T. Styles,
  - metamorphic rocks (RR 99-02) S. Robertson,
  - sedimentary rocks (RR 99-03) C.R. Hallsworth and R.W. O'B Knox,
  - artificial (man-made) ground and natural superficial deposits (RR 99-04) A.A. McMillan and J.H. Powell.

=> see also IUGS ?

*matter_solid*_components_comments [*matter*_components_comments]	blob	U [m]	MatSol	F	--	Additional comments on the component(s) of the mineral matter

Solid matter global density

*matter_solid*_compacity [*layer/matter*_compacity]	float	U [m]	MatSol	F	*no*	Compacity of the solid matter (fraction of solid material volume per matter volume unit) *Note:* compacity = (1 – porosity) *Note:* value of the raw matter before any preparation for sample
*matter_solid*_compacity_error [*layer/matter*_compacity_error]	float	U [m]	MatSol	F	*no*	Absolute uncertainty on the compacity of the solid matter

*matter_solid*_density [*layer/matter*_density]	float	U [m]	MatSol	F	g/cm3	Density of the solid matter • stored in the database and provided to user in 'g/cm^3' unit *Note:* value for the raw matter before any preparation for sample
*matter_solid*_density_error [*layer/matter*_density_error]	float	U [m]	MatSol	F	g/cm3	Absolute uncertainty on the density of the solid matter • stored in the database and provided to user in 'g/cm^3' unit

Solid matter global texture

*matter_solid*_shape [*matter*_shape]	varchar(255)	U [m]	MatSol	F	--	Description of the macroscopic shape of the solid matter *Notes:* - mostly for single piece (compact or cemented/sintered granular textures) - write *'undefined (loose)'* for loose granular solids. *Exemples:* - thick slab, polished thin section, conchoidal fractured solid, …
*matter_solid*_texture [*layer/matter*_texture]	enum(text)	S1 [m]	MatSol	F	--	Macroscopic texture of the solid matter (at scale above material grains) OpenEnum: {muddy, earthy, pulverulent, loose fine grained, loose coarse grained, loose granular, sintered granular, cemented granular, mixed granular, compact, compact glassy, compact poor grained, compact fine grained, compact coarse grained, compact lamellar, compact fibrous, compact crystal, compact mixed, single grain, individual grains, aggregated grains, isolated aerosols, aggregated aerosols, clusters, liquid, gaseous, other, unknown} *Definitions: see "layer*_texture*"* *Note:* a rock is considered here as one type of 'compact' matter
*matter_solid*_porosity_type [*layer/matter*_porosity_type]	enum(text)	S2 [!_m]	Mat	F	--	Type of porosity of the matter (at scale above material grains) OpenEnum: {particulate, porous, open pores, closed pores, without pores, other, unknown}

						*Definitions: voir "layer*_porosity_type*"*
Matter global grain size distribution and texture						
*matter_solid*_grain_size_unit [*sample/matter*_grain_size_unit]	enum(text)	U [£o_m]	MatSol	F	--	Unit for the solid matter and material grain sizes (diameter) Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*matter_solid*_grain_size_min" OR "*matter_solid*_grain_size_max" has a value *Note DB:* all grain sizes data will be stored in 'mm' *Note:* used for "*matter_solid*_grain_size_min/_max" and "*material*_grain_size_min/_max"
*matter_solid*_grain_size_method [*material/matter*_grain_size_method]	blob	U [m]	MatSol	F	--	Description of the grain size (min/max) definition, and of the method of determination of the grain size distribution *Ex:* 'sieving by 2 stainless steel sieves with 50 and 100 µm meshs', 'microscope measurement of section'
matter_solid_grain_sizes	***List [L6]***	[O]				£: Size distribution of the solid matter grains *Note*: Used when only a global grain size distribution of the solid matter is available, but not for each of its materials
*matter_solid*_grain_size_median [*material/matter*_grain_size_median]	float	S3 [m]	MatSol L6	F	var.	Median size (diameter) of solid matter grains *Unit:* in "*matter_solid*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_solid*_grain_size_unit" *Note*: mostly used when only one median size is known for the matter grains
*matter_solid*_grain_size_width [*material/matter*_grain_size_width]	float	U [m]	MatSol L6	F	var.	Full width at half maximum of the size distribution (diameter) of solid matter grains *Unit:* in "*matter_solid*_grain_size_unit"

						• converted in 'm' unit in the database but provided to user in "*matter_solid*_grain_size_unit" *Note*: mostly used when only one median size and its distribution is known for the matter grains
*matter_solid*_grain_size_min [*material/matter*_grain_size_min]	float	S3 [m]	MatSol L6	F	var.	Smallest size (diameter) of solid matter grains of this size range *Unit:* in "*matter_solid*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_solid*_grain_size_unit"
*matter_solid*_grain_size_max [*material/matter*_grain_size_max]	float	S3 [m]	MatSol L6	F	var.	Largest size (diameter) of solid matter grains of this size range *Unit:* in "*matter_solid*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_solid*_grain_size_unit"
*matter_solid*_grain_size_fraction [*material/matter*_grain_size_fraction]	float	U [m]	MatSol L6	F	*no*	Mass fraction of solid matter grains comprised between size min and size max (diameter) *Note:* value between 0 and 1
*matter_solid*_grain_size_fraction_error [*material/matter*_grain_size_fraction_error]	float	U [m]	MatSol L6	F	*no*	Absolute uncertainty on the mass fraction of solid matter grains comprised between size min and size max (diameter)
*matter_solid*_grain_size_shape [*material/matter*_grain_size_shape]	enum(text)	S2 [m]	MatSol L6	F	--	Dominant shape of the solid matter grains (granular matter) or crystals (compact matter) of this size range Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions: voir "material*_grain_size_shape*"*

*matter_solid*_grain_size_distribution [*material/matter*_grain_size_distribution]	blob	U [m]	MatSol	F	--	Description and parameters of the size distribution of the matter grains *Note:* see "*material*_grain_size_distribution"
*matter_solid*_grain_texture [*material/matter*_grain_texture]	openum(text)	S2 [m]	MatSol	F	--	Description of the major grain texture of the solid matter OpenEnum: {clay-like, silt-like, compact, compact with defects, compact with bubbles, compact porous, compact microporous, lamellar, fibrous, compact mixed, complex, other, unknown, …} *Definitions: voir "material*_grain_size_shape*"*
*matter_solid*_grain_compacity [*material/matter*_grain_compacity]	float	U [m]	MatSol	F	*no*	Compacity of the grains of the solid matter (fraction of solid volume per grain volume unit) *Note:* compacity = (1 – porosity)
*matter_solid*_grain_compacity_error [*material/matter*_grain_compacity_error]	float	U [m]	MatSol	F	*no*	Absolute uncertainty on the compacity of the grains of the solid matter
*matter_solid*_grain_density [*material/matter*_grain_density]	float	U [m]	MatSol	F	g/cm^3	Mean bulk density of the grains of the solid matter • stored in the database and provided to user in 'g/cm^3' unit
*matter_solid*_grain_density_error [*material/matter*_grain_density_error]	float	U [m]	MatSol	F	g/cm^3	Absolute uncertainty on the mean bulk density of the grains of the solid matter • stored in the database and provided to user in 'g/cm^3' unit
*matter_solid*_texture_comments [*material/matter*_texture_comments]	blob	U [m]	MatSol	F	--	Experimentalist additional information or comments about the texture of the solid matter *Ex:* …

Solid matter global oxides composition *Note*: Used when only a global oxide composition is available, but not for each of its solid

						(otherwise describe it for each material in '*matter_solid*_material_oxides')
matter_solid_oxides	***List [L7]***	[O]				£: Description of the oxides composition of the solid matter
*matter_solid*_oxide_formula [*material/matter*_oxide_formula]	CS- enum(text)	U [m]	MatSol L7	F	--	Formula of the different oxides composing the solid matter Enum: *see mineral*_oxide_formula *Note:* - mostly used for minerals (a common method for composition determination), but can be applied to most solids containing O atoms - did not distinguish non-natural isotopic species
*matter_solid*_oxide_mass_fraction [*material/matter*_oxide_mass_fraction]	float	U [m]	MatSol L7	F	%	Mass fraction (in %) of each type of oxide composing the solid matter *Note:* value between 0 and 100
*matter_solid*_oxides_comments [*material/matter*_oxides_comments]	blob	U [m]	MatSol	F	--	Any additional information (sum of oxides …) or comments on the oxides composition of the solid matter *Note:* also additional information on impurities not measured by oxides

Solid matter composition

Note: Whatever are the materials that constitute the solid matter they will be always defined from the ”material” level (link(s) with “*matter_solid*_material_index”) through their “constituents” and “species”, exactly as for sample. or through other matter(s). All the structure is taken from sample and only their type of material mixing is repeated here.

*matter_solid*_materials_mixing [+] [*matter*_materials_mixing]	enum(text)	S2 [!_m]	MatSol	F	--	How the different materials are mixed in the solid matter Enum: {single material, homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, spatial distribution...} *Definitions:* cf. “*layer*_materials_mixing”
*matter_solid*_materials_number [+][-xml]	int(10)	U [!_c]	MatSol	F	*no*	Number of different materials mixed in the solid matter ➔ calculated from " *matter_solid*_materials" list

[*matter*_materials_number]

matter_solid_matters	***List [L8a]***	[!]				£: matters constituting this solid matter
*matter_solid*_matter_index [*][-xml] [*matter*_matter_index]	int(10) [Internal link]	B [!_g]	MatSol MatXxx L8a	F	--	ID of the matters(s) constituting the 'solid matter' *Note xml:* in practice the description of the material(s) is done directly under "*matter_solid*" without providing the ID link

➢ Same structure as "*sample*"

matter_solid_materials	***List [L8b]***	[!]				£: materials constituting this solid matter
*matter_solid*_material_index [*][-xml] [*matter*_material_index]	int(10) [Internal link]	B [!_g]	MatSol Mater L8b	F	--	ID of the material(s) constituting the 'solid matter' *Note:* The different solids (fundamental phases or custom constituents) composing the solid matter are described inside this materials structure at the constituent level. *Note:* For solid solutions or n-hydrated minerals ("*mineral*_classification_level" = {variable mineral, unique mineral} or "*mineral*_hydration_series" = 'true') the modifications of the mineral solid solution parameters (VM) (composition and properties) are described at the species level *Notes:* - Case of '*glasses'*: amorphised forms of a (or a mixture of) solid phases. They are defined as amorphous solid constituents that refer to the equivalent crystalline solid/mineral phase(s), with modification of "*solid/mineral*_crystal_system" = 'amorphous', "*solid/mineral*_crystal_class/_symbol/_spacegroup" = 'N/A', and modification of some variables parameters (VS/VM) (composition and properties) - Case of *'clays/silts'* (complex mix and disordered): mineral matters or sedimentary rocks made of one or more clay minerals (+ possible impurities) filled with interlayer water. They are described as a solid matter with mineral phases defined

➢ Same structure as "*sample*"

						inside the matter structure at the constituent level and water defined as another constituent inserted inside layers of each mineral phase ("*constituent*_phase_type" = 'interlayer' + "*constituent*_sorption_constituent_uid"). If there are several clay mineral phases intimately mixed, they should be defined inside one multi-species constituent. *Note xml:* in practice the description of the material(s) is done directly under "*matter_solid*" without providing the ID link
*matter_solid*_comments [*matter*_comments]	blob	U [m]	MatSol	F	--	Additional information on the solid matter (minor impurities in substitution or in crystal defects, …) or comments on the composition and formula of the actual solid phases composing the solid matter
Precursor materials		[O]				*Condition:* description of precursor materials is optional but strongly recommended. *Note:* "*material*_is_precursor" = 'true' *Note:* refer to the same table as "*materials*" in the sample structure but without the "material arrangement and abundance" bloc *Note:* Precursor materials which are not matter(s) are defined here through the "material(s)/constituent(s)/specie(s)" structure. They are used in "processing" through links with their "*matter*_precursor_material_uid". Precursors which are "*matters*" (gas bottle, liquid matters, …) are directly linked in "*processing*". Their mixing and processing step(s) up to the formation of the final matter are described in "*matter*_processings".
matter_solid_precursor_materials [matter_precursor_materials]	***List [L9]***	[O]				£: Precursor materials used to create the solid matter
*matter_solid*_precursor_material_index [*][-xml] [*matter*_precursor_material_index] ➢ Same structure as "*materails*" but without the "material arrangement and abundance" bloc	int(11) [Internal link]	B [O!!_g]	MatSol PreMater L9	F	--	ID of the different precursor materials used to create the 'solid matter' *Note:* determined automatically during import *Note:* a precursor material is a "*simple material"* described through the material/constituent(s) and specie(s) structure. When the precursor material is a "*matter*" then no need to describe it here because it can be linked directly as a matter (with its "*matter*_uid") in the processings with "*matter*_processing_precursor_matter_uid"

Note xml: in practice the description of the precursor material(s) is done directly under the "*matter_solid*" structure without providing the ID link

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Solid matter processings: step [O] *Condition:* only when there is processing of materials or parent matter/sample

Note: refer to the same table as "*processings*" in the sample structure but with a few restrictions (no sample layer, …) and with "*Layer/Sample*" replaced by "*Matter*".

Note: They can be processings of materials (atoms, molecules, solids, minerals, …) to form a synthetic solid matter, or processing of a natural mineral phase, or processing of a matter to form another solid matter.

Note: the new matter should be available for future experiments (at least two). Otherwise (processings for a single experiment) these processings will be described directly in the sample description using the parent matter with no new matter created.

Note: the physical units are used only as text in "*processing*_process" and are not specified in "matters" (contrary to "sample") but it is requested to express all them in an homogeneous way by choosing ONE of each of the following units:

- Temperature: {K, °C}
- Pressure: {Pa, hPa, mbar, bar, atm, torr}
- Time: {s, min, h, d}
- Energy: {J, kJ, eV, keV, MeV, A, nm, micron, cm-1}

matter_solid_processings	***List [L10]***	[O]				£: Processings of the matter.
*matter_solid*_processing_index [*§][-xml]	int(11) [Internal Links]	B [O!!_g]	MatSol Process L10	F	--	ID of the processing(s) of the matter. *Note:* determined automatically during import

- Use the same structure as for "*Sample processings*" with only a few changes (noted in "*Sample processings*")
  - Not used for matters: "*processings*_product_sample_uid", "*processings*_product_sample_uid", "*processings*_chronology"
  - Used only for matters: *processings*_product_matter_uid

Solid matter documentation and references

matter_solid_documentations	***List [L11]***	[O]				£: Documentations about the solid matter
*matter_solid*_documentation_name	varchar(255)	U [m]	MatSol L11	F	--	Name of the documentation describing the solid matter

[*sample_documentation_name*]						*Note:* this name will appear as the documentation title in the database *Ex:* 'Optical properties of Jacobsite'
*matter_solid*_documentation_filename [*sample_documentation_filename*]	varchar(255)	U [m]	MatSol L11	F	--	File name (with extension) of the documentation describing the solid matter *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database
matter_solid_links	***List [L12]***	[O]				£: Web pages describing the solid matter and its properties
*matter_solid*_link_name [*matter*_link_name]	varchar(255)	U [m]	MatSol L12	F	--	Name of the web page(s) describing the solid matter and its properties. *Ex:* 'Clay Mineral Society', …
*matter_solid*_link_url [*matter*_link_url]	CS-varchar(255)	U [m]	MatSol L12	F	--	URL address(es) of the web page(s) describing the solid matter and its properties *Notes:* - useful when the solid matter comes from a mineral database, a stable commercial supplier, ... - can also link to various types of measurements made on this matter - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
matter_solid_publications	***List [L13]***	[O]				£: Publications describing the solid matter and its properties.
*matter_solid*_publication_uid [*] [*matter*_publication_uid]	varchar(255)	S2 [m]	MatSol Publi L13	F	--	Link to the existing UID of the publication(s) describing the solid matter(s) and its properties. *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter', at least

7.4 Carbonaceous Matters (Natural and synthetic) Table

Root of the table: ***matter_carbonaceous***

Data type: 'Matter'

Definition: '*carbonaceous matter'* is any complex natural (from Earth or planetary bodies) or synthetic matter made of organic species or of a carbonaceous macromolecular structure , excluding extraterrestrial carbonaceous materials from meteorite, micrometeorites, IDPs or cosmic dust (asteroidal and cometary dust, …).

Notes:

- Carbonaceous mineral matters (carbon, coal, anthracite, lignite, …) will be preferentiably entrered as "carbonaceous matters" as the KW are more adapted.
- Organic bio-minerals, such as amber, will be also preferentiably entrered as "carbonaceous matters"
- Natural terrestrial organic fluids, such as petroleum and derivatives, will be also preferentiably entrered as "carbonaceous matters"
- Extraterrestrial carbonaceous matters extracted from meteorite, micrometeorites, IDPs or cosmic dust will be entrered as "extraterrestrial matters"
- Any other carbonaceous matters collected at the surface or in the atmosphere of planetary bodies (planets, satellites, asteroids, comets, TNO, …) will be entered as "carbonaceous matters"

Key-word	Type	Level	Table	Exp	Unit	Description
Carbonaceous matter import						
*matter_carbonaceous*_import_mode [*matter*_import_mode]	enum(text)	P [!!_m]	MatCarb	F	--	Mode of import of the "carbonaceous matter" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*matter_carbonaceous*_xml_filename [-xml] [*matter*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	MatCarb	(V)	--	Name of the storage copy of the xml import file of the "*matter_carbonaceous*" metadata ➔ determined automatically during import (from "*matter_carbonaceous*_uid" ?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to

						apply correction
Carbonaceous matter indexes						
*matter_carbonaceous*_index [**][-xml] [*matter*_index]	int(10)	B [!!_g]	MatCarb	F	--	Automatic random but unique number (ID) given to new carbonaceous matter
*matter_carbonaceous*_uid [**] [*matter*_uid]	varchar(255)	P/U [!!_m]	MatCarb	F	--	Unique identifier code (UID) given to the carbonaceous matter table (to be created) *Nomenclature:* Create this UID with 'MATCARB_' very accurately in order to be simple and unique - It should be of the style 'MATCARB_CarbonaceousMatter_AB_yyyymmdd' where 'CarbonaceousMatter' is the matter name (part of *matter_carbonaceous*_name) or the main carbonaceous material/constituent name, 'AB' are the initials of the person preparing the import, or of the experimentalist preparing the matter (*experimentalist*_acronym of *matter_carbonaceous*_experimentalist), 'yyyymmdd' is the full date of creation of the matter (from *matter_carbonaceous*_date) or the date of the day. *Note*: use lowercases for 'CarbonaceousMatter' *Note*: if several matters are created the same day with the same carbonaceous material then add some distinguishing property after 'CarbonaceousMatter'. *Ex:* - 'MATCARB_tholins-SA98_EQ_20131003' - 'MATCARB_kerogen_PB_20130828'
matter_carbonaceous_owner_databases	***List [L0]***	[!!]				£: databases which manage this matter
*matter_carbonaceous*_owner_database_uid [*] [*matter*_owner_database_uid]	varchar(255)	P/U [!!o_m]	MatCarb DatBas	F	--	Link(s) to the existing UID(s) of the database which owns and manages this matter information

			L0				*Condition:* at least one database *Note:* For common 'reference' matters and for matters from external laboratories (not managed by a database), it should be 'DB_SSHADE'
Carbonaceous matter experimentalist							
matter_carbonaceous_experimentalists	***List [L1]***	[O]					£: experimentalists who prepared the matter
*matter_carbonaceous*_experimentalist_uid [*] [*matter*_experimentalist_uid]	varchar(255)	P/U [m]	MatCarb Exper L1	F	--		Link to the existing UID of the experimentalist(s) which prepared the matter *Condition:* can be no experimentalist when the matter is stored as it is delivered
Carbonaceous matter family and description							
*matter_carbonaceous*_family [-xml] [*matter*_family]	enum(text)	S [!!_g]	MatCarb	F	--		Family of the carbonaceous matter Enum: {carbonaceous} *Default* = 'carbonaceous' *Definitions:* - '*carbonaceous'*: matters made primarily of natural or synthetic carbonaceous materials
*matter_carbonaceous*_name [*matter*_name]	varchar(255)	S [!!_m]	MatCarb	F	--		Common or given name of the carbonaceous matter *Notes:* – It should contain explicit info on the matter and constituting materials/constituent/species: name(s) and some typical properties of the matter (phase type, components, preparation, …). – It maybe the name of the main carbonaceous compound (if pure, almost pure, or the major component) or a name describing the main carbonaceous components if mixed – It is used as the title of the matter page on the SSHADE interface

						Ex: 'sulfurous planktonic kerogen (II) - Liptinite', 'Titan tholins SA98 - 2% CH4'
*matter_carbonaceous*_date [*matter*_date]	date	P [!_m]	MatCarb	F	YYYY-MM-DD	Date of creation of the carbonaceous matter *Note:* This date can be the date of collection or delivery for natural matters, or of creation for synthetic ones, or of end of processing(s) in the case of a matter generated by processing another one (parent matter).
*matter_carbonaceous*_parent_matter_uid [*] [*matter*_parent_matter_uid]	varchar(255)	S2/S1i [$o_m]	MatCarb MatXxx	F	--	Link to the existing UID of the parent matter (if present in the database) used to create this one by some processing (e.g. thermal cycle, irradiation, sieving, …) *Recommendation:* Strongly recommended when already exist in the database. *Ex:* a granular matter sieved to a specific grain size range gives a daughter matter from the parent unsieved matter.
*matter_carbonaceous*_first_parent_matter_uid [*] [-xml] [*matter*_first_parent_matter_uid]	varchar(255)	S2/S1i [!o_c]	MatCarb MatXxx	F	--	Link to the existing UID of the first parent of the generation of matters (present in the database) that has been initially used to create this one by a series of processes. *Condition:* when "*matter_carbonceous*_parent_matter_uid" ≠ Φ ➔ calculated recursively using "*matter_carbonaceous*_parent_matter_uid", when it exist
Carbonaceous matter origin						
*matter_carbonaceous*_level [*matter*_level]	enum(text)	S2 [!_m]	MatCarb	F	--	Level of the carbonaceous matter Enum: {from sample return mission, from international repository, from laboratory repository, from commercial supplier, local matter, other} *Definitions:* cf. *"matter_solid*_level"
*matter_carbonaceous*_origins	***List [L2]***	[!!]				£: Origins of the carbonaceous matter

*matter_carbonaceous*_origin [*matter*_origin]	enum(text)	S [!!_m]	S	MatCarb Miner L2	F	--	--	Origin of the carbonaceous matter Enum: {natural terrestrial, extraterrestrial, planetary, laboratory, commercial, simulated} *Definitions: cf. "matter_solid*_origin" *Notes:* – a carbonaceous matter should be predominantly synthetic (laboratory or commercial), – it may also be mixed with some natural material as long as this material is not the main focus of the matter (e.g. darkening material, dilution/matrix material, …) – it may also be simulated (numerical simulation)

Carbonaceous matter provider

*matter_carbonaceous*_provider [*matter*_provider]	varchar(255)	S [!_m]	U	MatCarb Miner L1	F	--	--	Provider name, address, … of the carbonaceous matter *Note:* Organic repository, commercial company, individual + laboratory name, ... *Ex:* 'Exxon oil company'
*matter_carbonaceous*_provider_reference_code [*matter*_provider_reference_code]	varchar(255)	S [m]	S1/S1bs	MatCarb Miner L1	F	--	--	Reference number or name given by the provider of the carbonaceous matter *Ex:* 'SA90'
*matter_carbonaceous*_igsn_code [*matter*_igssn_code]	varchar(255)	S [m]	S1/S1bs	MatFluid Miner L1	F	--	--	'International Geo Sample Number'code (*IGSN*) of the carbonaceous matter *Constraint:* only when *"matter_carbonaceous*_origin" = {natural terrestrial, extraterrestrial} *Definition*: The IGSN is an alphanumeric code that uniquely identifies samples from our natural environment and related sampling features (http://www.geosamples.org) *Ex:* 'IEJEN00CH'

*matter_carbonaceous*_igsn_url [-xml] [*matter*_igssn_url]	varchar(255)	S [!o_c]	U	Mineral Fluid	F	--	--	url address of the information page for carbonaceous matters with an IGSN code *Condition:* mandatory when "*matter_carbonaceous*_igsn_code" ≠ Ø ➔ *Calculated* with https://app.geosamples.org/sample/igsn/"*matter_carbonaceous*_igsn_code" *Ex*: 'https://app.geosamples.org/sample/igsn/IEJEN00CH' for IGSN='IEJEN00CH'
*matter_carbonaceous*_local_reference_code [*matter*_local_reference_code]	varchar(255)	S [m]	S1/S1bs	Mineral Fluid	F	--	--	Local reference number or name given by local experimentalists to the carbonaceous matter *Ex: '*SA90-120212'

Natural carbonaceous matter: planetary body

*matter_carbonaceous_body*_uid [*] [-xml] [*matter*_body_uid]	varchar(255)	S [!!o_c]	S1/S1s	Mineral Fluid Body	F	--	--	Link to the existing UID of the planetary body from which the natural matter originates *Condition:* absolute mandatory when *"matter_carbonaceous*_origin" = {natural terrestrial, planetary} ➔ Calculated: ⇨ = 'BODY_planet_Earth' when "*matter_carbonaceous*_origin" = {natural terrestrial} ⇨ = *"matter_carbonaceous_body*_object_uid" / "*object_planetary_body*_uid" when *"matter_carbonaceous*_origin" = {planetary} *Note:* - added in order to be able to set "body" automatically to 'Earth' for 'natural terrestrial' matters who did not have a mandatory 'planetary object') - not used for laboratory, commercial and simulated matters

*matter_carbonaceous*_body_object_uid [*] [*matter*_body_object_uid]	varchar(255)	S1/S1s [!!o_m]	MatCarb Matter Object	F	--	--	Link to the existing UID of the planetary object from which the natural matter originates *Condition:* absolute mandatory when *"matter_carbonaceous*_origin" = {planetary, extraterrestrial} *Notes:* see "*matter_solid*_body_object_uid"
*matter_carbonaceous*_body_terrain_type [*matter*_body_terrain_type]	openum(text)	S2 [!o_m]	MatCarb Matter	F	--	--	Type of geological/geophysical terrain on the planetary body where the natural matter is/was situated. OpenEnum: {mineral surface, icy surface, organic surface, liquid surface, mixed surface types, mineral subsurface, icy subsurface, organic subsurface, liquid subsurface, mixed subsurface types, atmosphere, other, unknown} *Condition:* mandatory when *"matter_carbonaceous*_origin" = {natural terrestrial, extraterrestrial} *Definitions:* see *"matter_solid*_body_terrain_type" *Note:* the precise type and location on the planetary body is described in "*matter_carbonaceous*_geolocation_xxx"
*matter_carbonaceous*_body_coordinate_system [*matter*_body_coordinate_system]	openum(text)	U [!o_m]	MatCarb	F	--		Coordinate system on the planetary body of the geographic location of the natural matter OpenEnum: {WGS84, Mars 2000, Moon 2000, Pluto 2015, …} *Condition:* mandatory when "*matter_carbonaceous_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Definitions*: see "*experiment*_body_coordinate_system" *Notes*: - Prefer 'Planetocentric latitude with east longitude' coordinate systems approved by the International Astronomical Union - currently only 'WGS84' system for Earth

Natural carbonaceous matter: geolocation

*matter_carbonaceous*_geolocation_place [*matter*_geolocation_place]	varchar(255)	S1b [!o_m]	MatCarb	F	--	--	Geologic source and geographic location on the planetary body of the natural matter (geologic type, place and area names) *Condition:* mandatory when *"matter_carbonaceous*_origin" = {natural terrestrial, extraterrestrial} *Ex:* -
*matter_carbonaceous*_geolocation_region [*matter*_geolocation_region]	varchar(255)	S1b [!o_m]	MatCarb	F	--	Region, state, province or county (administrative location) on Earth of the natural matter *Condition:* mandatory and only when "*matter_carbonaceous_body*_uid" = 'BODY_planet_Earth' *Ex:* - 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi' (Earth)
*matter_carbonaceous*_geolocation_country_code [*matter*_geolocation_country_code]	enum(text)	S1b [!o_m]	MatCarb	F	--	2-digit code of the country of the geographic location on Earth of the natural matter Enum: {CH, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory and only when "*matter_carbonaceous_body*_uid" = 'BODY_planet_Earth' *Definitions:* see "*laboratory*_address_country_code"
*matter_carbonaceous*_geolocation_type [*matter*_geolocation_type]	enum(text)	U [!!o_m]	MatCarb	F	--	Type of geographic location the natural matter Enum: {point, line, box, polygon} *Condition:* mandatory when "*matter_carbonaceous_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_carbonaceous*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_geolocation_type"

matter_carbonaceous_geolocation_coordinates [*matter_geolocation_coordinates*]	***List [L3]***	[!O]				£: Geolocation on the planetary body of the natural matter *Condition:* mandatory when "*matter_carbonaceous_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition*: absolute mandatory when "*matter_carbonaceous*_geolocation_type" ≠ Ø *Conditions:* on the number of long/lat couple: see *"experiment*_geolocation_coordinates" *Note DB*: will be stored in shapefile format ?
*matter_carbonaceous*_geolocation_coordinate_latitude [*matter*_geolocation_coordinate_latitude]	float	S3 [!o_m]	MatCarb L3	F	deg	Latitude of the geographic location on the planetary body of the natural matter *Format*: in N 'decimal degrees' in "*matter_carbonaceous*_body_coordinate_system" *Condition:* mandatory when "*matter_carbonaceous_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_carbonaceous*_geolocation_coordinate_longitude [*matter*_geolocation_coordinate_longitude]	float	S3 [!o_m]	MatCarb L3	F	deg	Longitude of the geographic location on the planetary body of the natural matter *Format*: in E 'decimal degrees' (in the E direction only) in "*matter_carbonaceous*_body_coordinate_system" *Condition:* mandatory when "*matter_carbonaceous_body*_uid" / "*body*_family" = {planet, dwarf planet, satellite}
*matter_carbonaceous*_geolocation_coordinate_altitude [*matter*_geolocation_coordinate_altitude]	float	S3 [m]	MatCarb L3	F	m	Altitude of the geographic location on the planetary body of the natural matter *Format*: in 'meter' in "*matter_carbonaceous*_body_coordinate_system" *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*matter_carbonaceous*_geolocation_comments	blob	U	MatCarb	F	--	Any additional information or comments about the geolocation of this matter

[*matter*_geolocation_comments]		[m]				*Ex:* 'matter was collected within 100m of this point', 'very approximate coordinates (+/- 0.1°)'…

Carbonaceous matter images

matter_carbonaceous_images	***List [L4]***	[O]				£: Pictures of the carbonaceous matter
*matter_carbonaceous*_image_file name [*matter*_image]	varchar(255)	U [m]	MatCarb L4	F	--	File name(s) (with extension) of the picture(s) of the carbonaceous matter *Image formats:* .png, .jpg, (.gif) *Note:* this file will be imported in the database
*matter_carbonaceous*_image_caption [*matter*_image_caption]	varchar(255)	U [m]	MatCarb L4	F	--	Caption(s) or comment(s) on the picture(s) of the carbonaceous matter

Carbonaceous matter preparation and component types

*matter_carbonaceous*_preparation [*matter*_preparation]	enum(text)	U [!_m]	MatCarb	F		Type of preparation of the carbonaceous matter Enum: {raw, section, polished section, selected components, sieved fraction, extracted components} *Definitions:* - '*raw'*: piece of carbonaceous material without chemical treatment nor selection of a particular component nor other type of preparation (cutting, polishing, …) - '*section*': raw carbonaceous material cut and potentially polished by different ways - '*selected components'*: peculiar component (specific phase, ...) selected mechanically without any chemical treatment - '*sieved fraction'*: size fraction separated by sieving - '*extracted components'*: carbonaceous phase extracted using a chemical or physical treatment (Insoluble Organic Matter, Soluble Organic Matter, …)

*matter_carbonaceous*_method [*matter*_method]	varchar(255)	S U [m]	MatCarb L5	F	--	--	Method of extraction (natural) or synthesis of this carbonaceous matter *Ex:* 'raw coal extracted from a mine', 'photolysis of CH4:N2 gas mixture'
*matter_carbonaceous*_storage_condition [*matter*_storage_condition]	varchar(255)	S U [m]	MatCarb L5	F	--	--	Storage condition of this carbonaceous matter *Ex:* 'stored at 20°C in 1 bar of pure and dry Ar gas since field collection', … *Notes*: see "*matter_solid*_storage_condition"
*matter_carbonaceous*_phase_type [*matter*_phase_type]	enum(text)	S0/S2s [!_m]	MatCarb	F	--		Type of phase of the carbonaceous matter Enum: {solid, liquid, gas} *Note:* if there are several phase types, then give the main here and add a comment in "*matter_carbonaceous*_comments"
matter_carbonaceous_components [*matter_components*]	***List [L5]***	[!]					£: Components type and group of synthetic carbonaceous matter
*matter_carbonaceous*_component_type [*matter*_component_type]	enum(text)	S [!_m]	MatCarb L5	F	--		Type of carbonaceous matter Enum: {living organism or its products, soil organic compounds, sedimentary organic compounds, organic mineral, natural abiotic carbonaceous matter, semisynthetic organic matter, synthesized carbonaceous matter, pure carbon allotrope, molecular organic, mixed types, other, unknown} *Definitions:* For biotic terrestrial carbonaceous matters: - '*living organism or its products'*: any part of living organisms (plant, animal, …) or their products (ex: bee wax, musc...) - '*soil organic compounds'*: undecomposed, partly decomposed and completely decomposed remains of live organisms as well as products of their transformation. - *'sedimentary organic compounds'*: kerogen, coal, petroleum, natural gas - '*organic mineral'*: any type of natural organic mineral (salts of organic

						acids and hydrocarbons: Amber, Mellite, Ravatite, …) For natural abiotic or synthetic carbonaceous matters: - '*natural abiotic carbonaceous matter*': mostly extraterrestrial carbonaceous matter *Note*: carbonaceous matter of meteorite, micrometeorites, IDPs, cometary dust, … will be described in 'extraterrestrial matter' - '*semisynthetic organic matter'*: any type of complex organic matters formed by reaction on chemical compounds isolated from natural sources. *cf.:* https://en.wikipedia.org/wiki/Semisynthesis - *'synthesized carbonaceous matter':* any type of complex carbonaceous matters formed by irradiation(s) or thermal chemical reactions of simple molecules (total synthesis) - '*pure carbon allotrope*': any type of natural or synthetic carbon allotrope (diamond, graphite, fullerene, nanotube, amorphous or disordered carbon, …) - *'molecular organic'*: simple condensed (solid or liquid) organic molecule or molecular mixture. Others: - '*mixed types'*: more than one of the above carbonaceous types mixed in the carbonaceous matter (put information on the types in "*matter_carbonaceous*_comments") - '*other*': any other type of carbonaceous matter, either natural or synthetic (put information in "*matter_carbonaceous*_comments") - '*unknown*': unknown type of carbonaceous matter *Note:* although some of the 'pure carbon allotropes' and most of the 'organic minerals' are classified as minerals (Carbon polymorph (Dana group 01.03.06) & Salts of organic acids and hydrocarbons (Dana class 50)) the matters containing them are described in "carbonaceous matter" because its description keywords are more relevant for matters mainly made of these species (atomic composition instead oxides composition, …).
*matter_carbonaceous*_component_group [*matter*_component_group]	openum(text)	S [!_mo]	MatCarb L5	F	--	Group of carbonaceous matter. OpenEnum: {plant, plant product, animal, animal product, fungi, protist, bacteria, soil organic matter, kerogen, coal, petroleum, natural gas, organic

acid salt, hydrocarbon mineral, natural abiotic carbonaceous matter, photolysis product, radiolysis product, plasma deposited product, heating process product, diamond, graphite, fullerene, amorphous or disordered carbon, other carbon allotrope, molecular organic, mixed organics, other, unknown}

Definitions:

For 'living organism or its product':

- '*plant*': any type of plant (lichen, …), part of plant (leave, root, spores, …)
- '*plant product':* product of plants (resin, copal, amber, …)
- '*animal*': any type of animal (…) or part of animal (…)
- *'animal product'*: animal products (bee wax, musc, grey amber, …)
- *'fungus':* mushrooms and any member of eukaryotic organisms, also including microorganisms such as yeasts and molds, that form the kingdom of Fungi.
- *'protist':* large and diverse group of eukaryotic microorganisms, which belong to the kingdom Protista.
- *'bacteria':* prokaryotic microorganisms.

For 'soil organic compound'

- '*soil organic matter'*: non-living components which are a heterogeneous mixture composed largely of products resulting from microbal and chemical transformations of organic debris. Include unaltered materials, transformed products (humus: humic and non-humic substances, pyrogenic carbon, …).

For 'sedimentary organic':

- *'kerogen'*: Mixture of organic chemical compounds (sedimentary carbonaceous matter) (sub-types: I, II, III)
    - '*sapropelic kerogen (I)*':
    - '*planktonic kerogen (II)*': (or liptinite)
    - '*sulphurous kerogen (II)*':
    - '*humic kerogen (III)*': (or votrinite)
    - '*kerogen residue (IV)*': (or inertinite)
- *'coal'*: combustible black or brownish-black sedimentary rock usually occurring in rock strata in layers or veins (sedimentary carbonaceous matter). Coal is composed primarily of carbon along with variable quantities of other elements, chiefly hydrogen, sulfur, oxygen, and

nitrogen

- ‘*peat’*: (or turf) accumulation of partially decayed vegetation (sub-types: fibric, hemic, sapric)
- ‘*lignite*’: (or brown coal) lowest rank of coal (C = 25-35%)
- ‘*sub-bituminous coal’*: whose properties range from those of lignite to those of bituminous coal
- ‘*bituminous coal’*: (or black coal) dense sedimentary rock, usually black, but sometimes dark brown. Relatively soft coal containing a tarlike substance called bitumen.
- ‘*steam coal’*: grade between bituminous coal and anthracite
- ‘*anthracite*’: hard, compact, glossy black coal (C = 92-98%)
- ‘*graphite*’: highest rank of coal

- *‘petroleum’*: naturally occurring flammable liquid consisting of a complex mixture of hydrocarbons of various molecular weights and other liquid organic compounds, that are found in geologic formations beneath the Earth's surface (sedimentary carbonaceous matter) (C = 83-87%)
  - ‘*crude oil’*: unrefined petroleum
  - ‘*paraffins*’: (or alkanes) white or colourless soft solid (C = 20-40), liquid kerosene (C=6-16)
  - ‘*naphthenes*’: (or cycloalkanes) types of alkanes that have one or more rings of carbon atoms in the chemical structure of their molecules
  - ‘*aromatics*’:
  - ‘*asphalt*’: (or bitumen) sticky, black and highly viscous liquid or semi-solid form of petroleum
- *‘natural gas’*: naturally occurring hydrocarbon gas mixture consisting primarily of methane, but commonly including varying amounts of other hydrocarbons, carbon dioxide, nitrogen and hydrogen sulfide (sedimentary carbonaceous matter)
  - ‘*natural gas’*: low molecular weight components of gas contained in crude oil
  - ‘*natural gas liquid’*: higher molecular weight components components of gas contained in crude oil

- ‘*town gas’*: gaseous fuel made by the destructive distillation of coal and contains a variety of calorific gases including hydrogen, carbon monoxide, methane and other volatile hydrocarbons together with small quantities of non-calorific gases such as carbon dioxide and nitrogen
- ‘*bio gas’*: produced by the anaerobic decay of non-fossil organic matter (biomass)
- ‘*shale gas’*:
- ‘*methane clathrate’*: naturally occurring clathrate hydrate from seabed, bottom of lake or permafrost consisting primarily of methane and commonly including varying amounts of other hydrocarbons, carbon dioxide, nitrogen and hydrogen sulphide (sedimentary organic matter),

For ‘organic mineral’:

- ‘*organic acid salt’*: salts of organic acids: oxalates, mellitates, citrates, cyanates, and acetates (50.01, 50.02 and 50.04 Dana types)
- ‘*hydrocarbon mineral’*: with formula CxHy (50.03 and 50.00 Dana types)

For ‘natural abiotic carbonaceous matter’:

- ‘*natural abiotic carbonaceous matter’*:
  - *meteorite organic*: organic extracts from meteorites (with a “matter_meteorite” as parent matter)
  - *solar system dust organic*: organic extracts from solar system dust: IDPs, cometary dust, micrometeorites…

For ‘synthesized carbonaceous matter’

- *‘photolysis product’:* carbonaceous matter produced by photolysis of simpler molecules
- *‘radiolysis product’:* carbonaceous matter produced by radiolysis of simpler molecules
- *‘plasma deposited product’:* carbonaceous matter produced by plama deposition
- *‘heating process product’:* carbonaceous matter resulting from heating processes (pyrolysis)

  *Note: Tholin*s are heteropolymer molecules formed by irradiation (UV, electrons, …) of simple organic compounds such as methane

or ethane. So they are either ‘photolysis product’, ‘radiolysis product’ or *‘plasma deposited product’*.

For ‘pure carbon allotrope’:

- ‘*diamond*’: metastable allotrope of carbon, where the carbon atoms are arranged in a variation of the face-centered cubic crystal structure.
- ‘*graphite*’: allotrope of carbon, where the carbon atoms are arranged in a layered planar structure.
- ‘*fullerene*’: molecules of varying sizes composed entirely of carbon, which take the form of a hollow sphere, ellipsoid, or tube and many other shapes.
- ‘*amorphous or disordered carbon’*: carbon that does not have any crystalline structure
- ‘*other carbon allotrope’*: carbon allotrope not listed above,
  ex: Lonsdaleite, Chaoite, …
  cf. http://en.wikipedia.org/wiki/Allotropes_of_carbon

For ‘molecular organics’

- ‘*molecular organic’*: simple condensed (solid or liquid) organic molecule or molecular mixture.

Others:

- ‘*mixed organics’*: more than one of the above organics mixed in the carbonaceous matter (put information on groups in “*matter_carbonaceous*_comments”)
- ‘*other*’: any other organic matter, either natural or synthetic (put information in “*matter_carbonaceous*_comments”)
- ‘*unknown*’: unknown group of carbonaceous matter

http://en.wikipedia.org/wiki/Organic_matter
http://en.wikipedia.org/wiki/Soil_organic_matter
http://en.wikipedia.org/wiki/Kerogen
http://en.wikipedia.org/wiki/Coal
http://en.wikipedia.org/wiki/Petroleum
http://en.wikipedia.org/wiki/Allotropes_of_carbon
http://en.wikipedia.org/wiki/Tholin

*matter_carbonaceous*_component	blob	U	MatCarb	F	--	Additional comments on the component(s) of the carbonaceous matter

s_comments [*matter*_components_comments]		[m]				

Carbonaceous matter global density

*matter_carbonaceous*_compacity [*layer/matter*_compacity]	float	U [m]	MatCarb	F	*no*	Compacity of the carbonaceous matter (fraction of solid material volume per matter volume unit) *Note:* compacity = (1 – porosity) *Note:* value of the raw matter before any preparation for sample
*matter_carbonaceous*_compacity_error [*layer/matter*_compacity_error]	float	U [m]	MatCarb	F	*no*	Absolute uncertainty on the compacity of the carbonaceous matter
*matter_carbonaceous*_density [*layer/matter*_density]	float	U [m]	MatCarb	F	g/cm3	Density of the carbonaceous matter • stored in the database and provided to user in 'g/cm^3' unit *Note:* value of the raw matter before any preparation for sample
*matter_carbonaceous*_density_error [*layer/matter*_density_error]	float	U [m]	MatCarb	F	g/cm3	Absolute uncertainty on the density of the carbonaceous matter • stored in the database and provided to user in 'g/cm^3' unit

Carbonaceous matter global texture

*matter_carbonaceous*_shape [*matter*_shape]	varchar(255)	U [m]	MatCarb	F	--	Description of the macroscopic shape of the carbonaceous matter, mostly for sedimentary organic rocks (compact or cemented/sintered granular textures) *Note:* for loose granular carbonaceous matters: *'undefined (loose)'.* *Exemples:* - For naturally occurring carbonaceous matters: aggregates, dendritic, … - For sedimentary rock: massive, foliated, lamellar, mossy, nodular, … - For (semi-)prepared sedimentary rocks: thick slab, polished thin section, …

*matter_carbonaceous*_texture [*layer/matter*_texture]	enum(text)	U [m]	MatCarb	F	--	Macroscopic texture of the carbonaceous matter (at scale above material grains) OpenEnum: {muddy, earthy, pulverulent, loose fine grained, loose coarse grained, loose granular, sintered granular, cemented granular, mixed granular, compact, compact glassy, compact poor grained, compact fine grained, compact coarse grained, compact lamellar, compact fibrous, compact crystal, compact mixed, single grain, individual grains, aggregated grains, isolated aerosols, aggregated aerosols, clusters, liquid, gaseous, other, unknown} *Definitions: see "layer*_texture*"*
*matter_carbonaceous*_porosity_type [*layer/matter*_porosity_type]	enum(text)	S [!_m]	Mat	F	--	Type of porosity of the matter (at scale above material grains) OpenEnum: {particulate, porous, open pores, closed pores, without pores, other, unknown} *Definitions: voir "layer*_porosity_type*"*

Matter global grain size distribution and texture

*matter_carbonaceous*_grain_size_unit [*sample/matter*_grain_size_unit]	enum(text)	U [£o_m]	MatCarb	F	--	Unit for the carbonaceous matter and material grain sizes (diameter) Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*matter_carbonaceous*_grain_size_min" OR "*matter_carbonaceous*_grain_size_max" has a value *Note DB:* all grain sizes data will be stored in 'mm' *Note:* used for "*matter_carbonaceous*_grain_size_min/_max" and "*material*_grain_size_min/_max" *Note:* the other units are only used in formation and processing conditions ("*matter_carbonaceous*_material_processing_xxx") as text. But it is requested to expres all these units in an homogeneous way by choosing one of each of the following units: • Temperature: {K, °C} • Pressure: {Pa, hPa, mbar, bar, atm, torr} • Time: {s, min, h, d}

						• Energy: {J, kJ, eV, keV, MeV, A, nm, micron, cm-1}
*matter_carbonaceous*_grain_size_method [*material/matter*_grain_size_method]	blob	U [m]	MatCarb	F	--	Description of the grain size (min/max) definition, and of the method of determination of the grain size distribution *Ex:* 'sieving by 2 stainless steel sieves with 50 and 100 µm meshs', 'microscope measurement of section'
matter_carbonaceous_grain_sizes	***List [L6]***	[O]				£: Size distribution of the carbonaceous matter grains *Note*: Used when only a global grain size distribution of the carbonaceous matter is available, not for each of its materials
*matter_carbonaceous*_grain_size_median [*material/matter*_grain_size_median]	float	S3 [m]	MatCarb L6	F	var.	Median size (diameter) of carbonaceous matter grains *Unit:* in "*matter_carbonaceous*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_carbonaceous*_grain_size_unit" *Note*: mostly used when only one median size is known for the matter grains
*matter_carbonaceous*_grain_size_width [*material/matter*_grain_size_width]	float	U [m]	MatCarb L6	F	var.	Full width at half maximum of the size distribution (diameter) of carbonaceous matter grains *Unit:* in "*matter_carbonaceous*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_carbonaceous*_grain_size_unit" *Note*: mostly used when only one median size and its distribution is known for the matter grains
*matter_carbonaceous*_grain_size_min [*material/matter*_grain_size_min]	float	S3 [m]	MatCarb L6	F	var.	Smallest size (diameter) of carbonaceous matter grains of this size range *Unit:* in "*matter_carbonaceous*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_carbonaceous*_grain_size_unit"

*matter_carbonaceous*_grain_size_max [*material/matter*_grain_size_max]	float	S3 [m]	MatCarb L6	F	var.	Largest size (diameter) of carbonaceous matter grains of this size range *Unit:* in "*matter_carbonaceous*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_carbonaceous*_grain_size_unit"
*matter_carbonaceous*_grain_size_fraction [*material/matter*_grain_size_fraction]	float	U [m]	MatCarb L6	F	*no*	Mass fraction of carbonaceous matter grains comprised between size min and size max (diameter) *Note:* value between 0 and 1
*matter_carbonaceous*_grain_size_fraction_error [*material/matter*_grain_size_fraction_error]	float	U [m]	MatCarb L6	F	*no*	Absolute uncertainty on the mass fraction of carbonaceous matter grains comprised between size min and size max (diameter)
*matter_carbonaceous*_grain_size_shape [*material/matter*_grain_size_shape]	enum(text)	S2 [m]	MatCarb L6	F	--	Dominant shape of the carbonaceous matter grains (granular matter) or crystals (compact matter) of this size range Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions:* - see "*matter_solid_grain_size_shape*"
*matter_carbonaceous*_grain_size_distribution [*material/matter*_grain_size_distribution]	blob	U [m]	MatCarb	F	--	Description and parameters of the size distribution of the matter grains *Note:* see "*material*_grain_size_distribution"
*matter_carbonaceous*_grain_texture [*material/matter*_grain_texture]	openum(text)	U [m]	MatCarb	F	--	Description of the major grain texture of the carbonaceous matter OpenEnum: {clay-like, silt-like, compact, compact with defects, compact with bubbles, compact porous, compact microporous, lamellar, fibrous, compact mixed, complex, other, unknown, …} *Definitions:*

							- see ”*matter_solid*_grain_texture”
*matter_carbonaceous*_grain_compacity [*material/matter*_grain_compacity]	float		U [m]	MatCarb	F	*no*	Compacity of the grains of the carbonaceous matter (fraction of solid volume per grain volume unit) *Note:* compacity = (1 – porosity)
*matter_carbonaceous*_grain_compacity_error [*material/matter*_grain_compacity_error]	float		U [m]	MatCarb	F	*no*	Absolute uncertainty on the compacity of the grains of the carbonaceous matter
*matter_carbonaceous*_grain_density [*material/matter*_grain_density]	float		U [m]	MatCarb	F	g/cm^3	Mean bulk density of the grains of the carbonaceous matter • stored in the database and provided to user in ‘g/cm^3’ unit
*matter_carbonaceous*_grain_density_error [*material/matter*_grain_density_error]	float		U [m]	MatCarb	F	g/cm^3	Absolute uncertainty on the mean bulk density of the grains of the carbonaceous matter • stored in the database and provided to user in ‘g/cm^3’ unit
*matter_carbonaceous*_texture_comments [*material/matter*_texture_comments]	blob		U [m]	MatCarb	F	--	Experimentalist additional information or comments about the texture of the carbonaceous matter *Ex:* …
Carbonaceous matter global composition							*Condition*: Used when only a global elemental composition is available, not for each of its constituents
matter_carbonaceous_atoms	***List [L7]***		[O]				£: Global elemental (atomic) composition of the carbonaceous matter.
*matter_carbonaceous*_atom_uid [*] [*material/matter*_atom_uid]	varchar(255)		S1i [!!o_m]	MatCarb Atom	F	--	Link to the existing UID of the atom(s) (natural or isotopic atomic species) composing the carbonaceous matter *Condition:* absolute mandatory when

			L7			*"matter_carbonaceous*_atom_mole_fraction" or "*matter_carbonaceous*_atom_mole_fraction" ≠ Ø *Note:* it is mostly 'C', 'H', 'O', 'N' and 'S', but also can be any other atom.
*matter_carbonaceous*_atom_mole_fraction [+] [*material/matter*_atom_mole_fraction]	float	U [mc]	MatCarb L7	F	*no*	Mole fraction of each type of atom (natural or isotopic atomic species) composing the carbonaceous matter *Constraint*: only when "*matter_carbonaceous*_atom_mass_fraction" = {Ø, NULL} ➔ calculated when "*matter_carbonaceous*_atom_mass_fraction" ≠ {Ø, NULL} for all "*matter_carbonaceous*_atom_uid" ≠ {Ø, NULL} ⇨ "_atom_mole_fraction(atom_j)" = ("_atom_mass_fraction(atom_j)" / "*atom*_molar_mass(atom_j))/ Σi ("_atom_mass_fraction(atom_i)" / "*atom*_molar_mass(atom_i)") ⇨ molar masses of all atoms in the matter => in "*atom species*" table: "*atom*_molar_mass" of each "*matter_carbonaceous*_atom _uid" *Notes:* - value between 0 and 1 - For natural atoms it is the total fraction for this chemical element (no specific isotope).
*matter_carbonaceous*_atom_mass_fraction [*material/matter*_atom_mass_fraction]	float	U [m_co]	MatCarb L7	F	-	Mass fraction of each type of atom (natural or isotopic atomic species) composing the carbonaceous matter *Constraint*: only when "*matter_carbonaceous*_atom_mole_fraction" = {Ø, NULL} ➔ calculated when "*matter_carbonaceous*_atom_mole_fraction" ≠ {Ø, NULL} for all "*matter_carbonaceous*_atom_uid" ≠ {Ø, NULL} ⇨ "_atom_mass_fraction(atom_j)" = ("_atom_mole_fraction(atom_j)" * "*atom*_molar_mass(atom_j)) / Σi ("_atom_mole_fraction(atom_i)" * "*atom*_molar_mass(atom_i)") ⇨ molar masses of all atoms in the matter => in "*atom species*" table:

						“*atom*_molar_mass” of each “*matter_carbonaceous*_atom _uid” *Notes:* - value between 0 and 1 - for natural atoms it is the total fraction for this chemical element (no specific isotope).
*matter_carbonaceous*_H_C_ratio [*matter*_H_C_ratio]	float	S3 [m_co]	MatCarb	F	--	Elemental H/C ratio of the carbonaceous matter ➔ calculated when "*matter_carbonaceous*_atom_mole_fraction" ≠ {Ø, NULL} for “*matter_carbonaceous*_atom_uid” = {ATOM_C, ATOM_ H} ⇨ = “_atom_mole_fraction” [“_atom_uid”= ‘ATOM_ H’] / “_atom_mole_fraction” [“_atom_uid”= ‘ATOM_ C’] OR when *“matter_carbonaceous*_atom_mass_fraction” ≠ {Ø, NULL} ⇨ = 12.0107/1.00794 * “_atom_mass_fraction” [“_atom_uid”= ‘ATOM_ H’] / “_atom_mass_fraction” [“_atom_uid”= ‘ATOM_ C’] *Note:* used in Van Krevelen maturity diagram (H/C versus O/C) http://en.wikipedia.org/wiki/Van_Krevelen_diagram
*matter_carbonaceous*_O_C_ratio [*matter*_O_C_ratio]	float	S3 [m_co]	MatCarb	F	--	Elemental O/C ratio of the carbonaceous matter ➔ calculated when "*matter_carbonaceous*_atom_mole_fraction" ≠ {Ø, NULL for “*matter_carbonaceous*_atom_uid” = {ATOM_C, ATOM_O} ⇨ = “_atom_mole_fraction” [“_atom_uid”= ‘ATOM_ O’] / “_atom_mole_fraction” [“_atom_uid”= ‘ATOM_ C’] OR when *“matter_carbonaceous*_atom_mass_fraction” ≠ {Ø, NULL ⇨ = 12.0107/15.9994 * “_atom_mass_fraction” [“_atom_uid”= ‘ATOM_ O’] / “_atom_mass_fraction” [“_atom_uid”= ‘ATOM_ C’] *Note:* used in Van Krevelen maturity diagram (H/C versus O/C)
*matter_carbonaceous*_N_C_ratio [*matter*_N_C_ratio]	float	S3 [m_co]	MatCarb	F	--	Elemental N/C ratio of the carbonaceous matter ➔ calculated when "*matter_carbonaceous*_atom_mole_fraction" ≠ {Ø, NULL

						for "*matter_carbonaceous*_atom_uid" = {ATOM_C, ATOM_N} ⇨ = "_atom_mole_fraction" ["_atom_uid"= 'ATOM_ N'] / "_atom_mole_fraction" ["_atom_uid"= 'ATOM_ C'] OR when "*matter_carbonaceous*_atom_mass_fraction" ≠ Ø ⇨ = 12.0107/14.0067 * "_atom_mass_fraction" ["_atom_uid"= 'ATOM_ N'] / "_atom_mass_fraction" ["_atom_uid"= 'ATOM_ C']
*matter_carbonaceous*_S_C_ratio [*matter*_S_C_ratio]	float	S3 [m_co]	MatCarb	F	--	Elemental S/C ratio of the carbonaceous matter ➔ calculated when "*matter_carbonaceous*_atom_mole_fraction" ≠ {Ø, NULL for "*matter_carbonaceous*_atom_uid" = {ATOM_C, ATOM_S} ⇨ = "_atom_mole_fraction" ["_atom_uid"= 'ATOM_ S'] / "_atom_mole_fraction" ["_atom_uid"= 'ATOM_ C'] OR when "*matter_carbonaceous*_atom_mass_fraction" ≠ {Ø, NULL ⇨ = 12.0107/32.065 * "_atom_mass_fraction" ["_atom_uid"= 'ATOM_ S'] / "_atom_mass_fraction" ["_atom_uid"= 'ATOM_ C']
*matter_carbonaceous*_sp2_sp3_ratio [*matter*_sp2_sp3_ratio]	float	S3 [m]	MatCarb	F	--	sp2/sp3 ratio of the carbon of the carbonaceous matter *Definition:*
*matter_carbonaceous*_gap_Tauc [*matter*_gap_Tauc]	float	S3 [m]	MatCarb	F	--	Tauc Gap of the carbonaceous matter *Definition:* the optical band gap refers to the energy difference (in electron volts) between the top of the valence band and the bottom of the conduction band in insulators and semiconductors. http://en.wikipedia.org/wiki/Tauc_plot
*matter_carbonaceous*_gap_E04 [*matter*_gap_E04]	float	S3 [m]	MatCarb	F	eV	Band gap E04 of the carbonaceous matter *Definition:* the band gap E04 is the energy at which the absorption coefficient reaches 10^4 cm^{-1}

*matter_carbonaceous*_composition_comments [*matter*_composition_comments]	blob	U [m]	MatCarb	F	--	Any additional information or comments on the composition of the carbonaceous matter *Ex:* sum of atomic fractions, vitrinite reflectance VR (in oil: %Ro) of coal carbonaceous matter, … *Note:* also additional information on impurities not measured

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Carbonaceous matter composition

Note: Whatever are the materials that constitute the carbonaceous matter they will be always defined from the ”material” level (link(s) with “*matter_carbonaceous*_material_index”) through their “constituents” and “species”, or through other matter(s). Only their type of mixing is described here.

*matter_carbonaceous*_materials_mixing [+] [*matter*_materials_mixing]	enum(text)	S2 [!_m]	MatCarb	F	--	How the different materials are mixed in the carbonaceous matter Enum: {single material, homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, spatial distribution...} *Definitions:* cf. “*layer*_materials_mixing”
*matter_carbonaceous*_materials_number [+][-xml] [*matter*_materials_number]	int(10)	U [!_c]	MatCarb	F	*no*	Number of different materials mixed in the carbonaceous matter ➔ calculated from " *matter_carbonaceous*_materials" list
matter_carbonaceous_matters	***List [L8a]***	[!]				£: matters constituting this carbonaceous matter
*matter_carbonaceous*_matter_index [*][-xml] [*matter*_matter_index] ➢ Same structure as “*sample*”	int(10) [Internal link]	B [!_g]	MatCarb MatXxx L8a	F	--	ID of the matters(s) constituting the ‘carbonaceous matter’ *Note xml:* in practice the description of the material(s) is done directly under “*matter_carbonaceous*” without providing the ID link
matter_carbonaceous_materials	***List [L8b]***	[!]				£: materials constituting this carbonaceous matter
*matter_carbonaceous*_material_index [*][-xml] [*matter*_material_index]	int(10) [Internal link]	U/S [!_g]	MatCarb Mater	F	--	ID of the material(s) constituting the ‘carbonaceous matter’ *Note:* The different organic solids (fundamental phases or custom constituents) composing the carbonaceous matter are described inside this materials

➢ Same structure as "*sample*"			L8b				structure at the constituent level. The different, molecules, chemical functions (chemical description) and/or atoms (elemental composition) composing the extraterrestrial matter are described at the species level. *Note xml:* in practice the description of the matter-material(s) is done directly under "matter_carbonaceous" without providing the ID link
*matter_carbonaceous*_comments [*matter*_comments]	blob		U [m]	MatCarb	F	--	Additional information on the carbonaceous matter (minor impurities, …) or comments on the composition of the actual organic species or functions of the carbonaceous matter

Precursor materials .

Note: "*material*_is_precursor" = 'true'

Note: refer to the same table as "*materials*" in the sample structure but without the "material arrangement and abundance" bloc

See definitions and notes in "*Mineral matter*"

matter_carbonaceous_precursor_materials *[matter_precursor_materials]*	***List [L9]***	[O]	MatCarb PreMater L9	£: Precursor materials used to create the carbonaceous matter *Condition:* description of precursor materials is optional

- Use exactly the same structure as for "*Mineral matter*"

Carbonaceous matter processings

matter_carbonaceous_processings *[matter_processings]*	***List [L10]***	[O]	MatCarb L10	£: Processing steps of the precursor materials/matters *Condition:* only when there is processing of materials or parent matter/sample

- Use exactly the same structure as for "*Mineral matter*"

Carbonaceous matter documentation and references

matter_carbonaceous_documentations	***List [L11]***	[O]		£: Documentations about the carbonaceous matter

*matter_carbonaceous*_documentation_name [*sample_documentation_name*]	varchar(255)	U [m]	MatCarb L11	F	--	Name of the documentation describing the carbonaceous matter *Note:* this name will appear as the documentation title in the database *Ex:* 'Analysis of PC2742 Coal'
*matter_carbonaceous*_documentation_filename [*sample_documentation_filename*]	varchar(255)	U [m]	MatCarb L11	F	--	File name (with extension) of the documentation describing the carbonaceous matter *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database
matter_carbonaceous_links	***List [L12]***	[O]				£: Web pages describing the carbonaceous matter and its properties
*matter_carbonaceous*_link_name [*matter*_link_name]	varchar(255)	U [m]	MatCarb L12	F	--	Name of the web page(s) describing the carbonaceous matter and its properties. *Ex:* 'Institut Français du Pétrole', …
*matter_carbonaceous*_link_url [*matter*_link_url]	varchar(255)	U [m]	MatCarb L12	F	--	URL address(es) of the web page(s) describing the carbonaceous matter and its properties *Note:* useful when the carbonaceous matter comes from a organic database, a stable commercial supplier, a laboratory, ... *Notes*: - can also link to various types of measurements made on this matter - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
matter_carbonaceous_publications	***List [L13]***	[O]				£: Publications describing the carbonaceous matter and its properties.
*matter_carbonaceous*_publication_uid [*] [*matter*_publication_uid]	varchar(255)	S2 [m]	MatCarb Publi	F	--	Link to the existing UID of the publication(s) describing the carbonaceous matter(s) and its properties.

L13	*Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

7.5 Extraterrestrial matter Table

Root of the table: ***matter_extraterrestrial***

Data type: 'Matter'

Definition: '*extraterrestrial matter'* is any complex extraterrestrial matter made of organics and/or minerals found either on Earth (meteorite, micrometeorites), or collected in Earth atmosphere or in orbit (IDPs), or in interplanetary space (Cosmic dust: asteroidal and cometary dust, …), but excluding planetary bodies (planets, satellites, asteroids, comets, …).

Notes:

- Extraterrestrial minerals, carbonaceous matters, or fluids extracted from meteorite, micrometeorites, IDPs or cosmic dust will be entrered as "extraterrestrial matters"
- Any other minerals/rocks, carbonaceous matters, or fluids collected at the surface or in the atmosphere of planetary bodies (planets, satellites, asteroids, comets, TNO, …) will be entered as "fluid, solid or carbonaceous matters"

Key-word	Type	Level	Table	Exp	Unit	Description
Extraterrestrial matter import						
*matter_extraterrestrial*_import_mode [*matter*_import_mode]	enum(text)	P [!!_m]	MatExtra	F	--	Mode of import of the "extraterrestrial matter" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*matter_extraterrestrial*_xml_filename [-xml] [*matter*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	MatExtra	(V)	--	Name of the storage copy of the xml import file of the "*matter_extraterrestrial*" metadata ➔ determined automatically during import (from "*matter_extraterrestrial*_uid" ?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Extraterrestrial matter indexes						

*matter_extraterrestrial*_index [**][-xml] [*matter*_index]	int(11)	B [!!_g]	MatExtra	F	--	Automatic random but unique number (ID) given to new extraterrestrial matter
*matter_extraterrestrial*_uid [**] [*matter*_uid]	varchar(255)	P/U [!!_m]	MatExtra	F	--	Unique identifier code (UID) given to the extraterrestrial matter table (to be created) *Nomenclature:* Create this UID very accurately in order to be simple and unique. - It should be of the style 'MATXXX_ExtraterrestrialObject_AB_yyyymmdd' where o MATXXX is: – 'MATMET' for meteorites collected on Earth – 'MATIDP' for interplanetary dust particles (IDP) collected in Earth atmosphere – 'MATMICROMET' for micrometeorites collected on Earth – 'MATDUST' for cometary, asteroidal and interplanetary dust particle o 'ExtraterrestrialObject' is the name of the extraterrestrial object (ex: "*object_meteorite*_name"), 'AB' are the initials of the person preparing the import, or of the experimentalist preparing the matter ("*experimentalist*_acronym" of "*matter_extraterrestrial*_experimentalist"), 'yyyymmdd' is the full date of creation of the matter (from "*matter_extraterrestrial*_date"). *Note*: if several matters are created the same day with the same extraterrestrial object then add some distinguishing property after 'ExtraterrestrialName'. *Ex:* - 'MATMET_Allende_LB_20131003' - 'MATMICROMET_DC060937_LF_20130828'
matter_extraterrestrial_owner_databases	***List [L0]***	[!!]				£: databases which manage this matter

[*matter*_owner_database_uid]						
*matter_extraterrestrial*_owner_database_uid [*] [*matter*_owner_database_uid]	varchar(255)	P/U [!!o_m]	MatExtra DatBas L0	F	--	Link(s) to the existing UID(s) of the database which owns and manages this matter information *Condition:* at least one database *Note:* For common 'reference' matters and for matters from external laboratories (not managed by a database), it should be 'DB_SSHADE'
Extraterrestrial matter experimentalist						
matter_extraterrestrial_experimentalists	***List [L1]***	[O]				£: experimentalists who prepared the matter
*matter_extraterrestrial*_experimentalist_uid [*] [*matter*_experimentalist_uid]	varchar(255)	P/U [m]	MatExtra Exper L1	F	--	Link to the existing UID of the experimentalist(s) which prepared (section, selection, extraction, …) the extraterrestrial matter *Condition:* can be no experimentalist when the matter is delivered ready, or can be the person who prepared the piece at the repository lab.
Extraterrestrial matter family and description						
*matter_extraterrestrial*_family [-xml] [*matter*_family]	enum(text)	S [!!_g]	MatExtra	F	--	Family of the extraterrestrial matter Enum: {extraterrestrial} *Default* = 'extraterrestrial' *Definitions:* - '*extraterrestrial*': matters primarily made of extraterrestrial materials
*matter_extraterrestrial*_name [*matter*_name]	varchar(255)	S [!!_m]	MatExtra	F	--	Common or given name of the extraterrestrial matter *Notes:* – It should contain explicit info on the matter or constituting materials/constituent/species: name(s) and some typical properties of the matter (phase type, components, preparation, …). – It may be the name of the extraterrestrial object plus some feature

						– It is used as the title of the matter in the sample structure bloc of the SSHADE interface *Ex:* 'Allende slice', 'Nagoya powder', 'ALH8044 IOM extract', …
*matter_extraterrestrial*_date [*matter*_date]	date	P [!_m]	MatExtra	F	YYYY-MM-DD	Date of creation of the matter *Note:* This date can be the date of delivery of the extraterrestrial object (or the date of preparation of the piece at the repository lab), or of end of processing(s) in the case of a matter generated by some processing (selection, extraction, …) of a parent extraterrestrial matter
*matter_extraterrestrial*_parent_matter_uid [*] [*matter*_parent_matter_uid]	varchar(255)	S2/S1i [$o_m]	MatExtra MatXxx	F	--	Link to the existing UID of the parent matter (if present in the database) used to create this one by some processing (e.g. thermal cycle, irradiation, sieving, …) *Recommendation:* Strongly recommended when already exist in the database *Ex:* a granular matter sieved to a specific grain size range gives a daughter matter from the parent unsieved matter.
*matter_extraterrestrial*_first_parent_matter_uid [*] [-xml] [*matter*_first_parent_matter_uid]	varchar(255)	S2/S1i [!o_c]	MatExtra MatXxx	F	--	Link to the existing UID of the first parent of the generation of matters (present in the database) that has been initially used to create this one by a series of processes. *Condition:* when "*matter_extraterrestrial*_parent_matter_uid" ≠ Φ ➔ calculated recursively using "*matter_extraterrestrial*_parent_matter_uid", when it exist
Extraterrestrial matter origin						
*matter_extraterrestrial*_level [*matter*_level]	enum(text)	S2 [!_m]	MatExtra Matter	F	--	Level of the extraterrestrial matter Enum: {from sample return mission, from international repository, from laboratory repository, from commercial supplier, local matter, other} *Definitions:* cf. *"matter_solid*_level"

*matter_extraterrestrial*_origins	***List [L2b]***	[O]					£: Origins of the solid matter
*matter_extraterrestrial*_origin [*matter*_origin]	enum(text)	S [!!_m]	MatExtr Matter L2b	F	F	-- --	Origin of the extraterrestrial matter Enum: {natural terrestrial, extraterrestrial, planetary, laboratory, commercial, simulated} *Definitions: cf. "matter_solid*_origin" *Note:* - An extraterrestrial matter should be fully or predominantly either of extraterrestrial ot planetary origin - it may coexist with some natural terrestrial material such as in breccia - it may also be mixed with some natural terrestrial or synthetic material (e.g. darkening material, dilution/matrix material, glue …) - In some rare cases it may also be simulated (numerical simulation)

Extraterrestrial matter provider

*matter_extraterrestrial*_provider [*matter*_provider]	varchar(255)	S [!_m]	MatExtr Matter	F	F	-- --	origin of the extraterrestrial matter: extraterrestrial object repository, laboratory (name), commercial (name) + web address ...
*matter_extraterrestrial*_provider_reference_code [*matter*_provider_reference_code]	varchar(255)	S [m]	MatExtr Matter	F	F	-- --	Reference code (catalog number or name) given by the provider of the extraterrestrial matter (e.g., section number)
*matter_extraterrestrial*_igsn_code [*matter*_igssn_code]	varchar(255)	S [m]	MatSol Matter	F	F	-- --	'International Geo Sample Number'code (*IGSN*) of the extraterrestrial matter *Constraint:* only when *"matter_extraterrestrial*_origin" = {natural terrestrial, extraterrestrial} *Definition*: The IGSN is an alphanumeric code that uniquely identifies samples from our natural environment and related sampling features (http://www.geosamples.org) *Ex:* 'IEJEN00CH'

*matter_extraterrestrial*_igsn_url [-xml] [*matter*_igssn_url]	varchar(255)	SU [!o_c]	MatSol MatExtra	F	--	url address of the information page for extraterrestrial matters with an IGSN code *Condition:* mandatory when "*matter_extraterrestrial_* igsn_code" ≠ Ø ➔ *Calculated* with https://app.geosamples.org/sample/igsn/"*matter_extraterrestrial*_igsn_code" *Ex*: 'https://app.geosamples.org/sample/igsn/IEJEN00CH' for IGSN='IEJEN00CH'
*matter_extraterrestrial*_local_reference_code [*matter*_local_reference_code]	varchar(255)	SU [m]	MatExtra Matter	F	--	Local reference number or name given by local experimentalists to the extraterrestrial matter *Note:* could be used to provide meteorite extract number, or type of preparation through this code…

Extraterrestrial matter: planetary body

*matter_extraterrestrial*_object_uid [*] [*matter*_object_uid]	varchar(255)	S1 [!o_m]	MatExtra Matter ObjMet	F	--	Link to the existing UID of the object to which the extraterrestrial matter belong *Condition:* absolute mandatory when *"matter_extraterrestrial*_origin" = {extraterrestrial, planetary} *Note:*

Extraterrestrial matter images

matter_extraterrestrial_images	***List [L2]***	[O]				£: Pictures of the extraterrestrial matter
*matter_extraterrestrial*_image_filename [*matter*_image]	varchar(255)	U [m]	MatExtra L2	F	--	File name(s) (with extension) of the picture(s) of the extraterrestrial matter *Image formats:* .png, .jpg, (.gif) *Note:* this file will be imported in the database
*matter_extraterrestrial*_image_caption	varchar(255)	U	MatExtra	F	--	Caption(s) or comment(s) on the picture(s) of the extraterrestrial matter

[*matter*_image_caption]		[m]	L2				

Extraterrestrial matter location

*matter_extraterrestrial*_grain_type [*matter*_grain_type]	enum(text)	S [!o_m]	S Matter	F	--	--	Type of extraterrestrial grains Enum: {single grain, grains cluster} *Condition*: only and mandatory when "*matter_extraterrestrial*_object_uid" / "*object_xxx*_family"= {micrometeorite, idp, planetary aerosol, planetary dust, interplanetary dust} *Definitions*: - '*single grain'*: individual IDPs with diameter ranging from 1–50 mm, although most are between 5 and 15 mm - '*grains cluster'*: large 50–500 mm diameter particles (10–20% of collected IDPs) that fragment into many pieces when they impact the flags *Ex*: 'single grain' for a Hayabusa grain, 'cluster' for IDP clusters, …
*matter_extraterrestrial*_location [*matter*_location]	varchar(255)	S1b [!o_m]	S Matter	F	--	--	Information on the location of the extraterrestrial matter on/in the object (meteorite, …) *Condition*: mandatory when "*matter_extraterrestrial*_object_uid" / object_xxx_family" = {meteorite} *Note*: - Mostly used for meteorites - it can be information on the piece of meteorite (catalog number and mass of the piece, …) that make the matter and its location on the wole meteorite object (if known) - for a fragment of a micrometeorite, you can say which part it is (if easy to describe!) *Ex:* - 'Crust of Allende meteorite': case of meteorite pieces (surface, interior, …) - 'fragment of the micrometeorite DC06-09-54': case of micrometeorite

							fragment
Extraterrestrial matter preparation and component types							
*matter_extraterrestrial*_preparation [*matter*_preparation]	enum(text)	U [!_m]	MatExtra	F			Type of preparation of the extraterrestrial matter Enum: {raw, section, polished section, selected components, sieved fraction, extracted components} *Definitions:* - '*raw'*: extraterrestrial object (or piece) without chemical treatment nor selection of a particular component nor other type of preparation (cutting, polishing, …) - '*section*': raw rock (or grain) cut and potentially polished by different ways - '*selected components'*: peculiar petrologic entity (chondrules, CAIs, metal grains, matrix grains, specific minerals...) selected mechanically without any chemical treatment - '*sieved fraction'*: size fraction separated by sieving - '*extracted components'*: meteoritic materials/phase extracted using a chemical or physical treatment (Insoluble Organic Matter, Soluble Organic Matter, …)
*matter_extraterrestrial*_method [*matter*_method]	varchar(255)	SU [m]	MatExtra Matter	F	--	--	Method of preparation or extraction of the extraterrestrial matter *Note:* short synthetic description only. Full description will be done in "processing(s)" *Ex:* 'meteorite powder prepared by crushing and sieving rock pieces', 'soluble organic matter extracted by chemical dissolution', …
*matter_extraterrestrial*_storage_condition [*matter*_storage_condition]	varchar(255)	SU [m]	MatExtra Matter	F	--	--	Storage condition of this extraterrestrial matter *Ex:* 'stored at 20°C in 1 bar of pure and dry Ar gas since field collection', … *Notes*: see "*matter_solid*_storage_condition"

*matter_extraterrestrial*_phase_type [*matter*_phase_type]	enum(text)	S0/S2s [!_m]	MatExtra	F	--	Type of phase of the extraterrestrial matter Enum: {solid, liquid, gas} *Note:* if there are several phase types, then give the main here and add a comment in "*matter_extraterrestrial*_comments"
matter_extraterrestrial_componen ts [*matter_components*]	***List [L3]***	[!]				£: Components type of the extraterrestrial matter
*matter_extraterrestrial*_componen t_type [*matter*_component_type]	enum(text)	S [!_m]	MatExtra L3	F	--	Type(s) of component(s) in the extraterrestrial matter Enum: {bulk, matrix, chondritic matrix, chondrules, CAI, presolar grains, extracted SOM, extracted IOM, minerals, metal, other} *Definitions:* For all: – '*bulk*': all components of the extraterrestrial object – 'matrix': material cimenting various petrographic units – '*minerals*': mineral grains (not identified as chondrules or CAI) or minerals in non-chondritic meteorite – '*metal*': metal grains – '*presolar grains'*: presolar grains – '*other*': all other types of components (describe in "comments") For chondritic extraterrestrial matter and primitive cosmic dust matter: – '*chondritic matrix*': fine-grained interchondrule matrix (organics and minerals) between high-temperature components or matrix rims around high-temperature components – '*chondrules*': chondrules (minerals) – '*CAI'*: Ca-Al-rich Inclusions (minerals) – '*presolar grains'*: presolar grains present in the matrix For extracted organics – '*extracted SOM'*: soluble organic matter (SOM) extracted from the bulk – '*extracted IOM'*: insoluble organic matter (IOM) extracted from the

						bulk
*matter_extraterrestrial*_componen ts_comments [*matter*_components_comments]	blob	U [m]	MatExtra	F	--	Additional comments on the component(s) of the extraterrestrial matter
Extraterrestrial matter global density						
*matter_extraterrestrial*_compacity [*layer/matter*_compacity]	float	U [m]	MatExtra	F	*no*	Compacity of the extraterrestrial matter (fraction of solid material volume per matter volume unit) *Note:* compacity = (1 – porosity) *Note:* value of the raw matter before any preparation for sample
*matter_extraterrestrial*_compacity _error [*layer/matter*_compacity_error]	float	U [m]	MatExtra	F	*no*	Absolute uncertainty on the compacity of the extraterrestrial matter
*matter_extraterrestrial*_density [*layer/matter*_density]	float	U [m]	MatExtra	F	g/cm3	Density of the extraterrestrial matter • stored in the database and provided to user in 'g/cm^3' unit *Note:* value of the raw matter before any preparation for sample
*matter_extraterrestrial*_density_er ror [*layer/matter*_density_error]	float	U [m]	MatExtra	F	g/cm3	Absolute uncertainty on the density of the extraterrestrial matter • stored in the database and provided to user in 'g/cm^3' unit
Extraterrestrial matter global texture						
*matter_extraterrestrial*_shape [*matter*_shape]	varchar(255)	U [m]	MatExtra	F	--	Description of the macroscopic shape of the extraterrestrial matter, mostly for compact pieces (compact or cemented/sintered granular textures) *Note:* for loose granular extraterrestrial objects: *'undefined (loose)'.* *Exemples:* - For naturally occurring meteorites: irregular, with faceted surfaces,

						cone-shaped, shrapnel, with flow features, with regmaglypts, … - For (semi-)prepared meteorites: thick slab, polished thin section, raw fractured meteorite, flat fractured meteorite (roughness of the order of the grain size), conchoidal fractured meteorite, …
*matter_extraterrestrial*_texture [*layer/matter*_texture]	enum(text)	U [m]	MatExtra	F	--	Macroscopic texture of the extraterrestrial matter (at scale above material grains) OpenEnum: {muddy, earthy, pulverulent, fluffy fine grained, fine grained, fine grained scoriaceous, scoria, loose fine grained, loose coarse grained, loose granular, sintered granular, cemented granular, mixed granular, compact, compact glassy, compact poor grained, compact fine grained, compact coarse grained, compact lamellar, compact fibrous, compact crystal, compact mixed, single grain, individual grains, aggregated grains, isolated aerosols, aggregated aerosols, clusters, liquid, gaseous, other, unknown} *Definitions:* - See "*layer*_texture" For micrometeorites - '*fluffy fine grained'*: - '*fine grained'*: - '*fine grained scoriaceous'*: - '*scoria*':
*matter_extraterrestrial*_porosity_type [*layer/matter*_porosity_type]	enum(text)	S [!_m]	Mat	F	--	Type of porosity of the matter (at scale above material grains) OpenEnum: {particulate, porous, open pores, closed pores, without pores, other, unknown} *Definitions: see "layer*_porosity_type*"*

Matter global grain size distribution and texture

*matter_extraterrestrial*_grain_size_unit [*sample/matter*_grain_size_unit]	enum(text)	U [£o_m]	MatExtra	F	--	Unit for the extraterrestrial matter and material grain sizes Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*matter_extraterrestrial*_grain_size_min" OR

						"*matter_extraterrestrial*_grain_size_max" has a value *Note DB:* all grain sizes data will be stored in 'mm' *Note:* used for "*matter_extraterrestrial*_grain_size_min/_max" and "*matter_extraterrestrial*_material_grain_size_min/_max" *Note:* the other units are only used in formation and processing conditions ("*matter_extraterrestrial*_material_processing_xxx") as text. But it is requested to expres all these units in an homogeneous way by choosing one of each of the following units: • Temperature: {K, °C} • Pressure: {Pa, hPa, mbar, bar, atm, torr} • Time: {s, min, h, d} • Energy: {J, kJ, eV, keV, MeV, A, nm, micron, cm-1}
*matter_extraterrestrial*_grain_size_method [*material/matter*_grain_size_method]	blob	U [m]	MatExtra	F	--	Description of the grain size (min/max) definition, and of the method of determination of the grain size distribution *Ex:* 'sieving between 2 stainless steel sieves with 50 and 100 µm meshs', 'microscope measurement of section'
matter_extraterrestrial_grain_sizes	***List [L4]***	[O]				£: Size distribution of the extraterrestrial matter grains *Note*: Used when only a global grain size distribution of the extraterrestrial matter is available, not for each of its materials
*matter_extraterrestrial*_grain_size_median [*material/matter*_grain_size_median]	float	S3 [m]	MatExtra L4	F	var.	Median size (diameter) of extraterrestrial matter grains *Unit:* in "*matter_extraterrestrial*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_extraterrestrial*_grain_size_unit" *Note*: mostly used when only one median size is known for the matter grains
*matter_extraterrestrial*_grain_size_width [*material/matter*_grain_size_widt	float	U [m]	MatExtra L4	F	var.	Full width at half maximum of the size distribution (diameter) of extraterrestrial matter grains *Unit:* in "*matter_extraterrestrial*_grain_size_unit"

h]						• converted in 'm' unit in the database but provided to user in "*matter_extraterrestrial*_grain_size_unit" *Note*: mostly used when only one median size and its distribution is known for the matter grains
*matter_extraterrestrial*_grain_size_min [*material/matter*_grain_size_min]	float	S3 [m]	MatExtra L4	F	var.	Smallest size (diameter) of extraterrestrial matter grains of this size range *Unit:* in "*matter_extraterrestrial*_grain_size_unit" (will be 'micron' by default if you did not filled this unit) • converted in 'm' unit in the database but provided to user in "*matter_extraterrestrial*_grain_size_unit"
*matter_extraterrestrial*_grain_size_max [*material/matter*_grain_size_max]	float	S3 [m]	MatExtra L4	F	var.	Largest size (diameter) of extraterrestrial matter grains of this size range *Unit:* in "*matter_extraterrestrial*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*matter_extraterrestrial*_grain_size_unit"
*matter_extraterrestrial*_grain_equivalent_diameter	float	U [mc]	MatExtra L4	F	µm	Equivalent diameter, Deq, of extraterrestrial matter grains *Unit:* micrometers *Condition*: use either 'equivalent diameter' or 'size_min/max' *Note*: this equivalent diameter can be either measured or calculated from 'size_min/max': ➔ when 'size_min/max' have values, then • Deq= $(max \times min^2)^{1/3}$
*matter_extraterrestrial*_grain_size_fraction [*material/matter*_grain_size_fraction]	float	U [m]	MatExtra L4	F	*no*	Mass fraction of extraterrestrial matter grains comprised between size min and size max (diameter) *Note:* value between 0 and 1
*matter_extraterrestrial*_grain_size_fraction_error	float	U [m]	MatExtra L4	F	*no*	Absolute uncertainty on the mass fraction of extraterrestrial matter grains

[*material/matter*_grain_size_fraction_error]						comprised between size min and size max (diameter)
*matter_extraterrestrial*_grain_size_shape [*material/matter*_grain_size_shape]	enum(text)	S2 [m]	MatExtra L4	F	--	Dominant shape of the extraterrestrial matter grains (granular matter) or crystals (compact matter) of this size range Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions:* - cf. "*matter_solid*_grain_size_shape"
*matter_extraterrestrial*_grain_size_distribution [*material/matter*_grain_size_distribution]	blob	U [m]	MatExtra	F	--	Description and parameters of the size distribution of the matter grains *Note:* see "*material*_grain_size_distribution"
*matter_extraterrestrial*_grain_texture [*material/matter*_grain_texture]	openum(text)	U [m]	MatExtra	F	--	Description of the major grain texture of the extraterrestrial matter OpenEnum: {clay-like, silt-like, compact, compact with defects, compact with bubbles, compact porous, compact microporous, lamellar, fibrous, compact mixed, complex, other, unknown, …} *Definitions:* - See "*matter_solid*_grain_texture"
*matter_extraterrestrial*_grain_compacity [*material/matter*_grain_compacity]	float	U [m]	MatExtra	F	*no*	Compacity of the grains of the extraterrestrial matter (fraction of solid volume per grain volume unit) *Note:* compacity = (1 – porosity)
*matter_extraterrestrial*_grain_compacity_error [*material/matter*_grain_compacity	float	U [m]	MatExtra	F	*no*	Absolute uncertainty on the compacity of the grains of the extraterrestrial matter

_error]						
*matter_extraterrestrial*_grain_density [*material/matter*_grain_density]	float	U [m]	MatExtra	F	g/cm^3	Mean bulk density of the grains of the extraterrestrial matter • stored in the database and provided to user in 'g/cm^3' unit
*matter_extraterrestrial*_grain_density_error [*material/matter*_grain_density_error]	float	U [m]	MatExtra	F	g/cm^3	Absolute uncertainty on the mean bulk density of the grains of the extraterrestrial matter • stored in the database and provided to user in 'g/cm^3' unit
*matter_extraterrestrial*_texture_comments [*material/matter*_texture_comments]	blob	U [m]	MatExtra	F	--	Experimentalist additional information or comments about the texture of the extraterrestrial matter *Ex:* …
Extraterrestrial matter global oxides composition						*Note*: Used when only a global composition is available, and not for each of its extraterrestrial object mineral materials
matter_extraterrestrial_oxides	***List [L5a]***	[O]				£: Description of the oxides composition of the mineral materials of the extraterrestrial matter
*matter_extraterrestrial*_oxide_formula [*material/matter*_oxide_formula]	CS- enum(text)	U [m]	MatExtra L5a	F	--	Formula of the different oxides composing the the mineral materials of the extraterrestrial matter Enum: *see mineral*_oxide_formula *Note:* did not distinguish non-natural isotopic species
*matter_extraterrestrial*_oxide_mass_fraction [*material/matter*_oxide_mass_fraction]	float	U [m]	MatExtra L5a	F	%	Mass fraction (in %) of each type of oxide composing the mineral materials *Note:* value between 0 and 100
*matter_extraterrestrial*_oxides_comments	blob	U	MatExtra	F	--	Any additional information (sum of oxides …) or comments on the oxides

[*material/matter*_oxides_comments]		[m]				composition of the extraterrestrial matter *Note:* also additional information on impurities not measured by oxides
Extraterrestrial matter global composition						*Condition*: Used when only a global elemental composition is available, not for each of its constituents
matter_extraterrestrial_atoms	***List [L5b]***	[O]				£: Global elemental (atomic) composition of the carbonaceous matter.
*matter_extraterrestrial*_atom_uid [*] [*material/matter*_atom_uid]	varchar(255)	S1i [!!o_m]	MatExtra Atom L5b	F	--	Link to the existing UID of the atom(s) (natural or isotopic atomic species) composing the carbonaceous extraterrestrial matter *Condition:* absolute mandatory when *"matter_extraterrestrial*_atom_mole_fraction" or "*matter_extraterrestrial*_atom_mole_fraction" ≠ Ø *Note:* it is mostly 'C', 'H', 'O', 'N' and 'S', but also can be any other atom.
*matter_extraterrestrial*_atom_mole_fraction [+] [*material/matter*_atom_mole_fraction]	float	U [mc]	MatExtra L5b	F	*no*	Mole fraction of each type of atom (natural or isotopic atomic species) composing the carbonaceous extraterrestrial matter *Constraint*: only when "*matter_extraterrestrial*_atom_mass_fraction" = {Ø, NULL} ➔ calculated when "*matter_extraterrestrial*_atom_mass_fraction" ≠ {Ø, NULL} for all "*matter_extraterrestrial*_atom_uid" ≠ {Ø, NULL} See calculation in "*matter_carbonaceous*_atom_mole_fraction" *Notes:* - value between 0 and 1 - For natural atoms it is the total fraction for this chemical element (no specific isotope).
*matter_extraterrestrial*_atom_mass_fraction [*material/matter*_atom_mass_fraction]	float	U [mc]	MatExtra L5b	F	-	Mass fraction of each type of atom (natural or isotopic atomic species) composing the carbonaceous extraterrestrial matter *Constraint*: only when "*matter_extraterrestrial*_atom_mole_fraction" = {Ø,

						NULL} ➔ calculated when "*matter_extraterrestrial*_atom_mole_fraction" ≠ {Ø, NULL} for all "*matter_extraterrestrial*_atom_uid" ≠ {Ø, NULL} See calculation in "*matter_carbonaceous*_atom_mass_fraction" *Notes:* - value between 0 and 1 - For natural atoms it is the total fraction for this chemical element (no specific isotope).
*matter_extraterrestrial*_H_C_ratio [*matter*_H_C_ratio]	float	S3 [mc]	MatExtra	F	--	Elemental H/C ratio of the carbonaceous extraterrestrial matter ➔ calculated when "*matter_extraterrestrial*_atom_mole_fraction" ≠ {Ø, NULL} for "*matter_extraterrestrial*_atom_uid" = {ATOM_C, ATOM_ H} See calculation in "*matter_carbonaceous*_H_C_ratio" *Note:* used in Van Krevelen maturity diagram (H/C versus O/C) http://en.wikipedia.org/wiki/Van_Krevelen_diagram
*matter_extraterrestrial*_O_C_ratio [*matter*_O_C_ratio]	float	S3 [mc]	MatExtra	F	--	Elemental O/C ratio of the carbonaceous extraterrestrial matter ➔ calculated when "*matter_extraterrestrial*_atom_mole_fraction" ≠ {Ø, NULL} for "*matter_extraterrestrial*_atom_uid" = {ATOM_C, ATOM_ O} See calculation in "*matter_carbonaceous*_O_C_ratio" *Note:* used in Van Krevelen maturity diagram (H/C versus O/C)
*matter_extraterrestrial*_N_C_ratio [*matter*_N_C_ratio]	float	S3 [mc]	MatExtra	F	--	Elemental N/C ratio of the carbonaceous extraterrestrial matter ➔ calculated when "*matter_extraterrestrial*_atom_mole_fraction" ≠ {Ø, NULL} for "*matter_extraterrestrial*_atom_uid" = {ATOM_C, ATOM_ N} See calculation in "*matter_carbonaceous*_N_C_ratio"
*matter_extraterrestrial*_S_C_ratio [*matter*_S_C_ratio]	float	S3 [mc]	MatExtra	F	--	Elemental S/C ratio of the carbonaceous extraterrestrial matter ➔ calculated when "*matter_extraterrestrial*_atom_mole_fraction" ≠ {Ø,

						NULL} for "*matter_extraterrestrial*_atom_uid" = {ATOM_C, ATOM_ S} See calculation in "*matter_carbonaceous*_S_C_ratio"
*matter_extraterrestrial*_sp2_sp3_ratio [*matter*_sp2_sp3_ratio]	float	S3 [m]	MatExtra	F	--	sp2/sp3 ratio of the carbon of the carbonaceous extraterrestrial matter *Definition:*
*matter_extraterrestrial*_gap_Tauc [*matter*_gap_Tauc]	float	S3 [m]	MatExtra	F	--	Tauc Gap of the carbonaceous extraterrestrial matter *Definition:* the optical band gap refers to the energy difference (in electron volts) between the top of the valence band and the bottom of the conduction band in insulators and semiconductors. http://en.wikipedia.org/wiki/Tauc_plot
*matter_extraterrestrial*_gap_E04 [*matter*_gap_E04]	float	S3 [m]	MatExtra	F	eV	Band gap E04 of the carbonaceous extraterrestrial matter *Definition:* the band gap E04 is the energy at which the absorption coefficient reaches 10^4 cm^{-1}
*matter_extraterrestrial*_composition_comments [*matter*_composition_comments]	blob	U [m]	MatExtra	F	--	Any additional information or comments on the composition of the carbonaceous extraterrestrial matter *Ex:* sum of atomic fractions, vitrinite reflectance VR (in oil: %Ro) of coal carbonaceous extraterrestrial matter, … *Note:* also additional information on impurities not measured

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Extraterrestrial matter composition

Note: Whatever are the materials that constitute the extraterrestrial matter they will be always defined from the "materials" level (link(s) with "*matter_extraterrestrial*_material_index") through their "materials", "constituents" and "species", or through other matter(s). Only their type of mixing is described here.

*matter_extraterrestrial*_materials_mixing [+] [*matter*_materials_mixing]	enum(text)	S2 [!_m]	MatExtra	F	--	How the different materials are mixed in the extraterrestrial matter Enum: {single material, homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, spatial distribution...}

						Definitions: cf. "*layer*_materials_mixing"
*matter_extraterrestrial*_materials_number [+][-xml] [*matter*_materials_number]	int(10)	U [!_c]	MatExtra	F	*no*	Number of different materials mixed in the extraterrestrial matter ➔ calculated from " *matter_extraterrestrial*_materials" list
matter_extraterrestrial_matters	***List [L6a]***	[!]				£: matters constituting this extraterrestrial matter
*matter_extraterrestrial*_matter_index [*][-xml] [*matter*_matter_index] ➢ Same structure as "*sample*"	int(10) [Internal link]	B [!_g]	MatExtra MatXxx L6a	F	--	ID of the matters(s) constituting the 'extraterrestrial matter' *Note xml:* in practice the description of the material(s) is done directly under "*matter_extraterrestrial*" without providing the ID link
matter_extraterrestrial_materials	***List [L6b]***	[!]				£: materials constituting this extraterrestrial matter
*matter_extraterrestrial*_material_index [*][-xml] [*matter*_material_index] ➢ Same structure as "*sample*"	int(10) [Internal link]	U/S [!_g]	MatExtra Mater L6b	F	--	ID of the material(s) constituting the "extraterrestrial matter" *Note:* The different solids (fundamental phases or custom constituents) composing the extraterrestrial matter are described inside this materials structure at the constituent level. The different, molecules, chemical functions (chemical description) and/or atoms (elemental composition) composing the extraterrestrial matter are described at the species level. *Note:* For mineral solid solutions or n-hydrated minerals ("*mineral*_classification_level" = {variable mineral, unique mineral} or "*mineral*_hydration_series" = 'true') the modifications of the mineral solid solution parameters (VM) (composition and properties) are described at the species level. *Note:* Case of '*glasses'* and *'clays/silts':* see *"matter_solid*_material_index" *Note xml:* in practice the description of the material(s) is done directly under "*matter_extraterrestrial*" without providing the ID link
*matter_extraterrestrial*_comments [*matter*_comments]	blob	U [m]	MatExtra	F	--	Additional information on the extraterrestrial matter *Ex:* comments on the composition and formula of the actual molecular or

							mineral phases composing the extraterrestrial matter
Precursor materials *Note:* "*material*_is_precursor" = 'true' *Note:* refer to the same table as "*materials*" in the sample structure but without the "material arrangement and abundance" bloc See definitions and notes in "*Mineral matter*"		[O]					*Condition:* description of precursor materials is optional.
matter_extraterrestrial_precursor_materials *[matter_precursor_materials]*	***List [L7]***	[O]	MatExtra PreMater L7				£: Precursor materials used to create the extraterrestrial matter *Condition:* description of precursor materials is optional
➢ Use exactly the same structure as for "*Mineral matter*"							
Extraterrestrial matter processings		[O]					*Condition:* only when there is processing of materials or parent matter/sample
matter_extraterrestrial_processings *[matter_processings]*	***List [L8]***		MatExtra L8				£: Processing steps of the precursor materials/matters
- Use exactly the same structure as for "*Mineral matter*"							
Extraterrestrial matter documentation and references							
matter_extraterrestrial_documentations	***List [L9]***	[O]					£: Documentations about the extraterrestrial matter
*matter_extraterrestrial*_documentation_name [*sample_documentation_name*]	varchar(255)	U [m]	MatExtra L9	F	--		Name of the documentation describing the extraterrestrial matter *Note:* this name will appear as the documentation title in the database *Ex:* 'Certificate of Allende meteorite'
*matter_extraterrestrial*_documentation_filename [*sample_documentation_filename*]	varchar(255)	U [m]	MatExtra L9	F	--		File name (with extension) of the documentation describing the extraterrestrial matter

						File formats: .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database
matter_extraterrestrial_links	***List [L10]***	[O]				£: Web pages describing the extraterrestrial matter and its properties
*matter_extraterrestrial*_link_name [*matter*_link_name]	varchar(255)	U [m]	MatExtra L10	F	--	Name of the web page(s) describing the extraterrestrial matter and its properties. *Ex:* 'Museum Histoire Naturelle', …
*matter_extraterrestrial*_link_url [*matter*_link_url]	CS-varchar(255)	U [m]	MatExtra L10	F	--	URL address(es) of the web page(s) describing the extraterrestrial matter and its properties *Note:* useful when the extraterrestrial matter comes from a meteorite database, a stable commercial supplier, ... *Notes*: - can also link to various types of measurements made on this matter - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
matter_extraterrestrial_publications	***List [L11]***	[O]				£: Publications describing the extraterrestrial matter and its properties.
*matter_extraterrestrial*_publication_uid [*] [*matter*_publication_uid]	varchar(255)	S2 [m]	MatExtra Publi L11	F	--	Link to the existing UID of the publication(s) describing the extraterrestrial matter(s), its preparation and its properties. *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

8. Plantetary bodies

8.1 Definition

The **planetary bodies** are the bodies of the solars system: planets, satellites, asteroids, comets, KBO, interplanetary dust, …

The generic information on these “bodies”is described by a set of key-words.

8.2 Planetary bodies Table

Root of the table: ***body***

Data type: 'Body'

Key-word	Type	Level	Table	Exp	Unit	Description
Planetary body import						
*body*_import_mode [*body*_import_mode]	enum(text)	P [!!_m]	ObjPla	F	--	Mode of import of the "planetary body" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*body*_xml_filename [-xml] [*body*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ObjPla	(V)	--	Name of the storage copy of the xml import file of the "*body*" metadata ➔ determined automatically during import (from "*body*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Planetary body indexes						
*body*_index [**][-xml] [*body*_index]	int(10)	B [!!_g]	ObjPla	F	--	Automatic random but unique number given to new planetary body
*body*_uid [**] [*body*_uid]	varchar(255)	S0/S1s [!!_m]	ObjPla	F	--	Unique identifier code given to the planetary body table (to be created) *Nomenclature:* Create this code name with 'BODY_' and be very accurately in order to be simple and unique. It should be of the style 'BODY_planetaryFamily_PlanetaryName' where 'planetaryFamily' is the family of planetary body and 'PlanetaryName' is the common name of the planetary body, with all non-basic ASCII characters (é, ù, -, …), and space removed or transformed in '_' or '-'. *Note:* use UPPERCASES for the 'MissionName', uppercases for the first letter of 'PlanetaryName' and lowercases for the ramining and for the

						‘planetaryFamily’ *Ex*: - ‘BODY_planet_Earth’, - ‘BODY_satellite_Moon’, - ‘BODY_comet_Wild2’, …
Planetary body description						
*body*_name [*body*_name]	varchar(255)	S0/S1s [!!_m]	ObjPla	F	--	Full official name of the planetary body *Ex.:* Europa, Moon, 67P/Chuyrimov-Gerasimenko, 1/Ceres …
body_secondary_names	***List [L0]***	[O]				£: Alternative names used for the planetary body
*body*_secondary_name [*body*_secondary_name]	varchar(255)	S0/S1s [m]	ObjPla L0	F	--	Alternative name used for the planetary body *Ex.:* ‘Jupiter II’ for Europa ‘1P/1682 Q1’ for 1P/Halley's comet ‘Tempel 2’ for 10P/Tempel comet *Notes:* – start with a capital letter
Planetary body origin						
*body*_discovery_date [*body*_recovery_year]	varchar(255)	S2/Us [!_m]	ObjPla	F	--	Date or year of discovery of the planetary body Ex: ‘2012’, ‘8 January 1610’
*body*_discoverer [*body*_discoverer]	varchar(255)	S2/Us [m]	ObjPla	F	--	Discoverer(s) of the planetary body Ex: ‘Galileo Galilei’
Planetary body family						

*body*_family	enum (text)	S1/S1s [!!_m]	ObjPla	F	--	Family of the planetary body Enum: {star, planet, dwarf planet, satellite, ring system, asteroid, distant minor planet, comet, interplanetary dust, other, unclassified} *Definitions:* - '*star*': the sun - '*planet*': the 8 planets of the solar system - '*dwarf planet'*: a dwarf planet is a planetary-mass body that is neither a planet nor a natural satellite. IAU recognizes five dwarf planets: Ceres in the asteroid belt, and Pluto, Haumea, Makemake, and Eris in the outer solar system.[- '*satellite'*: a natural satellite or moon is an astronomical body that orbits a planet or minor planet, or another small Solar System body (asteroid, TNO, …). - '*ring system*': a ring system is a disc or rings orbiting an astronomical object that is composed of solid material such as dust and moonlets, - '*asteroid'*: asteroid of the solar system - '*distant minor planet'*: a minor planet found in the outer Solar System that is not commonly thought of as an "asteroid". Include the populations of centaurs, Neptune trojans, and trans-Neptunian objects. A distant object has a semi-major axis greater than 6 AU (just beyond Jupiter.) - '*comet'*: - '*interplanetary dust'*: all type of dust in the interplanetary space, close or far to its source object, or with unknown source - '*other*': object classified in a family different from the list above. Need to give the family in "*body*_comment" - '*unclassified*': object not yet classified in a family
*body*_dynamic_family [*body*_dynamic_family]	openum(text)	S1/S1s [!_m]	ObjPla	F		Dynamic familly of the planetary body OpenEnum: {star, planet, inner moon, regular, irregular, planetary ring system, minor planet ring system, near-Earth asteroid, Earth trojan, Mars trojan, inner asteroid belt, middle asteroid belt, outer asteroid belt, Jupiter trojan, centaur, Neptune trojan, classical Kuiper belt, resonant Kuiper belt, scattered disk object, detached object, Jupiter family, Halley-type, long-period,

asteroidal dust, cometary dust, other dust, other, undefined}

Constaint: To be chosen in the list depending on "*body*_family"

Definitions:

For family = 'star':
- '*star*'

For family = 'planet':
- '*planet*'

For family = 'dwarf planet':
- '*middle asteroid belt'*: for Ceres
- '*resonant Kuiper belt'*: for Pluto, Haumea,
- '*classical Kuiper belt':* for Makemake,
- '*scattered disk objects'*: for Eris

For family = 'satellite':
- *'inner moon'* satellite following a prograde, low-inclination orbit inwards of the large satellites of the parent planet.
- *'regular moon':* (or main-group) the large satellites of the parent planet with nearly circular orbits near the plane of the equator of the central object
- *'irregular moon':* with elliptical and inclined orbit relative to the plane of the equator of the central object

For family = 'ring system':
- '*planetary ring system'*: a ring system around a planet is called a planetary ring system (the 4 giant planets)
- '*minor planet ring system'*: ring system around a distant minor planet (centaurs Chariklo and Chiron, TNO Haumea)
  Ref: https://en.wikipedia.org/wiki/Ring_system

For family = 'asteroid':
- '*near-Earth asteroid':* or NEAs, are asteroids that have orbits that pass close to that of Earth. Asteroids that actually cross Earth's orbital path are known as Earth-crossers.
  Notes:
  - '*Near-Earth - Apohele'*: orbit inside of Earth's perihelion distance and thus are contained entirely within the orbit of Earth..

        - ‘*Near-Earth - Aten’*: asteroids with a semi-major axes of less than Earth's and aphelion greater than 0.983 AU.
        - ‘*Near-Earth - Apollo’*: asteroids with a semimajor axis greater than Earth's, while having a perihelion distance of less than 1.017 AU.
        - ‘*Near-Earth - Amor’*: near-Earth asteroids that approach the orbit of Earth from beyond, but do not cross it.
    - ‘*Earth trojan’*: asteroids sharing Earth's orbit and gravitationally locked to it.
    - *‘Mars trojan’: asteroids sharing Mars's orbit and gravitationally locked to it.*

  Asteroid belt: follow roughly circular orbits between Mars and Jupiter.
    - ‘*inner asteroid belt*’: inside of the strong Kirkwood gap at 2.50 AU due to the 3:1 Jupiter orbital resonance.
    - ‘*middle asteroid belt*’: between the 3:1 and 5:2 Jupiter orbital resonances, the latter at 2.82 AU.
    - ‘*outer asteroid belt’:* between the 5:2 and 2:1 Jupiter orbital resonances.
    - ‘*Jupiter trojan’*: asteroids sharing Jupiter's orbit and gravitationally locked to it.

  For family = ‘distant minor planet’:
    - ‘*centaur*’: bodies in the outer Solar System between Jupiter and Neptune (5.4 – 30 AU)
    - ‘*Neptune trojan*’: bodies sharing Neptune's orbit and gravitationally locked to it.
    - ‘*classical Kuiper belt’:* also known as Cubewanos, are in primordial, relatively circular orbits that are not in resonance with Neptune (40.5 – 47.7 AU).
    - ‘*resonant Kuiper belt’:* in mean-motion orbital resonance with Neptune, excepted 1:1 resonance of Neptune trojans (include ‘Plutinos’ (resonance 2:3), ‘twotinos’ (resonance 1:2), … sub-families
    - ‘*scattered disk object’*: with high-inclination, high-eccentricity orbits. Thought to have been scattered by Neptune.
    - ‘*detached object’:* with both aphelia and perihelia outside the Kuiper belt. with generally highly elliptical, very large orbits of up to a few hundred AU and a perihelion too far from Neptune's orbit.

Note: the last four families are also known collectively as 'trans-neptunian objects'

For family = 'comet':

- '*Jupiter family'*: short-period comets with orbital periods less than 20 years and low inclinations (up to 30 degrees) to the ecliptic
- '*Halley-type'*: short-period comets with orbital periods of between 20 and 200 years and inclinations extending from zero to more than 90 degrees.
- '*long-period'*: Long-period comets have highly eccentric orbits and periods ranging from 200 years to thousands of years

For family = 'interplanetary dust':

- '*asteroidal dust*': dust at close proximity of an asteroid
- '*cometary dust*': dust at close proximity and in the dust tail of a comet (and in the orbit of a comet)
- '*other dust'*: dust in the general interplanetary space without clear origin

For family = 'asteroid, distant minor planet, comet, other, unclassified':

- '*other*':
- '*undefined*':

Note:

Planetary body satellites and rings

*body*_ring_system [*body*_ring_system]	boolean	S3 [!o_m]	ObjPla	F	--	Flag telling if the planetary body has a ring system BoolEnum: {yes, no} or {true, false} *Condition*: Mandatory only for "*body*_family" = {planet, dwarf planet} *Note:* a planet, a dwarf planet, an asteroid, a TNO… can have a ring system
*body*_satellites_number [*body*_satellite_number]	int(4)	S3 [!o_m]	ObjPla	F	--	Number of satellites orbiting around this planetary body *Condition*: Mandatory only for "*body*_family" = {planet, dwarf planet} *Note:*

*body*_central_body_uid [*] [*body*_central_body_uid]	varchar(255)	S2 [!o_m]	ObjPla ObjPla	F	--	Link to the existing UID of the central object around which this planetary body orbits *Condition*: Mandatory and only for "*body*_family" = {satellite, ring system} *Note:* can orbit around a planet, a dwarf planet, an asteroid, a TNO, …
*body*_source_body_uid [*] [*body*_source_body_uid]	varchar(255)	S2 [!o_m]	ObjPla ObjPla	F	--	Link to the existing UID of the source object producing this dust 'body' *Condition*: Mandatory for "*body*_dynamic_family" = {asteroidal dust, cometary dust} *Note:* can orbit around a planet, a dwarf planet, an asteroid, a TNO, …

Planetary body types

*body*_physical_type [*body*_physical_type]	openum(text)	S1 [!_m]	ObjPla	F	--	Physical type of the planetary body OpenEnum: {telluric, gaseous, rocky, icy, carbonaceous, stony, metallic, other, unknown} *Constaint:* To be chosen in the list depending on "*body*_family" For family = 'planet': - *'telluric':* Planets mainly composed of rock (Mercury, Venus, Earth and Mars) - *'gaseous':* planets primarily composed of hydrogen and helium (Jupiter, Saturn, Uranus and Neptune) For family = 'satellite': - '*rocky*': with surface and interior predominantly made of rock (Io, …) - '*icy*': with surface and interior predominantly, or largely made of ice (Europa, Triton, …) For family = 'ring system': - '*rocky*': with particles predominantly made of rock (Jupiter) - '*icy*': with particles predominantly made of ice (Saturn, Uranus) - '*carbonaceous*': with particles predominantly made of organics (Neptune) For family = 'asteroid' and 'dwarf planet' (Ceres): - *'carbonaceous:* C-group (B, F, G, C-types)

- *'stony'*: S-type (silicaneous)
- *'metallic':* X-group (M, E, P-types)
- *'other':* A, D, T, Q, R, V-types

For family = 'dwarf planet, distant minor planet, comet':
- '*rocky*': with surface and interior predominantly made of rock (Ceres, …)
- '*icy*': with surface and interior predominantly, or largely made of ice (Pluto, …)

For family = 'interplanetary dust':
- '*rocky*': with particles predominantly made of rock (?)

For family = 'o*ther*' & ' *undefined*':
- '*other*': physical type not described above
- '*unknown*':

Note:

*body*_minor_planet_spectral_type	openum(text)	S2 [!o_m]	ObjPla	F	--	Spectral type of the minor planets OpenEnum: {BB, RR, BR, IR, other} *Condition*: Mandatory and only for "*body*_family" = {distant minor planet} *Definitions:* Spectral classification - *'BB':* blue, average B−V = 0.70, V−R = 0.39 (e.g. Orcus) - *'RR':* very red, B−V = 1.08, V−R = 0.71 (e.g. Sedna) - *'BR':* intermediate class, differ mostly in the infrared bands I, J and H. - *'IR':* intermediate class differ mostly in the infrared bands I, J and H. - *'other':* *Note:*
*body*_asteroid_spectral_group	openum(text)	S2 [!o_m]	ObjPla	F	--	Spectral group of the asteroid (Bus-DeMeo classification) OpenEnum: {C, S, X, endmembers} *Condition*: Mandatory and only for "*body*_family" = 'asteroid' *Definitions:* Based on Bus-DeMeo 2009 spectral classification

- *'C:* dark carbonaceous objects
- *'S':* silicaceous (or "stony") objects.
- *'X':* metallic objects
- *'endmembers':* other objects

Note:

*body*_asteroid_spectral_type	openum(text)	S2 [!o_m]	ObjPla	F	--	Spectral type of the asteroid (Bus-DeMeo classification) OpenEnum: {A, B, C, Cb, Cg, Cgh, Ch, D, K, L, O, Q, R, S, Sa, Sq, Sr, Sv, Sw, T, V, Vw, X, Xc, Xe, Xk} *Condition*: Mandatory and only for "*body*_family" = 'asteroid' *Definitions:* Based on Bus-DeMeo 2009 spectral classification (24 classes) For C-group dark carbonaceous objects: - A-type - B-type (2 Pallas) - C-type (10 Hygiea) the remaining majority of 'standard' C-type asteroids. - Cb-subtype - Cg-subtype - Cgh-subtype - Ch-subtype For S-group silicaceous (or "stony") objects: - S-type (15 Eunomia, 3 Juno) - Sa-subtype - Sq-subtype - Sr-subtype - Sv-subtype For X-group: - X-type - Xc-subtype - Xe-subtype - Xk-subtype For Endmembers:

- D-type (624 Hektor)
- K-type
- L-type
- O-type
- Q-type
- R-type
- T-type (96 Aegle)
- V-type

Note:

*body*_comments [*body*_comments]	blob	U [m]	ObjPla	F	--	Additional information on the planetary body

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Planetary body images

body_images	***List [L1]***	[O]				£: Pictures of the planetary body
*body*_image_filename [*body*_image_filename]	varchar(255)	P/U [m]	ObjPla L1	F	--	File name(s) (with extension) of picture(s) of the planetary body *Image formats:* .png, .jpg, (.gif) *Note:* this file will be imported in the database

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Planetary body orbital properties

*body*_orbit_periapsis [*body*_orbit_periapsis]	float	U [!_m]	ObjPla	F	*km*	Periapsis of the orbit of the planetary body • Unit: km *Notes*: - noted Perihelion for an object orbiting the Sun - will be either displayed in AU (and km) for heliocentric objects or just in km for satellites & rings.
*body*_orbit_apoapsis	float	U	ObjPla	F	*km*	Apoapsis of the orbit of the planetary body

[*body*_orbit_apoapsis]		[!_m]				• Unit: km *Notes*: - noted Aphelion for an object orbiting the Sun - will be either displayed in AU (and km) for heliocentric objects or just in km for satellites & rings.
*body*_orbit_semimajor_axis [*body*_orbit_semimajor_axis]	float	U [!o_m]	ObjPla	F	*km*	Semi-major axis of the orbit of the planetary body *Condition*: Mandatory only for "*body*_family" = {planet, dwarf planet, asteroid, distant minor planet, comet} • Unit: km *Note*: will be either displayed in AU (and km) for heliocentric objects or just in km for satellites & rings.
*body*_orbit_eccentricity [*body*_orbit_eccentricity]	float	U [!_m]	ObjPla	F	--	Eccentricity of the orbit of the planetary body *Note*:
*body*_orbit_inclination_ecliptic [*body*_orbit_inclination_ecliptic]	float	U [!_m]	ObjPla	F	*deg*	Inclination of the orbit of the planetary body relative to the ecliptic *Note*:
*body*_orbit_inclination_central_body [*body*_orbit_inclination_central_body]	float	U [!o_m]	ObjPla	F	*deg*	Inclination of the orbit of the planetary body relative to the equator of the central object. *Condition*: Mandatory only for "*body*_family" = {satellite, ring system} *Note*:
*body*_orbit_direction [*body*_orbit_direction]	openum(text)	S2 [!_m]	ObjPla	F	--	Direction of rotation of the orbit of the planetary body relative to the rotation of the central object. OpenEnum: {prograde, retrograde} *Note:*

*body*_orbit_synchronous [*body*_orbit_synchronous]	boolean	U [!o_m]	ObjPla	F	--	Flag telling if the orbit of the planetary body is synchronous to the rotation of the central object around which it orbits BoolEnum: {yes, no} or {true, false} *Condition*: Mandatory only for "*body*_family" = {satellite} *Definition*: a synchronous orbit means that the orbital period of the object is the same as the rotation period of the central object and that the orbit direction is 'prograde' *Note*: for synchronous
*body*_orbit_period [*body*_orbit_period]	float	U [!_m]	ObjPla	F	*day*	Orbital period of orbit of the planetary body relative to the central object (sun, planet, …)

Planetary body rotation properties

*body*_rotation_synchronous [*body*_rotation_synchronous]	boolean	U [!_m]	ObjPla	F	--	Flag telling if the rotation of the planetary body around its axis is synchronous to its orbit BoolEnum: {yes, no} or {true, false} *Definition*: a synchronous rotation means that the rotation period of the object is the same as the orbital period and in the same direction *Note*: not for "family" = 'interplanetary dust'
*body*_rotation_obliquity [*body*_rotation_obliquity]	float	U [!_m]	ObjPla	F	*deg*	Tilt (called obliquity) of the rotation axis relative to the orbital axis of the planetary body *Note*: not for "family" = 'interplanetary dust'
*body*_rotation_period [*body*_rotation_period]	float	U [!o_m]	ObjPla	F	*day*	Rotation period of the planetary body around its axis *Condition*: Mandatory only for "family" = {planet, dwarf planet, satellite, asteroid} *Note*: not for "family" = 'interplanetary dust'

Planetary body physical properties

*body*_dimensions [*body*_dimensions]	varchar(255)	U [£o_m]	ObjPla	F	*km*	Dimensions of the planetary body along its 3 principal axes, with uncertainty *Condition*: Compulsory only for irregular objects such as satellites, asteroids, distant minor planets, and comets *Note*: give the dimensions in decreasing order *Ex*: '125 (+/-5) x 53 (+/- 3) x (22 (+/-2)'
*body*_mean_radius [*body*_mean_radius]	float	U [!_m]	ObjPla	F	*km*	Mean radius of the planetary body *Note*: - will be either displayed in km, or also in Earth-radius for large objects - Earth mean radius = 6371.0 km
*body*_mass [*body*_mass]	float	U [m]	ObjPla	F	*kg*	Mass of the planetary body *Note*: - will be either displayed in kg, or also in Earth-mass for large objects - Earth mass = 5.97237×10^{24} kg
*body*_mean_density [*body*_mean_density]	varchar(255)	S3 [!_m]	ObjPla	F	*g/cm3*	Mean density of the planetary body, with uncertainty *Note*: *Ex*: '2.15 (+/-0.15)'

Planetary body surface properties

*body*_surface_gravity [*body*_surface_gravity]	float	U [m]	ObjPla	F	*m/s2*	Gravity at the surface of the planetary body
*body*_surface_albedo_geometric_visual [*body*_surface_albedo_geometric_visual]	varchar(255)	S3 [!_m]	ObjPla	F	--	Visual geometric albedo (or albedo range or with uncertainty) of the surface of the planetary body *Definition:* ratio of the actual brightness of the object as seen from the light

						source (i.e. at zero phase angle) to that of an idealized flat, fully reflecting, diffusively scattering (Lambertian) disk with the same cross-section, and integrated over the visible spectrum. *Note*: *Ex*: '0.72 (+/-0.05)', '0.65 – 0.83'
*body*_surface_albedo_bond [*body*_surface_albedo_bond]	varchar(255)	S3 [m]	ObjPla	F	--	Bond albedo (or albedo range or with uncertainty) of the surface of the planetary body *Definition:* fraction of power in the total electromagnetic radiation incident on an astronomical body that is scattered back out into space. *Note*: *Ex*: '0.72 (+/-0.05)', '0.65 – 0.83'
*body*_surface_temperature [*body*_surface_temperature]	varchar(255)	U [m]	ObjPla	F	*K*	Temperature range of the surface of the planetary body (with K unit) *Note*: temperature can vary with season, within a day, with latitude and with altitude of the surface *Ex*: '150 K (polar night) – 300 K (mid-day equator)'
*body*_surface_pressure [*body*_surface_pressure]	varchar(255)	U [m]	ObjPla	F	*bar, mbar*	Atmospheric pressure (or pressure range) at the surface of the planetary body (with unit) *Note*: pressure can vary with season (Mars, Pluto, …) and with altitude of the surface *Ex*: '6 - 8 mbar at altitude zero'
*body*_properties_comments [*body*_properties_comments]	blob	U [m]	ObjPla	F	--	Any additional information or comments on the physical properties of the planetary body *Note:*

Planetary body atmosphere composition

body_composition_atmosphere_species	***List [L2]***	[O]				£: Description of the species and solid or liquid phases identified in the atmosphere of the planetary body
*body*_composition_atmosphere_specie_name [*body*_composition_specie_name]	varchar(255)	S2 [o!!_m]	ObjPla L2	F	--	Formula and/or name of the specie (atom, molecule, …) or phase (liquid, solid, …) identified in the atmosphere of the planetary body *Notes:* - For gaseous species provide the formula with the chemical name in parenthesis - For solid and liquid phases (aerosols, clouds) provide their formula or phase name with type of phase *Ex*: - 'H$_2$O (water)' - 'CO$_2$ (carbon dioxide)' - 'Ar (Argon)' - 'H$_2$O amorphous ice' - 'solid HC$_3$N' (Titan polar stratosphere)
*body*_composition_atmosphere_specie_state [*body*_composition_specie_state]	enum(text)	U [o!!_m]	ObjPla L2	F	--	State of the specie (gas) or phase (liquid, solid) identified in the atmosphere of the planetary body Enum: {gas, liquid, solid} *Note:*
*body*_composition_atmosphere_specie_mole_fraction [*body*_composition_specie_mole_fraction]	float	U [m]	ObjPla L2	F	%	Mole fraction (in %) of the specie identified in the atmosphere of the planetary body *Note*: value between 0 and 100
*body*_composition_atmosphere_specie_location [*body*_composition_specie_location]	varchar(255)	U [m]	ObjPla L2	F	--	Type of location of the specie identified in the atmosphere of the planetary body FreeList: {atmosphere, troposphere, stratosphere, polar stratosphere, mesosphere, thermosphere, exosphere, tropospheric clouds, tropospheric aerosols, stratospheric aerosols, jet, coma, …}

						Definitions: - *'atmosphere':* in several parts of the atmosphere - *'troposphere':* - *'stratosphere':* - *'polar stratosphere':* stratosphere over the poles - *'mesosphere':* - *'thermosphere:* - *'exosphere':* - *tropospheric clouds,* - *tropospheric aerosols,* - *stratospheric aerosols,* - *'jet':* within any type of transcient jet coming from the subsurface of te object (geyser, cometary jet, …) - *'coma':* of a comet or any sublimating body - ... *Note*: one or several attributes can be chosen and separated by a coma when a specie or phase is present at different places
*body*_composition_atmosphere_comments [*body*_composition_comments]	blob	U [m]	ObjPla	F	--	Any additional information or comments on the species or phases indentified in the atmosphere of the planetary body *Ex*: 'include unknown amount of other hydrocarbons and nitriles'

Planetary body surface composition

body_composition_surface_species	***List [L3]***	[O]				£: Description of the species and solid or liquid phases identified on the surface or in the subsurface of the planetary body
*body*_composition_surface_specie_name [*body*_composition_specie_name]	varchar(255)	S2 [o!!_m]	ObjPla L3	F	--	Formula and/or name of the specie (atom, molecule, …) or phase (liquid, solid, …) identified at the (sub)surface of the planetary body *Ex*: - 'beta-N_2:CH_4:CO ice', 'CH4-rich ice, phase I' - 'liquid CH_4:C_2H_6:N_2 mixture'

- ‘CO_2 clathrate hydrate’

*body*_composition_surface_specie_state [*body*_composition_specie_state]	enum(text)	U [!_m]	ObjPla L3	F	--	State of the specie (gas) or phase (liquid, solid) identified at the (sub)surface of the planetary body Enum: {gas, liquid, solid}
*body*_composition_surface_specie_mole_fraction [*body*_composition_specie_mole_fraction]	float	U [m]	ObjPla L3	F	%	Mole fraction (in %) of the specie identified at the (sub)surface of the planetary body *Note*: value between 0 and 100
*body*_composition_surface_specie_location [*body*_composition_specie_location]	varchar(255)	U [m]	ObjPla L3	F	--	Type of location of the mineral/solid/liquid on the (sub)surface of the planetary body FreeList: {surface, subsurface, crust, mantle, N polar cap, S polar cap, glaciers, seasonal snow, permafrost, seas, lakes, rivers, …} *Definitions:* - *surface,* - *subsurface,* - *crust,* - *mantle,* - *N polar cap,* - *S polar cap,* - *glaciers,* - *seasonal snow,* - *permafrost,* - *seas,* - *lakes,* - *rivers,* - *…* *Note*: one or several attributes can be chosen and separated by coma when a specie or phase is present at different places

*body*_composition_surface_comments [*body*_composition_comments]	blob	U [m]	ObjPla	F	--	Any additional information or comments on the species or phases indentified at the (sub)surface of the planetary body
Planetary body references						
body_links	***List [L4]***	[O]				£: Web pages describing the planetary body and its properties
*body*_link_name [*body*_link_name]	varchar(255)	U [m]	ObjPla L4	F	--	Name of the web site(s) describing the planetary body and its properties. *Ex:* 'Meteoretical Bulletin Database', …
*body*_link_url [*body*_link_url]	CS-varchar(255)	U [m]	ObjPla L4	F	--	URL address(es) of the web page(s) describing the planetary body. *Notes*: - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
body_publications	***List [L5]***	[O]				£: Publications describing the planetary and its properties.
*body*_publication_uid [*] [*body*_publication_uid]	varchar(255)	U [m]	ObjPla Publi L5	F	--	Link to the existing UID of the publication(s) describing the planetary(s) and its properties. *Note:* mostly publications describing the planetary body, its composition, properties, … *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

9. Natural Objects

9.1 Definition

The **Objects** are the geologic objects from which some natural matters (terrestrials or extraterrestrials) come from (e.g. “meteorites”, “micrometeorites”, “IDPs”, “planetary”…).

The generic information on these “objects”is described by a set of key-words.

9.2 Meteorite objects Table

Root of the table: ***object_meteorite***

Data type: 'Object'

Key-word	Type	Level	Table	Exp	Unit	Description
Meteorite object import						
*object_meteorite*_import_mode [*object*_import_mode]	enum(text)	P [!!_m]	ObjMet	F	--	Mode of import of the "meteorite object" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*object_meteorite*_xml_filename [-xml] [*object*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ObjMet	(V)	--	Name of the storage copy of the xml import file of the "*object_meteorite*" metadata ➔ determined automatically during import (from "*object_meteorite*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Meteorite object indexes						
*object_meteorite*_index [**][-xml] [*object*_index]	int(10)	B [!!_g]	ObjMet	F	--	Automatic random but unique number given to new meteorite object
*object_meteorite*_uid [**] [*object*_uid]	varchar(255)	S0/S1s [!!_m]	ObjMet	F	--	Unique identifier code given to the meteorite object table (to be created) *Nomenclature:* Create this code name with 'OBJMET_' and very accurately in order to be simple and unique. It should be of the style 'OBJMET_MeteoriteName' where 'MeteoriteName' is the common name of the meteorite object, with all non-basic ASCII characters (é, ù, -, …), and space removed or transformed in '_'. *Ex*: 'OBJMET_Cold_Bokkeveld', 'OBJMET_ALHA77307', …

Meteorite object name

*object_meteorite*_family [-xml] [*object*_family]	enum (text)	S0/S0s [!!_c]	ObjMet	F	--	Family of object Enum: {meteorite} *Default* = 'meteorite' *Definitions:* - '*meteorite*': extraterrestrial rocks larger than 2 mm in size collected at Earth surface
*object_meteorite*_name [*object*_name]	varchar(255)	S0/S1s [!!_m]	ObjMet	F	--	Full official name of the meteorite *Ex.:* Allan Hills A77307, Allende, …
*object_meteorite*_secondary_name [*object*_secondary_name]	varchar(255)	S0/S1s [m]	ObjMet	F	--	Alternative usual name(s) used for the meteorite *Notes:* – start with a capital letter – separate each name by a comma *Ex.:* 'ALHA77307' for Allan Hills A77307

Meteorite object origin

*object_meteorite*_recovery_status [*object*_recovery_status]	enum(text)	S1/S3s [!!_m]	ObjMet	F	--	Recovery status of the meteorite object Enum: {fall, find} *Definitions*: – '*fall*': meteorite recovered just after observation of its fall – '*find*': meteorite simply found "by chance" on the ground.
*object_meteorite*_recovery_year [*object*_recovery_year]	int(4)	S2/Us [!_m]	ObjMet	F	year	Year of recovery *Ex*: '2012'

*object_meteorite*_recovery_mass [*object*_mass]	float	S3/Us [m]	ObjMet	F	g	Total recovered mass of the meteorite object *Unit:* g

Meteorite object: planetary body

*object_meteorite*_recovery_body_uid [*] [*object*_recovery_body_uid]	varchar(255)	S2 [!!_m]	ObjMet Planet Body	F	--	-- Link to the existing UID of the planetary body from which the meteorite originates *Default:* 'BODY_planet_Earth' *Note:* - currently only for meteorites collected on Earth - will be possibly extended later for meteorites collected on the Moon or Mars.
*object_meteorite*_recovery_body_coordinate_system [*object*_recovery_body_coordinate_system]	openum(text)	U [!d_m]	ObjMet	F	--	Coordinate system on the planetary body of the geographic location of the recovery place of the meteorite OpenEnum: {WGS84, Mars 2000, Moon 2000, …} *Default*: 'WGS84' *Definitions*: see "*experiment*_body_coordinate_system" *Notes*: currently only 'WGS84' for Earth

Meteorite object: geolocation

*object_meteorite*_recovery_geolocation_place [*object*_recovery_geolocation_place]	varchar(255)	S1/Us [!_m]	ObjMet	F	--	Place of recovery of the meteorite on the planetary body *Note*: it is the name of geographic area or town (Earth) of recovery of the micrometeorite *Ex*: 'Chassigny (Haute-Marne)'
*object_meteorite*_recovery_geolocation_region [*object*_recovery_geolocation_region]	varchar(255)	S1/Us [m]	ObjMet	F	--	Region, state, province or county (administrative location) of the recovery place on Earth of the meteorite *Constraint:* only when "*object_meteorite*_recovery_body_uid" =

						‘BODY_planet_Earth’ *Ex:* ‘Murmanskaja Oblast’, ‘Sicilia’, ‘Rhône-Alpes’, ‘Arizona’, ‘Zambezi’
*object_meteorite*_recovery_geolocation_country_code [*object*_recovery_geolocation_country_code]	enum(text)	S1/Us [!o_m]	ObjMet	F	--	2-digit code of the country of the recovery place on Earth of the meteorite Enum: {AQ, AU, CH, CL, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see “*laboratory*_address_country_code” *Condition:* mandatory and only when “*object_meteorite*_recovery_body_uid” = ‘BODY_planet_Earth’ *Definitions:* see “*laboratory*_address_country_code” *Ex*: ‘AQ’ for Antarctica
*object_meteorite*_recovery_geolocation_type [*object*_recovery_geolocation_type]	enum(text)	U [!!o_m]	ObjMet	F	--	Type of geographic location of the recovery place of the meteorite Enum: {point, line, box, polygon} *Condition*: absolute mandatory when “*object_meteorite*_recovery_geolocation_coordinate_latitude” ≠ Ø *Definitions*: see “*experiment*_geolocation_type"
object_meteorite_recovery_geolocation_coordinates [*object_recovery_geolocation_coordinates*]	**List [L0]**	[O]				£: Geolocation (x,y,z coordinates) on the planetary body of the recovery place of the meteorite *Condition:* absolute mandatory when “*object_meteorite*_recovery_geolocation_type” ≠ Ø *Conditions:* on the number of long/lat couple: see *“experiment*_geolocation_coordinates”
*object_meteorite*_recovery_geolocation_coordinate_latitude [*object*_recovery_geolocation_coordinate_latitude]	float	S3 [O!_m]	ObjMet L0	F	deg	Latitude of the geographic location of the recovery place of the meteorite *Format*: in N ‘decimal degrees’ (negative value for S hemisphere) in “*object_meteorite*_recovery_body_coordinate_system” *Note*: 3 (100 m) to 5 decimals (1 m accuracy) are enough for Earth

						Ex: '12.12345' provides 1 m accuracy
*object_meteorite*_recovery_geolocation_coordinate_longitude [*object*_recovery_geolocation_coordinate_longitude]	float	S3 [O!_m]	ObjMet L0	F	deg	Longitude of the geographic location of the recovery place of the meteorite *Format*: in E 'decimal degrees' (in the E direction only) in "*object_meteorite*_recovery_body_coordinate_system" *Note*: same as for "*object_meteorite*_recovery_geolocation_coordinate_latitude" and even less at high latitude *Ex*: '12.12' provides 100 m accuracy at 85° latitude
*object_meteorite*_recovery_geolocation_coordinate_altitude [*object*_recovery_geolocation_coordinate_altitude]	float	S3 [m]	ObjMet L0	F	m	Altitude of the geographic location of the recovery place of the meteorite *Format*: in 'm' in "*object_meteorite*_recovery_body_coordinate_system" *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*object_meteorite*_recovery_comments [*object*_ recovery_comments]	blob	U [m]	ObjMet	F	--	Additional information or comments about the recovery of the meteorite *Ex*: 'collected jointly by ANSMET (US) and NIPR (Japan)', 'location accurate at +/- 1km', ', 'coordinates accurate at +/- 0.1°'
Meteorite object type						
*object_meteorite*_breccia	boolean	S3/Us [!!_m]	ObjMet	F	--	Flag to telling if the meteorite is a breccia or made of a single type/group/class BoolEnum: {yes, no} or {true, false} *Definitions:* - '*true*': the meteorite is a breccia possibly composed of several lithologies with different types/groups/classes - '*false*': the meteorite is of a single type/group/class
*object_meteorite*_breccia_type	enum(text)	S2/S2s	ObjMet	F	--	Breccia type of the meteorite

		[!o_m]				Enum: {regolith breccia, fragmental breccia, impact melt breccia, monomict breccia, polymict breccia, undefined} *Condition:* only when "*object_meteorite*_breccia" = 'true' *Definitions:* - '*regolith breccia'*: Fragmental debris on surface of body (contain solar-wind gases, solar flare tracks, agglutinates, etc.), usually have light-dark structure - '*monomict breccia'*: monomictic breccia results from rock deformation by shearing and granulation (cataclasis) in the process of tectonism or – more general – dislocation metamorphism *ref:* http://www.impact-structures.com/impact-rocks-impactites/the-impact-breccia-page/monomictic-breccia-monomictic-impact-breccia-monomictic-movement-breccia/ - '*polymict breccia'*: a breccia with clastic matrix or crystalline matrix (derived from the crystallization of impact melt) containing lithic and mineral clasts of different degree of shock metamorphism *ref:* http://www.impact-structures.com/impact-rocks-impactites/the-impact-breccia-page/polymictic-polymict-polygenetic-polylithologic-breccia/ - '*fragmental breccia'*: Fragmental debris with no regolith properties - '*impact melt breccia'*: Unmelted debris in igneous matrices - '*undefined*': not yet defined breccia type *Ref:* Classification of meteorites, Krot et al. (2003), p. 8 & 12
*object_meteorite*_category	enum (text)	S1/S1s [!!_m]	ObjMet	F	--	Category of the meteorite Enum: {chondritic, nonchondritic, differentiated planetary, unknown} *Definitions:* - '*chondritic*': Chondrites consist of four major components: chondrules, FeNi-metal, refractory inclusions (Ca–Al-rich inclusions (CAIs) and amoeboid olivine aggregates (AOAs)), and fine-grained matrix material. - '*nonchondritic*': Nonchondritic meteorites lack chondritic textures and are formed by partial or complete melting and differentiation of

chondritic precursor asteroids
- '*differentiated planetary'*: They are nonchondritic meteorites formed by planetary differentiation of large planetary bodies (Mars, Moon)
- '*unknown*': objects that has not been classified;
Note: objects that may not be meteorites, including the fusion crusts, should not be described as "*object_meteorite"*

Note: for breccia and silicate-bearing irons it is the type of the hosting (dominating) component. The type(s) of the other(s) component(s) should be given in "comments"

Meteoritical Bulletin Database: http://www.lpi.usra.edu/meteor/index.php
Wikipedia: http://en.wikipedia.org/wiki/Chondrite
http://en.wikipedia.org/wiki/Achondrite
http://en.wikipedia.org/wiki/Iron_meteorite
http://en.wikipedia.org/wiki/Stony-iron_meteorite
http://class.meteorites.com.au/

*object_meteorite*_group [*object*_group - ≠Enum]	openum(text)	S1/S1s [!!_m]	ObjMet	F	--	Group of the meteorite

OpenEnum: {carbonaceous chondrite, ordinary chondrite, enstatite chondrite, Kakangari-like chondrite, Rumuruti-like chondrite, ungrouped chondrite, primitive achondrite, differentiated achondrite, enstatite-rich achondrite, stony-iron, iron, ungrouped achondrite, martian, lunar, unknown}

Definitions: see Krot et al. (2003)
For category = 'chondritic':
- '*carbonaceous chondrite'*: a major class of chondrites that mostly have Mg/Si ratios near the solar value and oxygen isotope compositions that plot below the terrestrial fractionation line.
- '*ordinary chondrite'*: a major class of chondrites, distinguished by sub-solar Mg/Si and refractory/Si ratios, oxygen isotope compositions that plot above the terrestrial fractionation line, and a large volume percentage of chondrules, with only 10-15 vol% fine-grained matrix.
- '*enstatite chondrite'*: a major class of chondrites that mostly have sub-solar Mg/Si and refractory/Si ratios, oxygen isotope compositions that plot near the terrestrial fractionation line, and highly reduced mineral

assemblages (containing little FeO, Si-bearing metal, and sulfides of elements normally considered lithophile).

- '*Kakangari-like'*: a grouplet of chondrites with similarities to Kakangari, which do not fit into the major classes of chondrites such as carbonaceous, ordinary, or enstatite.
- '*Rumuruti-like'*: a group of chondrites that does not clearly belong to any of the major classes of chondrites (ordinary, carbonaceous, enstatite); R chondrites have sub-solar Mg/Si and refractory/Si ratios, oxygen isotope compositions that plot above the terrestrial fractionation line and ordinary chondrites, and highly oxidized mineralogy.
- '*ungrouped chondrite'*: chondrite well-enough characterized to determine that it do not fit into any of the above groups.

For category = 'nonchondritic':

- '*primitive achondrite'*: a meteorite that has lost its chondritic texture due to heating and partial melting, but still has nearly chondritic composition.
- '*differentiated achondrite'*: A stony meteorite that lacks chondrules and originated on a differentiated parent body.
- '*enstatite-rich achondrite'*: an enstatite-rich achondrite that has not yet been classified into one of the 4 achondrite groups
- '*stony-iron'*: A stony meteorite, mostly pallasite and mesosiderite
    - pallasite: A meteorite that is a mixture of metal and silicates (usually olivine grains).
    - mesosiderite: A brecciated meteorite containing subequal silicate and metallic components; the silicates are dominantly igneous rock fragments.
- '*iron*': A meteorite that is dominantly composed of Fe-Ni metal and that crystallized from a melt.
- '*ungrouped achondrite'*: an achondrite well-enough characterized to determine that it do not fit into any of the above groups.

For category = 'differentiated planetary':

- *'martian'*: Martian meteorites are martian rocks that were ejected from Mars by impacts and later fell to the Earth as meteorites. Three well-known types are shergottites (basaltic to lherzolitic igneous rocks,

named after the Shergotty, India, fall of 1865), nakhlites (clinopyroxenites or wehrlites, formed as cumulate rocks, and named after the Nakhla, Egypt, fall of 1911), and chassignites (dunitic cumulate rocks named after the Chassigny, France, fall of 1815).

- '*lunar*': Lunar meteorites are lunar rocks that were ejected from the Moon by impacts and later fell to the Earth as meteorites. .

For category = 'unknown':

- '*unknown*': objects that has not been classified;
  Note: objects that may not be meteorites, including the fusion crusts, should not be described as "*object_meteorite"*

Note:

- for breccia and silicate-bearing irons it is the group of the hosting (dominating) component. The group(s) of the other(s) component(s) should be given in "comments"

Ref: Classification of meteorites, Krot et al. (2003), in Treatise of Geochemistry, chap 1.05, pp. 1-52 (pdf)

*object_meteorite*_class [*object*_class - ≠Enum]	openum(text)	S1b/S1b ObjMets [!_m]	F	--	Class of the meteorite OpenEnum: {CI, CM, CR, CO, CV, CVOx, CVRed, CK, CH, CB, CBa, CBb, CH/CB, C ungrouped, H, H/L, L, L/LL, LL, EH, EL, K, R, acapulcoite, lodranite, acapulcoite-lodranite, winonaite, angrite, aubrite, brachinite, ureilite, howardite, eucrite, diogenite, pallasite, mesosiderite, IAB, IC, IIAB, IIC, IID, IIE, IIF, IIG, IIIAB, IIICD, IIIE, IIIF, IVA, IVB, shergottite, nacklite, chassignite, orthopyroxenite, augite-rich basalt, basalt, anorthite, basalt-anorthite, gabbro, feldspathic breccia, basaltic breccia, ungrouped, not classified, other} *Note:* To be chosen in a list depending on "*object_meteorite*_group" For category = 'chondritic': - '*carbonaceous chondrite'*: CI, CM, CR, CO, CV, CVOx, CVRed, CK, CH, CB, CBa, CBb, CH/CB, C ungrouped, not classified, other - '*ordinary chondrite'*: H, H/L, L, L/LL, LL, not classified (not yet, or not fully classified) , other - '*enstatite chondrite'*: EH, EL, not classified, other

- '*Kakangari-like'*: K
- '*Rumuruti-like'*: R
- '*ungrouped chondrite'*: not classified
- '*unknown chondrite'*: fusion crust (piece of fusion crust that became detached from a chondrite meteorite)

For category = 'nonchondritic':

- '*primitive achondrite'*: acapulcoite, lodranite, winonaite, acapulcoite-lodranite, other (silicate-bearing IAB, IIE and IIICD irons)
- '*differenciated achondrite*': angrite, aubrite, brachinite, ureilite, howardite, eucrite, diogenite, other
- *'enstatite achondrite'*: not classified
- '*stony-iron'*: pallasite, mesosiderite, not classified, other
- '*iron*': IAB, IC, IIAB, IIC, IID, IIE, IIF, IIG, IIIAB, IIICD, IIIE, IIIF, IVA, IVB, ungrouped (does not fit into any of the above chemical groups)
  Note: 'IIICD' a fusionné avec 'IAB'
- '*ungrouped achondrite'*: other (silicate-bearing IVA iron ?)

For category = 'differentiated planetary':

- '*martian*': shergottite, nakhlite, chassignite, orthopyroxenite, augite-rich basalt, other (for the breccias)
  Note: les 3 premiers sont parfois regroupé sous le terme 'SNC'
- '*lunar*': basalt, anorthite, basalt-anorthite, gabbro, norite, feldspathic breccia, basaltic breccia, other (for the other rock types and breccias: basaltic-gabbroic breccia, troctolitic anorthosite, olivine-bearing gabbro, olivine-bearing gabbronorite)

Definitions:

- All class definitions can be found in the Meteoritical Bulletin Database: https://www.lpi.usra.edu/meteor/metbull.php
- *'ungrouped':* a meteorite that belongs to none of the defined classes
- *'C ungrouped':* a meteorite that belongs to the general C class but to none of the defined C subclasses
- *'not classified':* a meteorite that most probably belongs to one of the defined classes but has not yet been classified

Note:

- for 'ungrouped' and 'other': need to write additional information in

					"*object_meteorite*_comments" - for breccia and silicate-bearing irons it is the class of the hosting (dominating) component. The class(es) of the other(s) component(s) should be given in "comments" (also their relative abundance(s), petrologic_type(s), weathering(s), … if relevant). When (very rarely) there are 2 or more components of similar abundances, then put your main component of interest and the information on the other(s) in "comments".
*object_meteorite*_chondrite_petrologic_type [*object*_type - ≠Enum]	varchar(255)	S1/S3s [!o_m]	ObjMet	F	--	Petrologic type of the chondritic meteorite FreeList: {1, 1/2, 1-2, 2, 2.0, 3, 3.0, 3.00, 3.05, 3.1, 3.10, 3.15, 3.1/3.4, 3.2, 3.3, 3.4, 3.5, 3.6, sup 3.6, 3.7, 3.8, 3.9, 3/4, 3-4, 3-5, 3-6, 4, 4/5, 5, 5/6, 6, 7, undefined, other, …} *Condition:* mandatory only when "object_*meteorite*_category" = 'chondritic' *Note:* range of values: - '*carbonaceous chondrite'* Cx: 1 to 7 - '*ordinary chondrite'* H, L, LL: 3 to 7 - '*enstatite chondrite'*: EH: 3 to 5, EL: 3 to 6 - '*ungrouped chondrite'*: 1 to 7 - '*Kakangari-like"* K: 3 - '*Rumuruti-like"* R: 3, 4 - '*undefined*': not yet defined petrologic type - '*other*': breccias with several different petrologic types - any type of range of type can be given (FreeList) such as 3-4, 4/5, ...
*object_meteorite*_achondrite_petrologic_type [*object*_type - ≠Enum]	varchar(255)	S1/S3s [!o_m]	ObjMet	F	--	Petrologic type or chemical group of the achondritic meteorite OpenEnum: {MG, sHH, sHL, sLH, sLL, sLM, A, A1, A2, A3, A4, B, B1, B2, B3, B4, C, C2, C3, PMG, PES, ungrouped, undefined, other} *Condition:* mandatory only when "object_*meteorite*_category" = 'nonchondritic' *Definitions:* For "Class" = 'IAB' [iron meteorite IAB complex}: - 'MG': main group

- ‘sHH’: high-Au, high-Ni subgroup
- ‘sHL’: high-Au, low-Ni subgroup
- ‘sLH’: low-Au, high-Ni subgroup
- ‘sLL’: low-Au, low-Ni subgroup
- ‘sLM’: low-Au, medium-Ni subgroup

For “Class” = ‘Mesosiderite’:
- ‘A’: petrologic class A (basaltic)
- ‘A1’: petrologic class A and metamorphic grade 1
- ‘A2’: petrologic class A and metamorphic grade 2
- ‘A3’: petrologic class A and metamorphic grade 3
- ‘A4’: petrologic class A and metamorphic grade 4
- ‘B’: petrologic class B (more ultrmafic)
- ‘B1’: petrologic class B and metamorphic grade 1
- ‘B2’: petrologic class B and metamorphic grade 2
- ‘B3’: petrologic class B and metamorphic grade 3
- ‘B4’: petrologic class B and metamorphic grade 4
- ‘C’: petrologic class C (orthopyroxenite)
- ‘C2’: petrologic class C and metamorphic grade 2
- ‘C3’: petrologic class C and metamorphic grade 3

For “Class” = ‘Pallasite’:
- ‘PMG’: main petrologic/chemical group.
- ‘PES’: Eagle Station petrologic/chemical group.
- ‘*ungrouped*’: does not fit into any of the above chemical groups
- ‘*undefined*’: not yet defined petrologic type
- ‘*other*’: breccias with several different petrologic types

*object_meteorite*_shock	enum(text)	S2/Us [m]	ObjMet	F	--	Shock metamorphism stage of the meteorite Enum: {S1, S2, S3, S4, S5, S6, S7, unshocked, very low, low, moderate, high, very high, severe, undefined} *Definitions:* For chondritic or nonchondritic meteorites: - *‘S1’* or *‘unshocked’:* unshocked - *‘S2’* or *‘very low’:* very weakly shocked - *‘S3’* or *‘low’:* weakly shocked

- *'S4'* or *'moderate':* moderately shocked
- *'S5'* or *'high':* strongly shocked
- *'S6'* or *'very high':* very strongly shocked
- *'S7'* or *'severe':* shock-melted
- *'undefined':* not yet determined shock metamorphism stage

Notes:

- the '*Sn*' notation is used for chondritic meteorites while the '*adjective*' notation is used for nonchondritic meteorites
- 'S7' is listed but not yet officially attributed to shock-melted meteorites
- shock as observed in olivine and plagioclase for chondrites, extended to orthopyroxene for Enstatite chondrites
- other terms used for nonchondritic meteorites should be translated:
  - 'strong', 'strongly shocked', 'highly shocked', => 'high'
  - 'extensive shock' => 'very high'
  - 'severely shocked' => 'severe'
- when intermediate or multi-stages occurs, put the first in *'object_meteorite*_shock' and the whole description in *'object_meteorite*_comments'
  ex: S2-4, S4/5, ...

Ref: Classification of meteorites, Krot et al. (2003), p. 8 & 12

*object_meteorite*_weathering	enum(text)	S2/Us [m]	ObjMet	F	--	Terrestrial weathering grade of the meteorite Enum: {A, B, C, D, Ae, Be, Ce, W0, W1, W2, W3, W4, W5, W6, minor, low, moderate, high, severe, undefined} *Definitions:* For hand specimens of Antarctic meteorites: - '*A*': minor rustiness - '*B*': moderate rustiness - '*C*': severe rustiness - '*D*': evaporite minerals visible to the naked eye - '*Ae*': minor rustiness with evaporate minerals - '*Be*': moderate rustiness with evaporate minerals - '*Ce*': severe rustiness with evaporate minerals

For meteorites in polished sections:
- '*W0*': no visible oxidation of metal or sulfides
- '*W1*': minor oxide veins and rims around metal and troilite
- '*W2*': moderate oxidation of B20–60% of metal
- '*W3*': heavy oxidation of metal and troilite, 60–95%being replaced
- '*W4*': complete oxidation of metal and troilite, but no oxidation of silicates
- '*W5*': beginning alteration of mafic silicates, mainly along cracks
- '*W6*': massive replacement of silicates by clay minerals and oxides

For nonchondritic meteorites:
- '*minor*':
- '*low*':
- '*moderate*':
- '*high*':
- '*severe*':

For all meteorites:
- '*undefined*': not yet defined weathering

Notes:
- other terms used for nonchondritic meteorites should be translated:
  - 'very low', 'minimal' => 'minor'
  - 'strong' => 'high'
- when intermediate or multi-grades occurs, put the first in *'object_meteorite_* weathering' and the whole description in *'object_meteorite_*comments'
  ex: A/B, A/Be, B/C, B/Ce, C/D, W0-1, W1-2, W1/2,...

Ref: Classification of meteorites, Krot et al. (2003), p. 8-9

*object_meteorite_*comments [*object_*comments]	blob	U [m]	ObjMet	F	--	Additional information on the meteorite object (information on intermediate classes (CM/CI, CO/CM, CK/CV, …), on iron old classification (hexahedrite (H), octahedrite (O), ataxite (D)), on 'ungrouped chondrite' or 'other class, on 'other' petrologic or chemical types), and also for the other type/group/classes present in breccia and silicate-bearing irons, … (+ relative abundance(s), petrologic_type(s), weathering(s), …)

Meteorite object images						
object_meteorite_images	***List [L1]***	[O]				£: Pictures of the meteorite
*object_meteorite*_image_filename [*object*_image]	varchar(255)	P/U [m]	ObjMet L1	F	--	File name(s) (with extension) of picture(s) of the meteorite object *Image formats:* .png, .jpg, (.gif) *Note:* this file will be imported in the database
*object_meteorite*_image_caption [*object*_image_caption]	varchar(255)	U [m]	ObjMet L1	F	--	Caption(s) of the picture(s) of the meteorite
Meteorite mineralogic composition						
object_meteorite_minerals	***List [L2a]***	[O]				£: Description of the global mineralogic composition of the meteorite object
*object_meteorite*_mineral_symbol [*object*_mineral_symbol]	CS- enum(text)	U [m]	ObjMet L2a	F	--	Geochemical symbol of the different basic minerals of the meteorite object Enum: {Fa, Fs, Wo, Ab, An, En, Or} *Definitions:* - *'Fa':* Fayalite (Fe_2SiO_4) - *'Fs':* Ferrosilite ($Fe_2Si_2O_6$) - *'Wo':* Wollastonite ($CaSiO_3$) - *'Ab':* Albite ($NaAlSi_3O_8$) - *'An':* Anorthite ($CaAl_2Si_2O_8$) - *'En':* Enstatite ($Mg_2Si_2O_6$) - *'Or':* Orthoclase ($KAlSi_3O_8$)
*object_meteorite*_mineral_mole_fraction [*object*_mineral_mole_fraction]	varchar(255)	U [m]	ObjMet L2a	F	%	Mole fraction or fraction range (in %) of each type of basic mineral composing the meteorite *Note*: values between 0 and 100 Ex: '40.5', '12-25', ...
Meteorite global oxides composition						

object_meteorite_oxides	***List [L2b]***	[O]				£: Description of the oxides composition of the mineral materials of the meteorite object
*object_meteorite*_oxide_formula [*object*_oxide_formula]	CS- enum(text)	U [m]	ObjMet L2b	F	--	Formula of the different oxides composing the mineral materials of the meteorite object Enum: *see mineral*_oxide_formula *Note:* did not distinguish non-natural isotopic species
*object_meteorite*_oxide_mass_fraction [*object*_oxide_mass_fraction]	float	U [m]	ObjMet L2b	F	*%*	Mass fraction (in %) of each type of oxide composing the mineral materials *Note*: value between 0 and 100
*object_meteorite*_oxides_comments [*object*_oxides_comments]	blob	U [m]	ObjMet	F	--	Any additional information (sum of oxides …) or comments on the mineralogic or oxides composition of the meteorite object *Note:* also additional information on impurities not measured by the basic minerals or oxides

Meteorite object references

object_meteorite_links	***List [L3]***	[O]				£: Web pages describing the meteorite object and its properties
*object_meteorite*_link_name [*object*_link_name]	varchar(255)	U [m]	ObjMet L3	F	--	Name of the web site(s) describing the meteorite object and its properties. *Ex:* 'Meteoretical Bulletin Database', …
*object_meteorite*_link_url [*object*_link_url]	CS- varchar(255)	U [m]	ObjMet L3	F	--	URL address(es) of the web page(s) describing the meteorite object. *Notes*: - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
object_meteorite_publications	***List [L4]***	[O]				£: Publications describing the meteorite and its properties.

*object_meteorite*_publication_uid [*] [*object*_publication_uid]	varchar(255)	U [m]	ObjMet Publi L4	F	--	Link to the existing UID of the publication(s) describing the meteorite(s) and its properties. *Note:* mostly publications describing the meteorite object, its composition, properties, … *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

9.3 Micrometeorite objects Table

Root of the table: ***object_micromet***

Data type: 'Object'

Key-word	Type	Level	Table	Exp	Unit	Description
Micrometeorite object import						
*object_micromet*_import_mode [*object*_import_mode]	enum(text)	P [!!_m]	ObjMM	F	--	Mode of import of the "micrometeorite object" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*object_micromet*_xml_filename [-xml] [*object*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ObjMM	(V)	--	Name of the storage copy of the xml import file of the "*object_micrometeorite*" metadata ➔ determined automatically during import (from "*object_micromet*_uid" ?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
Micrometeorite object indexes						
*object_micromet*_index [**][-xml] [*object*_index]	int(10)	B [!!_g]	ObjMM	F	--	Automatic random but unique number given to a new micrometeorite object
*object_micromet*_uid [**] [*object*_uid]	varchar(255)	S0 [!!_m]	ObjMM	F	--	Unique identifier code given to the micrometeorite object table (to be created) *Nomenclature:* Create this code name with 'OBJMM_' and be very accurately in order to be simple and unique. It should be of the style 'OBJMM_(Collection)MicrometeoriteName' where 'Collection' is an acronym for the sampling area, if not already present in 'MicrometeoriteName', and 'MicrometeoriteName' is the common name/number of the micrometeorite object (with all separators removed).

						Note: see note in "*object_micromet*_name" *Ex:* Name = 'Concordia DC 94-100-106' => uid = 'OBJMM_DC94100106'
Micrometeorite object name						
*object_micromet*_family [-xml] [*object*_family]	enum (text)	S0/S0s [!!_c]	ObjMM	F	--	Family of object Enum: {micrometeorite} *Default* = 'micrometeorite' *Definitions:* - '*micrometeorite*': extraterrestrial dust particles between 10µm and 2 mm in size collected at Earth's surface (in contrast to IDPs collected in the stratosphere)
*object_micromet*_name [*object*_name]	varchar(255)	S0/S1s [!!_m]	ObjMM	F	--	Name of the micrometeorite object *Note*: It should be typically 'Collection MicrometeoriteName' where 'Collection' is an acronym for the sampling area, if not already present in 'MicrometeoriteName', and 'MicrometeoriteName' is the common name/number of the micrometeorite object *Nomenclature*: for 'Collection': • DC = Concordia • TAM = Transantarctic Mountains • ATA = Atacama • SPWW = South Pole Water Well • DSS = Deep Sea Sediments • GL = Greenland • CP = Cap Prudhomme • ? *Note*: – the different collections of micrometeorites are currently more or less well organized, with not always a clear and unique nomenclature for their names. Frequently they just get an order number. – the above nomenclature tries to give a unique name by concatenating

						the acronym of the collection site with the order number. *Ex:* Concordia DC 94-100-106
*object_micromet*_secondary_name [*object*_secondary_name]	varchar(255)	S0/S1s [m]	ObjMM	F	--	Alternative name(s) used for the micrometeorite *Notes:* – for exemple, name used in a publication – start with a capital letter – separate each name by a semicolon
Micrometeorite object origin						
*object_micromet*_recovery_year [*object_meteor*_recovery_year]	int(4)	S2/S2s [!_m]	ObjMM	F	year	Year of recovery of the micrometeorite *Ex*: '2012'
Micrometeorite object: planetary body						
*object_micromet*_recovery_body_uid [*] [*object*_recovery_body_uid]	varchar(255)	S2 [!!_m]	ObjMM Miner Body	F	--	Link to the existing UID of Earth from which the micrometeorite originates *Default*: 'BODY_planet_Earth' *Note:* - only for micrometeorites collected on Earth
*object_micromet*_recovery_body_coordinate_system [*object*_recovery_body_coordinate_system]	openum(text)	U [!d_m]	ObjMM	F	--	Coordinate system on Earth of the geographic location of the recovery place of the micrometeorite OpenEnum: {WGS84} *Default*: 'WGS84' *Definitions*: see "*experiment*_body_coordinate_system" *Notes*: currently only 'WGS84' for Earth
Micrometeorite object: geolocation						

*object_micromet*_recovery_geolocation_place [*object*_recovery_geolocation_place]	varchar(255)	S1/Us [!_m]	ObjMM	F	--	Place of recovery on Earth of the micrometeorite *Note*: it is the name of geographic area or town of recovery of the micrometeorite *Ex*: 'Queen Alexandra range'
*object_micromet*_recovery_geolocation_region [*object*_recovery_geolocation_region]	varchar(255)	S1/Us [m]	ObjMM	F	--	Region, state, province or county (administrative location) of the recovery place on Earth of the micrometeorite *Constraint:* only when "*object_micromet*_recovery_body_uid" = 'BODY_planet_Earth' *Ex:* 'Murmanskaja Oblast', 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi'
*object_micromet*_recovery_geolocation_country_code [*object*_recovery_geolocation_country_code]	enum(text)	S1/Us [!o_m]	ObjMM	F	--	2-digit code of the country of the recovery place on Earth of the micrometeorite Enum: {AQ, AU, CH, CL, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory and only when "*object_micromet*_recovery_body_uid" = 'BODY_planet_Earth' *Definitions:* see "*laboratory*_address_country_code" *Ex*: 'AQ' for Antarctica
*object_micromet*_recovery_geolocation_type [*object*_recovery_geolocation_type]	enum(text)	U [!!o_m]	ObjMM	F	--	Type of geographic location of the recovery place of the micrometeorite Enum: {point, line, box, polygon} *Condition*: absolute mandatory when "*object_micromet*_recovery_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_geolocation_type"
object_micromet_recovery_geolocation_coordinates [*object_recovery_geolocation_coordinates*]	**List [L0]**	[!o]				£: Geolocation (x,y,z coordinates) on Earth of the recovery place of the micrometeorite *Condition*: absolute mandatory when "*object_micromet*_recovery_geolocation_type" ≠ Ø

						Conditions: on the number of long/lat couple: see *"experiment*_geolocation_coordinates"
*object_micromet*_recovery_geolocation_coordinate_latitude [*object*_recovery_geolocation_coordinate_latitude]	float	S3 [!!o_m]	ObjMM L0	F	deg	Latitude of the geographic location of the recovery place of the micrometeorite *Format*: in N 'decimal degrees' (negative value for S hemisphere) in WGS84 system *Note*: 3 (100 m) to 5 decimals (1 m accuracy) are enough *Ex*: '12.12345' provides 1 m accuracy
*object_micromet*_recovery_geolocation_coordinate_longitude [*object*_recovery_geolocation_coordinate_longitude]	float	S3 [!!o_m]	ObjMM L0	F	deg	Longitude of the geographic location of the recovery place of the micrometeorite *Format*: in E 'decimal degrees' (in the E direction only) in WGS84 system *Note*: same as for "*object_micromet*_recovery_geolocation_coordinate_latitude" and even less at high latitude *Ex*: '12.12' provides 100 m accuracy at 85° latitude
*object_micromet*_recovery_geolocation_coordinate_altitude [*object*_recovery_geolocation_coordinate_altitude]	float	S3 [m]	ObjMM L0	F	m	Altitude of the geographic location of the recovery place of the micrometeorite *Format*: in 'm' in WGS84 system *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*object_micromet*_recovery_comments [*object*_ recovery_comments]	blob	U [m]	ObjMM	F	--	Additional information or comments about the recovery of the micrometeorite *Ex*: 'collected jointly by ANSMET (US) and NIPR (Japan)', 'location accurate at +/- 1km', ', 'coordinates accurate at +/- 0.1°'
Micrometeorite object characteristics						
*object_micromet*_sampling_method	varchar(255)	U	ObjMM	F	--	Method to sample the micrometeorite (melting of snow, magnetic extraction…)

		[!_m]				
*object_micromet*_size_min	float	U [m]	ObjMM	F	µm	Smallest lateral dimension of the micrometeorite *Unit:* micrometers
*object_micromet*_size_max	float	U [m]	ObjMM	F	µm	Largest lateral dimension of the micrometeorite *Unit:* micrometers
*object_micromet*_equivalent_diameter	float	S3/Us [mc]	ObjMM	F	µm	Equivalent diameter, Deq *Unit:* micrometers *Condition*: use either 'equivalent diameter' or 'size_min/max' *Note*: this equivalent diameter can be either measured or calculated from 'size_min/max': ➔ when 'size_min/max' have values, then • Deq= $(max \times min^2)^{1/3}$
*object_micromet*_fragmented	boolean	S3/Us [m]	ObjMM	F	--	Flag telling if the micrometeorite is known to have been fragmented BoolEnum: {yes, no} or {true, false}

Micrometeorite object classification

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*object_micromet*_group [*object*_group - ≠Enum]	enum (text)	S1/S2s [!!_m]	ObjMM	F	--	Group of the micrometeorite Enum: {melted, partially melted, unmelted} *Definitions:* - '*melted*': particles that experienced large degrees of fusion of primary phases during atmospheric entry. - '*partially melted'*: represent a gradational series from the more intensely heated Cosmic Spherules to the least heated "unmelted particles"

						- '*unmelted*': dominated by a fine-grained porous groundmass of micron-sized mineral grains and are similar to the fine-grained matrices of chondritic matrices. Have broadly chondritic compositions.
*object_micromet*_class [*object*_class - ≠Enum]	openum (text)	S1/S1s [!!_m]	ObjMM	F	--	Class of the micrometeorite OpenEnum: {cosmic spherule, scoriaceous, mixed, fine-grained, coarse-grained, refractory, ultracarbonaceous} *Definitions:* For group = 'melted': - *'cosmic spherule':* spherical to subspherical particles formed as molten droplets during atmospheric entry For group = 'partially melted': - *'scoriaceous':* dominated by a mesostasis of microporphyritic olivine, usually with crystal sizes < 1µm, within an interstitial silicate glass phase. Often contain relict minerals and relict matrix areas. - *'mixed':* composite particles partially melted and including selvages of fine-grained matrix For group = 'unmelted': - *'fine-grained'*: dominated by a fine-grained porous groundmass of micron-sized mineral grains - '*coarse-grained*': dominated by anhydrous silicates with grain-sizes larger than several microns, often with glassy mesostasis - *'refractory':* unmelted MMs containing refractory minerals that are likely to be fragments of refractory inclusions. Contain isolated grains of spinel, perovskite, melilite, fassaite, and hibonite. - *'ultracarbonaceous':* contain higher abundances of carbon than CI chondrites, with heterogeneous compositions of silicates suggesting they are unequilibrated particles. *Ref:* The classification of micrometeorites. Genge et al. (2008) MAPS, 43(3) 497-515 (pdf)
*object_micromet*_type [*object*_type - ≠Enum]	openum (text)	S1/S1s	ObjMM	F	--	Type of the micrometeorite OpenEnum: {S-type, G-type, I-type, C1, C2, C3, FgF, FgC, chondritic

[o_m]

CgMMs, achondritic CgMMs, single crystal CgMMs, porous, compact, hydrated}

Constraint: only when "*object_micromet_*class"= {cosmic spherule, fine-grained, coarse-grained, refractory}

Definitions:

For class = 'cosmic spherule': Cosmic Spherule are subdivided into several chemical subtypes reflecting their principle mineralogy:

- '*S-type':* silicate-type spherules, the most common. Have broadly chondritic compositions.
- *'G-type':* spherules typically dominated by magnetite dendrites within a mesostasis of silicate glass with major element compositions intermediate between S- and I-types
- *'I-type':* iron-rich spherules dominated by FeO with minor amounts of other oxides.

For class = 'fine-grained':

- *'C1':* compact FgMMs with low apparent porosities that are chemically homogeneous over scales of 10 µm
- *'C2':* compact FgMMs with low porosities that are chemically heterogeneous in particular in their Fe/Mg, Fe/Si over scales of 10 µm
- *'C3':*porous FgMMs (porosity up to 50% by volume) that are dominated by subhedral magnesian olivine and pyroxene grains
- *'FgF':* unmelted micrometeorites with a fine-grained porous groundmass presenting textures similar to chondritic porous IDPs (//C3)
- *'FgC':* Fine-grained compact MMs, have a smooth compact texture (generally C1, C2) – in contrast to the fluffy particles

For class = 'coarse-grained':

- *'chondritic CgMMs':* coarse grained micrometeorites with igneous textures, dominated by pyroxene and/or olivine within a glassy mesostatis which can contain accessory metal, sulphide, and/or iron oxides. Have broadly chondritic mineral assemblages similar to chondrules or primitive achondrites.
- *'achondritic CgMMs':* very rare coarse grained micrometeorites

						with non-chondritic, non-refractory compositions and with textures and mineralogies suggesting derivation from differentiated parent body - *'single crystal CgMMs':* fragment of single crystals of olivine and pyroxene For class = 'refractory': - *'porous':* porous particles dominated by refractory minerals - *'compact':* compact particles dominated by refractory minerals - *'hydrated':* dominated by refractory minerals surrounded by Fe-rich phyllosilicates (or their thermal decomposition products) *Notes:* - to be chosen in a list depending on "*object_micromet*_class" - no "type" for classes = {scoriaceous, mixed, ultracarbonaceous}
*object_micromet*_subtype	openum(text)	S1/S2s [o_m]	ObjMM	F	--	Sub-type of the micrometeorite OpenEnum: {CAT, glass, cryptocrystalline, barred olivine, porphyritic olivine, coarse-grained, porphyritic olivine and/or pyroxene, granular olivine and/or pyroxene, radiate pyroxene, type I/type II} *Constraint:* only when "*object_micromet*_type"= {S-type, chondritic CgMMs} *Note:* only for types 'S-type' and 'chondritic CgMMs' *Definitions* For "type" = 'S-type': subdivided into several subclasses depending on their quench textures - '*CAT*': spherules with barred olivine texture, that lack Fe, have high Mg/Si ratios (> 1.7) and are enriched in Ca, Al, and Ti. - '*glass*': spherule lacking olivine microphenocrysts, usually spherical, can be highly vesiculated, some contain FeNi beads, consist almost entirely of glass - '*cryptocrystalline*': spherule dominated by submicron crystallites and can have significant submicron magnetite. - '*barred olivine'*: spherule dominated by parallel growth olivine within glass - '*porphyritic olivine'*: spherule dominated by olivine

						microphenocrysts with equant, euhedral or skeletal morphologies within a glassy mesostasis, usually with accessory magnetite and/or chromite. Relict-bearing varieties contain unmelted minerals. - '*coarse-grained'*: these spherules contain > 50 % volume relict minerals. For "type" = 'chondritic CgMMs' - '*porphyritic olivine and/or pyroxene'*: Igneous MMs dominated by pyroxene and/or pyroxene phenocrysts within glass. - '*granular olivine and/or pyroxene'*: Igneous MMs dominated by pyroxene and/or olivine without significant glass. - '*barred olivine'*: Igneous MMs dominated by parallel growth olivine within glass. - '*radiate pyroxene'*: Igneous MMs dominated by radiating pyroxene dendrites within glass. - '*type I/type II'*: Type I CgMMs are reduced particles containing Fs and/or Fa < 10 mol%. Type II CgMMs are oxidized particles with Fs and/or Fa > 10 mol%. *Notes:* - to be chosen in a list depending on "*object_micromet*_type" - "subtype" only for "type" = {S-type, chondritic CgMMs}
*object_micromet*_comments [*object*_comments]	blob	U [m]	ObjMM	F	--	Additional information on the micrometeorite object

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Micrometeorite object images

object_micromet_images	***List [L1]***	[O]				£: Pictures of the micrometeorite
*object_micromet*_image_filename [*object*_image]	varchar(255)	P/U [m]	ObjMM L1	F	--	File name(s) (with extension) of picture(s) of the micrometeorite object *Image formats:* .png, .jpg, (.gif) … *Note:* this file will be imported in the database
*object_micromet*_image_caption	varchar(255)	U [m]	ObjMM	F	--	Caption(s) on the picture(s) of the micrometeorite

[*object*_image_caption]		L1				

Micrometeorite global oxides composition

object_micromet_oxides	***List [L2]***	[O]				£: Description of the oxides composition of the mineral materials of the meteorite object
*object_micromet*_oxide_formula [*object*_oxide_formula]	CS- enum(text)	U [m]	ObjMM L2	F	--	Formula of the different oxides composing the micrometeorite object Enum: *see mineral*_oxide_formula *Note:* did not distinguish non-natural isotopic species
*object_micromet*_oxide_mass_fraction [*object*_oxide_mass_fraction]	float	U [m]	ObjMM L2	F	%	Mass fraction (in %) of each type of oxide composing the micrometeorite *Note*: value between 0 and 1
*object_micromet*_oxides_comments [*object*_oxides_comments]	blob	U [m]	ObjMM	F	--	Any additional information (sum of oxides …) or comments on the oxides composition of the micrometeorite object *Note:* also additional information on impurities not measured by oxides

Micrometeorite object references

object_micromet_links	***List [L3]***	[O]				£: Web pages describing the micrometeorite collection, object and properties
*object_micromet*_link_name [*object*_link_name]	varchar(255)	U [m]	ObjMM L3	F	--	Name of the web site(s) describing micrometeorite collection: sampling area and method *Ex:* 'Meteoritical Bulletin Database', …
*object_micromet*_link_url [*object*_link_url]	CS-varchar(255)	U [m]	ObjMM L3	F	--	URL address(es) of the web page(s) describing the micrometeorite collection Ex: https://www.lpi.usra.edu/meteor/metbull.php?sea=Allende&code=2278 *Notes*: - can link to a publication by giving its url address, preferably through its DOI.

						Ex: https://doi.org/10.1002/ejic.200700067
object_micromet_publications	***List [L4]***	[O]				£: Publications describing (i) the considered micrometeorite collection and sampling area, (ii) the considered micrometeorite and its properties
*object_micromet*_publication_uid [*] [*object*_publication_uid]	varchar(255)	U [m]	ObjMM Publi L4	F	--	Link to the existing UID of the publication(s) *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

9.4 IDPs objects Table

Root of the table: ***object_idp***

Data type: 'Object'

Key-word	Type	Level	Table	Exp	Unit	Description
IDP object import						
*object_idp*_import_mode [*object*_import_mode]	enum(text)	P [!!_m]	ObjIDP	F	--	Mode of import of the "IDP object" data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*object_idp*_xml_filename [-] [*object*_xml_filename]	varchar(255) [virtual KW]	P [!!_vc]	ObjIDP	(V)	--	Name of the storage copy of the xml import file of the "*object_IDP*" metadata ➔ determined automatically during import (from "*object_idp*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
IDP object indexes						
*object_idp*_index [**][-] [*object*_index]	int(10)	B [!!_a]	ObjIDP	F	--	Automatic random but unique number given to a new IDP object
*object_idp*_uid [**] [*object*_uid]	varchar(255)	S0/S1s [!!_m]	ObjIDP	F	--	Unique identifier code given to the IDP object table (to be created) *Nomenclature:* This code name should be of the style 'OBJIDP_IDPName' where 'IDPName' is the common name/number of the IDP object (with all separators removed) and specifying whether it is a cluster or not. *Note*: see "*object_idp*_name" *Ex:* 'OBJIDP_L2021D7', 'OBJIDP_L2055Clust2B3'

IDP object name

*object_idp*_family [-xml] [*object*_family]	enum (text)	S0/S0s ObjIDP [!!_c]	F	--	Family of object Enum: {idp} *Default* = 'idp' *Definitions:* - *'idp'* (Interplanetary Dust Particles): extraterrestrial dust particles collected in Earth's stratosphere (in opposition to micrometeorites recovered on Earth's surface and whose size range is typically slightly higher). *Note:* the word "IDP" only refers to dust sampled by high-altitude planes and orbital stations
*object_idp*_name [*object*_name]	varchar(255)	S0/S1s ObjIDP [!!_m]	F	--	Name of the IDP object *Definition for NASA*: ⇨ NASA: 'name of collector'-'name of particle': ex: 'Lxxxx Dyy' - 'name of collector': letter (L, U, W) + number (4): Lxxxx - 'name of the particle': letter + number (1 or 2) : 'Dyy' *Note*: there is a more complex way to name particles from clusters *Exemple*: - 'L2021 D7': collector L2021, particle D7
*object_idp*_secondary_name [*object*_secondary_name]	varchar(255)	S0/S1s ObjIDP [m]	F	--	Alternative name(s) used for the IDP *Notes*: - for example, the community working on presolar grains are used to give nicknames to the IDPs they are working on - start with a capital letter - separate each name by a semicolon *Exemple*: 'Andric' for U2108 B2 (Floss et al. 2011)

IDP object collection

*object_idp*_collector	varchar(255)	S1/S2s [!!_m]	ObjIDP	F	--	Name of the collector of the IDPs *Definition for NASA:* - *'name of collector':* letter (L, U, W) + number (4): LXxxxx or Uxxxx or Wxxxx *Notes:* - can be directly deduced from the IDP name - if unknow, then write 'unknown' *Exemple:* 'L2021' for L2021 D7
*object_idp*_collection_period [*object_meteor*_recovery_year]	varchar(255)	S2/Us [!_m]	ObjIDP	F	--	Periods when the stratospheric IDP collectors were flown *Note*: value from the 'introduction' of the NASA Cosmic dust Catalog" of the collector campain *Exemple*: 'between June 30 and July 30, 2008' (L2071)
*object_idp*_collection_duration	float	U [!_m]	ObjIDP	F	*hour*	Effective duration of collection of the IDPs • *Unit*: hour *Note*: value from the 'introduction' of the NASA Cosmic dust Catalog" of the collector campain *Exemple:* '50' for "50 hours of flight time" (L2071)
*object_idp*_collection_location	varchar(255)	S2/Us [!_m]	ObjIDP	F	--	Geographic area where the IDP collectors were flown *Note*: value from the 'introduction' of the NASA Cosmic dust Catalog" of the collector campain *Exemple:* in cosmic dust catalog vol. 18: - 'over the Eastern coast of the USA, the Great Lakes, and Canada' (L2071) - 'off the California coast' (L2076)

*object_idp*_targetted_collection	boolean	S3/Us [!_m]	ObjIDP	F	--	Flag telling if the IDP collection was targetted BoolEnum: {yes, no} or {true, false} *Note*: some collectors have been flown at specific times designed to coincide with the passage of the Earth through the dust trails of specific comets, in the hopes of collecting enhanced quantities of cometary dust over background extraterrestrial materials
*object_idp*_collection_target	varchar(255)	S1/S1b [!o_m]	ObjIDP	F	--	Name of the target (comet, …) of the IDP collection *Condition*: mandatory when "*object_idp*_targetted_collection" = 'yes' *Ex*: 'Tempel-Tuttle'; 'Grigg-Skjellerup'
*object_idp*_collection_comments [*object_* recovery_comments]	blob	U [m]	ObjIDP	F	--	Additional information or comments about the collection of the IDP *Ex*: 'collected jointly by ANSMET (US) and NIPR (Japan)'

IDP object classification

*object_idp*_provider	varchar(255)	S2/S2 [!_m]	ObjIDP	F	--	Provider of the IDP object *Note:* currently only 'NASA/Johnson Space Center Cosmic Dust Program'
*object_idp*_pre_type	openum (text)	S1/S2 [!_m]	ObjIDP	F	--	Pre-classification type of the IDP object given by the provider OpenEnum: {AOS, C, TCA, TCN, other, unknown} *Nomenclature*: - '*AOS*': Aluminum Oxide Sphere - '*C*': cosmic dust - '*TCA*': terrestrial contamination (artificial or man-made) - '*TCN*': terrestrial contamination (natural) - '*unknown*': unknown or uncertain identification - '*other*': none of the above pre-types. Provide information in "*object*_idp_comments" *Definition*: - this nomenclature is given as in "catalog format' of each NASA Cosmic Dust catalog: https://www-curator.jsc.nasa.gov/dust

						Ex: https://www-curator.jsc.nasa.gov/dust/cdcat20/basicinfo.cfm?vol=20,1&section=Format) *Note*: the pre-type of each particle is given as "Type" in NASA Cosmic Dust catalog
*object_idp*_chemical_group [*object*_group - ≠Enum]	enum(text)	S1/S1s [!_m]	ObjIDP	F	--	Chemical group of the IDP object Enum: {chondritic, non-chondritic} *Definitions*: - '*chondritic*': - '*non-chondritic*':
*object_idp*_morphological_type	enum(text)	S2/Us [!_m]	ObjIDP	F	--	Morphological type of the IDP object Enum: {porous, smooth} *Definitions*: - '*porous*': - '*smooth'*:
*object_idp*_mineralogical_class	enum(text)	S1/S1s [!_m]	ObjIDP	F	--	Mineralogical class of the IDP object (after their most abundant silicate minerals) Enum: {layer lattice silicates, pyroxene, olivine, pyroxene-olivine, FeO, FeS, FeO-FeS} *Definitions*: - '*layer lattice silicates'*: - '*pyroxene*': - '*olivine'*: - '*pyroxene-olivine'*: - '*FeO'*: - '*FeS'*: - '*FeO-FeS'*:
*object_idp*_comments	blob	U	ObjIDP	F	--	Additional information on the IDP object (comments from the NASA catalog

[*object*_comments]						for example specifying close spatial relationship between some particles)
IDP object characteristics						
*object_idp*_particle_type	enum	S1/S2s [!!_m]	ObjIDP	F	--	Type of IDP particle Enum: {unique particle, cluster of particles, particle from a cluster, unknown} - *Definitions*: - '*unique particle'*: individual particle - '*cluster of particles'*: cluster of several particles - '*particle from a cluster'*: particle picked out of a cluster
*object_idp*_shape	enum(text)	S2/Us [m]	ObjIDP	F	--	Description of the shape of the IDP object Enum: {irregular, spherical, equidimentional, irregular to spherical, irregular to equidimentional, spherical to equidimentional, various, unknown} *Notes:* - this information is given as 'Shape' {I: 'irregular', S: 'spherical', E: 'equidimentional' and combinations: I/S, I/E, S/E} in the NASACosmic Dust catalog - '*various*': used mostly for clusters when various types of shapes are present.
*object_idp*_size_min	float	U [m]	ObjIDP	F	µm	Smallest lateral dimension of the IDP • *Unit*: µm *Note*: the size of each particle is given as "size" (n or nxm) in NASA Cosmic Dust catalog
*object_idp*_size_max	float	U [m]	ObjIDP	F	µm	Largest lateral dimension of the IDP • *Unit*: µm *Note*: cf. note in "*object_idp*_size_min"
IDP object images						

object_idp_images	***List [L1]***	[O]				£: Pictures of the IDP object
*object_idp*_image_filename [*object*_image]	varchar(255)	P/U [m]	ObjIDP L1	F	--	File name(s) (with extension) of picture(s) of the IDP object *Image formats:* .png, .jpg, (.gif) … *Note:* - it can be the MEB image of the IDP object as provided by NASA. But this image can be accessed directly through the catalog (see "*object_idp_catalogs*") - it can be also an image recorded by researchers *Note DB:* this file will be imported in the database
*object_idp*_image_caption [*object*_image_caption]	varchar(255)	U [m]	ObjIDP L1	F	--	Caption(s) on the picture(s) of the IDP *Note*: the origin and credits of the image should be specified (ex: from NASA Catalog, or from another source: researcher, …)

IDP global oxides composition

object_idp_oxides	***List [L2]***	[O]				£: Description of the oxides composition of the mineral materials of the IDP object
*object_idp*_oxide_formula [*object*_oxide_formula]	CS-enum(text)	U [m]	ObjIDP L2	F	--	Formula of the different oxides composing the IDP object Enum: *see mineral*_oxide_formula *Note:* did not distinguish non-natural isotopic species
*object_idp*_oxide_mass_fraction [*object*_oxide_mass_fraction]	float	U [m]	ObjIDP L2	F	%	Mass fraction (in %) of each type of oxide composing the IDP object
*object_idp*_oxides_comments [*object*_oxides_comments]	blob	U [m]	ObjIDP	F	--	Any additional information (sum of oxides …) or comments on the oxides composition of the IDP object *Note:* also additional information on impurities not measured by oxides

IDP optical properties						*Note*: this information is given in the NASA Cosmic Dust catalog (https://www-curator.jsc.nasa.gov/dust/cdcat20/basicinfo.cfm?vol=20,1&section=Format)
*object_idp*_color	varchar(255)	S2/Us [m]	ObjIDP	F	--	Color nuance of the IDP object *Note:* this information is given as 'Color' {AM, BK, BL, BR, BZ, CL, CS, GN, GR, OR, RD, RU, SI, WH, YL} in the NASA Cosmic Dust catalog and can combine several. *Ex:* 'pale pinkish - green, pink, blue' Equivalence table between NASA 'color' and SSDM "*object_idp*_color": - BK = black - BL = blue - BR = brown - BZ = bronze - CL = colorless ? - CS = ? - GN = green - GR = gray - OR = orange - RD = red - RU = ? - SI = silver - WH = white - YL = yellow
*object_idp*_diaphaneity	enum(text)	S2/Us [m]	ObjIDP	F	--	Capacity of the IDP object to transmit light Enum: {transparent, transparent to translucent, transparent to opaque, translucent, translucent to transparent, translucent to opaque, opaque, opaque to transparent, opaque to translucent, various, unknown} *Notes:* - this information is given as 'Transparency' {transparent (T), translucent (TL), opaque (O) and combinations for intermediate:

						O/T, T/O, O/TL, TL/O, T/TL, TL/T} in the NASA Cosmic Dust catalog - '*various*': used mostly for clusters when various types of shapes are present.
*object_idp*_luster	enum(text)	S2/Us [m]	ObjIDP	F	--	Description of how and how much the surface of the IDP object reflects light. Enum: {dull, dull to submetallic, dull to metallic, dull to subvitreous, dull to vitreous, submetallic, submetallic to metallic, submetallic to subvitreous, submetallic to vitreous, metallic, metallic to vitreous, subvitreous, subvitreous to vitreous, vitreous, pearly, pearly to subvitreous, resinous, resinous to metallic, resinous to vitreous, other, various, unknown} *Definitions*: see "*mineral*_luster" for most of them - '*dull*': - '*subvitreous*': *Notes:* - this information is given as 'Luster' {Dull (D), Metallic (M), Submetallic (SM), Subvitreous (SV), and Vitreous (V), Pearly (P), Resinous (R) and some combinations for intermediate cases: D/SM, D/M, D/SV, D/V, SM/M, SM/SV, SM/V M/V, SV/V, P/SV, R/M, R/V} in the NASA Cosmic Dust catalog. - to reduce the high number of combinations, the opposite combinations have been merged, e.g. 'metallic to dull' (M/D) = 'dull to metallic' (D/M) - a few rare combinations (4 cases each) are not included in the list but can be associated to the closest description {M/SV => M/V, P/V => P/SV, R/SV => R/V} - a few other very rare combinations (1-2 cases each) are not included: (D/P, D/R, O?/SV, P/D, R/D, R/SM, SM/P} => 'other'

IDP object references

object_idp_links	***List [L3]***	[O]				£: Web pages describing the IDP object, collection and properties
*object_idp*_link_name [*object*_link_name]	varchar(255)	U [m]	ObjIDP L3	F	--	Name of the web site describing the IDP object and collection
*object_idp*_link_url [*object*_link_url]	CS-varchar(255)	U [m]	ObjIDP L3	F	--	URL address of the web page
object_idp_catalogs	***List [L4a]***	[O]				£: Catalog describing the IDP object, collection and properties
*object_idp*_catalog_uid [*] [*object*_catalog_uid]	varchar(255)	U [m]	ObjIDP Publi L4a	F	--	Link to the existing UID of the catalog publication *Notes*: - currently mostly the NASA catalogs. They correspond to one to several https://www-curator.jsc.nasa.gov/dust/catalogs/index.cfm collectors and contain preclassification type + size/shape/transparency/color/luster info + SEM image + EDS spectra - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067 *Note xml*: The pdf files of these catalogs should be ingested in SSHADE as "publication" prior the IDP object (to get an UID)
object_idp_publications	***List [L4b]***	[O]				£: Publications describing the IDP object and its properties
*object_idp*_publication_uid [*] [*object*_publication_uid]	varchar(255)	U [m]	ObjIDP Publi L4b	F	--	Link to the existing UID of the publication *Notes*: - scientific publication defining, among other data, the final classification of the considered cosmic dust - these papers should be in the bibliography database, with "*publication*_content" = 'planetary sciences'

10. SAMPLE

10.1 Introduction

The sample data model is the most complex part of the SSDM because it needs to describe the many different types of ***solid samples*** used in solid spectroscopy down to the atomic level, through a complete description of each of its ***layers***, of the ***materials*** (homogeneous collection of grains) constituting these layers, and of the ***constituents*** (minerals, molecular solids, ionic solids, liquids…) making up these materials, and then of the ***species*** (molecules, atoms) that compose the constituents. The mineral constiuents and molecular species are then described in term of ***atoms***.
For *complex solids* mostly a global description in terms of atoms is possible when an elemental analysis has been performed. But we also let the possibility to partly describe these solids in terms of chemical functions.

Amounts or mixtures of material(s) that is collected in the field (natural) of synthesized by chemical or physical processing (synthetic) are called *"**matters**"* (see ***). These matters are generally used a number of times within different samples and are described as material/constituent/species with additional information on the matter in specific keywords, including information on their origin. They can be directly used in sample as (set of) *materials*.

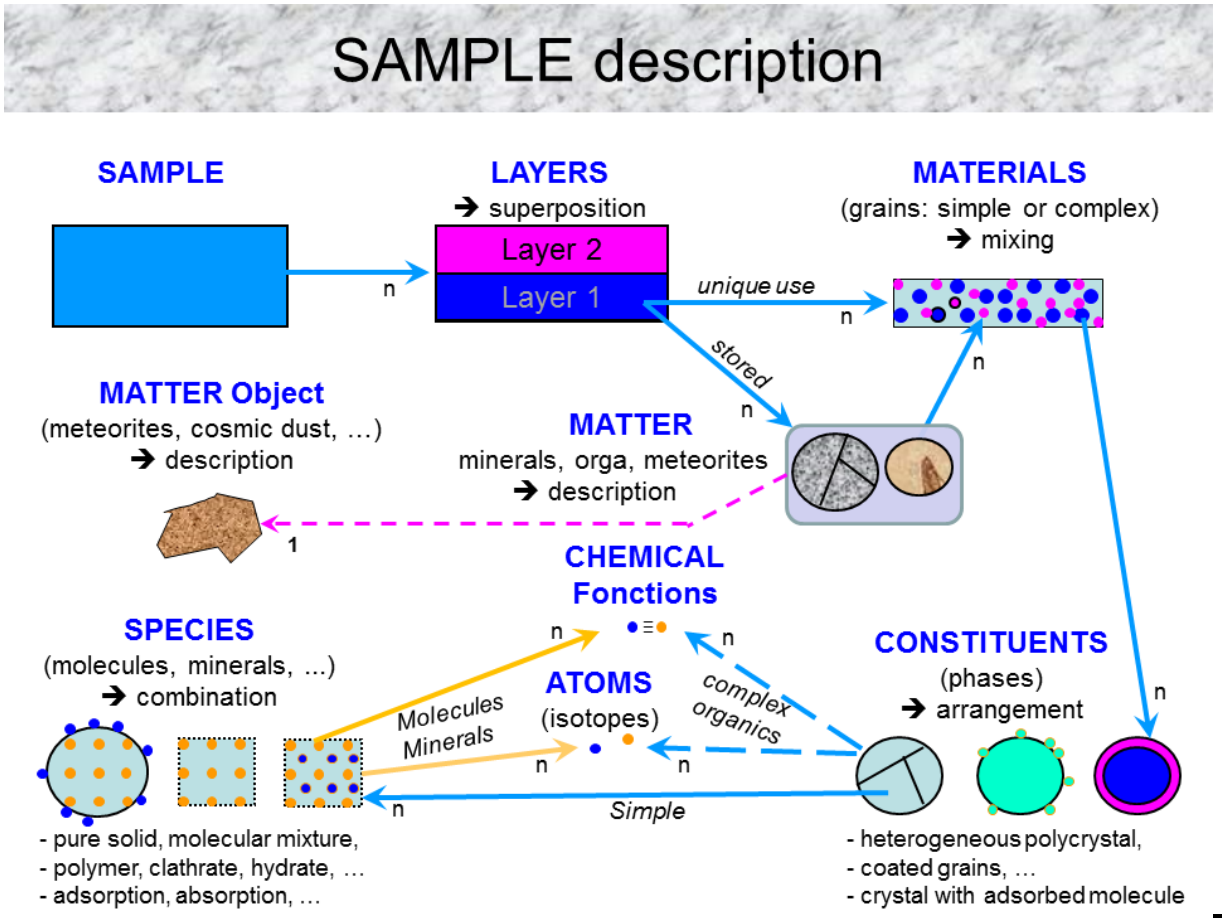


Figure 4: Sample structure from layers to atoms. The matter is a naturalor synthetic set of materials. It may be linked with a natural object.

10.2 Description

At each level of the sample description there are (see Figures 5a,b):

- parameters describing qualitatively how the lower levels are organized in this level in a relation " *this level n* with *m levels n-1* ": e.g. organization of *layers* in the sample, mixing of *materials* in each layer, organization of *constituents* in each material, of *species* in each constituent, and of *atoms* in each species) and

quantitatively (number of *layers* of the sample, number and list of *materials* of each layer, of *constituents* of each material, of *species* of each constituent, of *atoms* of each species or constituent).

- parameters describing how the current level is organized in the upper level in a relation "*this sub-level n-1* in *its level n*": e.g. *layer* order, type and thickness in the sample, *material* abundance and type (simple or *matter*) in its layer, *constituent* arrangement and abundance in its material, *species* state and abundance in its constituent, and *atom* abundance in its species).

- parameters specific to each level (its physical characteristics, state, texture, formation conditions, …).

In some more details:

Sample

* A solid **Sample** can have multiple ***layers*** added one on each other (films, granular layers,..).

- The sample has a *"name"* and possible "*provider*" or "*parent sample*". It is described by some macroscopic *"physical characteristics"* and by environment parameters (thermal, pressure, fluid, mechanical stress and/or irradiation) that can provide the state or can affect the sample prior to the experiment. The sample is then described in terms of its *"layers organization"*.

Layers

* Each **Layer** of a sample may have one or multiple ***materials*** mixed at grain level.

- Each **layer** is defined by its *"order"* in the sample, by its *"type"*, by *"physical characteristics"*, and by the *"formation conditions"* of the layer. Finaly the *"mixing of materials"* that constitute the layer is specified.

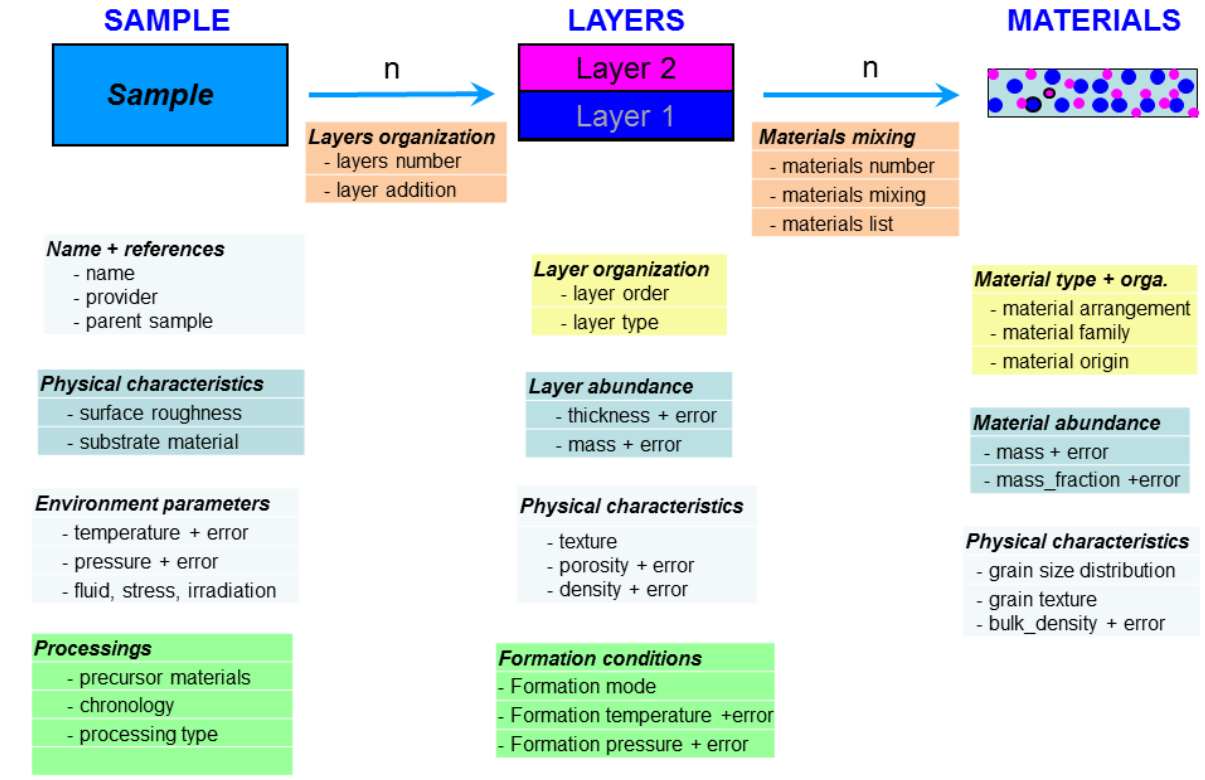
Materials

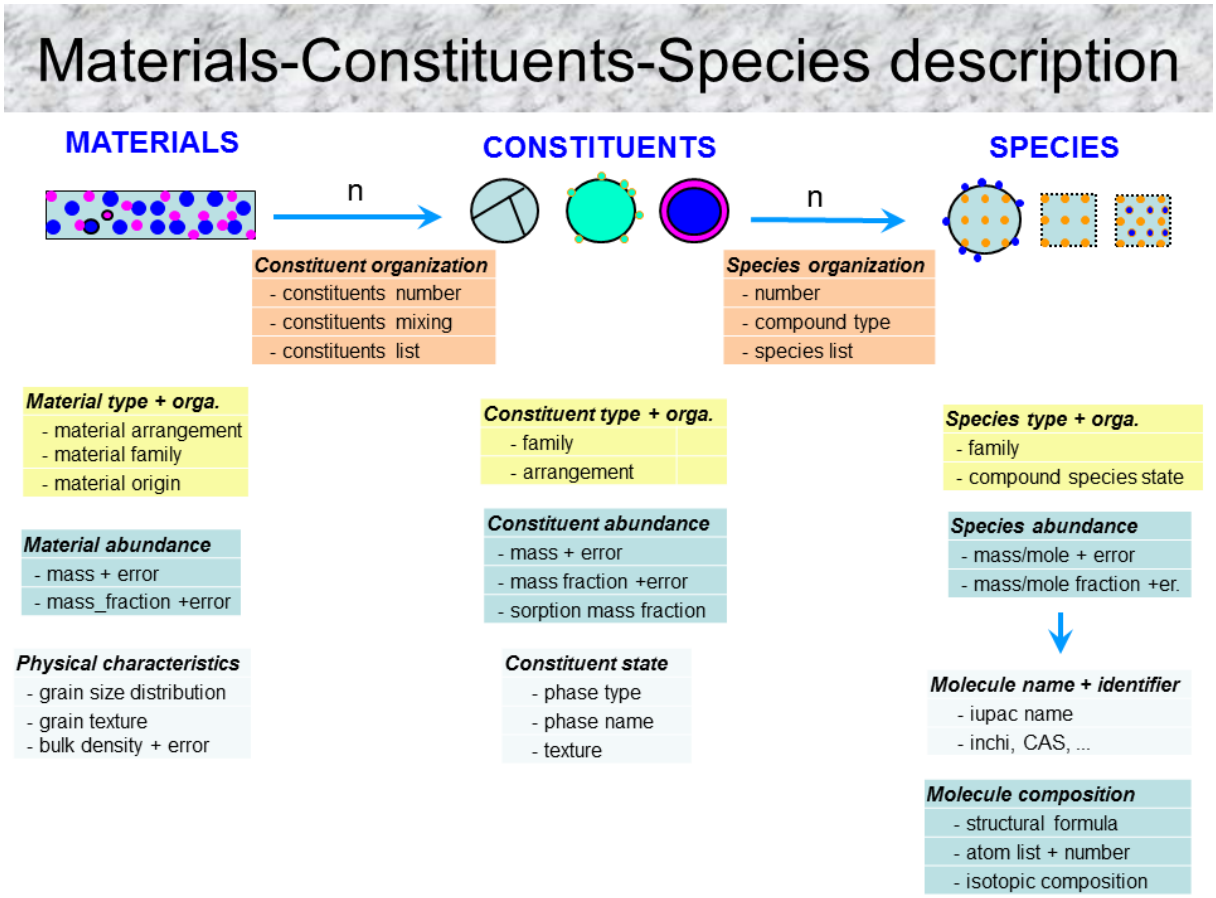
* The **Materials** of each layer are homogeneous collections of bulk pieces of solids such as "grains" (but can also be a single material such as a compact film or slice, a rock, …) that can each contains one or several different ***constituents*** (crystals, molecular phases, ...).

* When a material is composed of an homogeneous collection of solid pieces (grains, …) but each with complex composition that cannot be expressed in term of simple constituents (too complexes or too numerous), then it is called a ***"complex matter",*** described in a next step.

- Each **material** constituting each layer is described in terms of *"name and references"*, material *"type and family"*, "*abundances*" in the layer, and "*texture*". In the case of chemically or physically processed synthetic materials we can provide some details on *"formation conditions"* such as *"precursor materials, mixing and processing"*.
Finaly, for simple materials, the qualitative *"organization of constituents"* that constitutes the material is given.

Sample-Layers-Materials description





Figures 5a,b: "Sample to Species" organization of Keywords (only major KWs)

Constituents

* The bulk **Constituents** of a simple homogeneous material (natural or synthetic) are either mineral or/and molecular phases organized at sub-grain level (multi-phases poly-crystal, coated grain, with adsorption ...) that are composed of ***fundamental species*** (molecules, mineral, atoms) organized at molecular or at atomic levels.

* For the description of the complex matters, we define **"*complex constituents*"** to represent a single or a few clearly different complex constituents, composing their grains. These "complex constituents" are composed of either too complexes or too numerous species and can only be characterized by global elemental composition (***atoms***) and/or (partial) chemical (***chemical functions***) composition.

A constituent is thus either:

- **a molecular phase** composed of one or more ***species*** (molecules, isotopic species, atoms, ions, ...) that can be organized in different ways in the constituent: pure solid (one species), homogeneous molecular mixture, isotopic mixture, molecular compound (hydrate, clathrate hydrate, simple polymer, ...), ...
- **a molecular phase with molecules, ions or atoms adsorbed** on its surface or **absorbed** in its volume. This type of constituent is thus composed of two or more molecular ***species.***
- **a single mineral phase** (natural or synthetic). To simplify our nomenclature we will also call ***"species"*** all the pure fundamental mineral phases (see below).
- **a single mineral phase with molecules, ions or atoms adsorbed** on its surface or **absorbed** in its volume. This type of constituent is composed of one or more molecule/atom ***species*** and one mineral ***"species".***
- **the whole grain,** or a clearly different **part of a grain,** with complex composition(s) **of a complex matter** (cf ***complex constituent*** definition***)***
- *a complex constituent* of a complex "matter" (cf above) **with molecules, ions or atoms adsorbed** on its surface or **absorbed** in its volume.

- The different **constituents** composing each material are described in term of constituent *"family and organization"*, "*abundances*" in the material, *"state and texture"* as well as *"species organization"* in the constituent.

Species

* Each simple homogeneous constituent is composed of simple ***fundamental species: molecular, mineral*** and/or ***atomic.***

* Complex constituents from complex matters can only be described with ***atomic*** species and/or ***chemical functions*** (functional groups).

- The different **Species** composing each simple or complex constituent are described in term of species *"type and state"*, as well as "*abundances*" in the constituent.

We can also define ***"generic samples"*** for spectral data coming from the compilation of several measurements made on a series of samples (that we may not want to put all in the database). For such samples, generally made of one single constituent or a single material, the common parameters (composition, temperature, ...) are entered in the respective keywords, and the variable parameters are listed in "sample_comments".

There is also the possibility to define ***"simulated samples",*** for which we can simulate different types of spectra (absorption, reflection, …), from the complete definition of their layers, materials, constituents and species in radiative transfer models using the optical constants of the constituents. It is useful, for example, to provide reflectance spectra of a surface (with different grain sizes) when only optical constants are available. These simulations will be linked to the optical constants spectrum used (as "parent spectrum")

Precursor materials

Processings

10.3 Sample Table

Root of the table: ***sample***

Data type: 'Sample'

Key-word	Type	Level	Table	Exp	Unit	Description
Sample import mode and indexes						
*sample*_import_mode	enum(text)	P [!!_m]	Sampl	(V)	--	Mode of import of the "sample" metadata Enum: {first import, ignore, draft, no change, correction} *Definitions:* There are 2 levels of import: • '*first import'*: during first import of the metadata '*inherited*': takes the "import_mode" of the previous "import_mode" (only for "*layer*_import_mode", "*matter*_import_mode", "*material*_import_mode", "*constituent*_import_mode", and "*specie*_import_mode" => takes the value of "*sample*_import_mode". "spectrum import_mode" takes the value of "*experiment*_import_mode". "*band*_import_mode" takes the value of "*bandlist*_import_mode".) • '*use existing':* use an existing table specified by its UID. Need only to give this UID and some keyword values (not used for sample) There are 3 levels of 'no-correction': • *'ignore'*: fully ignore this metadata table. • *'draft'*: used for draft (not ready to be imported). Exactly same as 'ignore' but duplicated for practical reasons • '*no change'*: when there is no change in this table (for correction in other(s)) but it already exist in the database (checked) There are 1 level of correction: • '*correction':* used for data already imported in the database when values of metadata or links are corrected/added

*sample*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Sampl	(V)	--	Name of the storage copy of the xml import file of the sample metadata *Note:* determined automatically during export/(import) ➔ calculated using "*sample*_uid" ou "_index" ? *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*sample*_index [**][-xml]	int(11)	B [!!_g]	Sampl	F	--	Automatic incremental unique number (ID) given to new sample
*sample*_uid [**]	varchar(255)	S0 [!!_m]	Sampl	F	--	Unique identifier code (UID) given to the sample table (to be created) *Nomenclature:* This code name should start with 'SAMPLE_' and be very accurately formatted in order to be simple and unique It should be of the style 'SAMPLE_AB_yyyymmdd_123...' where 'AB' is initial of people preparing the import, 'yyyymmdd' is the full date of the day, and '123...' should be at the end and alphanumeric (only with '_'), with no more than 6 characters. *Ex:* 'SAMPLE_BS_20181006_059', 'SAMPLE_OB_20000101_01', 'SAMPLE _KD_20170712_X50A' *Notes:* - The post-fix '123...' may just be an incremental order number for that day, or may give a short description of the varying parameter of the sample. *Ex:* 'SAMPLE _KD_20170712_X50A'
sample_owner_databases	***List [L0]***	[!!]				£: databases which own this sample and manage its information
*sample*_owner_database_uid [*] [*matter*_owner_database_uid]	varchar(255)	S1 [!!o_m]	Sampl DatBas L0	F	--	Link(s) to the existing UID(s) of the database which owns and manages this sample information *Condition:* at least one database *Note:* For samples from experiments from external laboratories, not managed by a partner database, we will create specific database(s) (ex: 'DB_external')

						managed by the SSHADE managers
Sample experimentalists						
sample_experimentalists	***List [L1a]***	[!]				£: experimentalists which prepared the sample
*sample*_experimentalist_uid [*] [*matter*_experimentalist_uid]	varchar(255)	S1 [!_m]	Sampl Exper L1a	F	--	Link to the existing UID of the experimentalist(s) which prepared the sample *Notes*: - not mandatory to define and add 'experimentalists' (and their labs) from laboratories outside SSHADE partners - but recommended for major/regular external contributors that really prepared the sample (not just sent it!) - the others are acknowledged in "*sample*_provider"
Sample name and origin						
*sample*_name	varchar(255)	S0 [!!_m]	Sampl	F	--	Name of sample given by experimentalist *Note:* – It should contain explicit info on the sample or main constituting materials: name(s) and some typical properties of the sample (thickness, …). – It is used as the title of the sample in the sample structure bloc of the SSHADE interface
*sample*_date [*matter*_date]	date	S1 [!_m]	Sampl	F	YYYY-MM-DD	Date of creation of the sample, or of end of its processing(s) in the case of a sample generated by processing another one (parent sample).
*sample*_provider [*matter*_provider]	varchar(255)	S1b [m]	Sampl Manip	F	-- --	Provider name and laboratory/institute of the sample (or part of it) *Notes:* - individual + laboratory name, industrial/commercial company, ... - you can put your own lab when home made - 'sample_experimentalist' will give link to the major/regular external sample providers (not mandatory to add 'experimentalist' from labs

outside SSHADE partners)
- if one (or more) of the sample material(s) is provided by an external individual/lab, then list it(them) together with the material name, but not mandatory when this material is already described as a matter (which already contain 'provider').

Ex:
- 'Mathieu Gounelle, MNHM (siderite pellet) [whole sample provided]
- 'IPAG' [home made]
- 'Nathalie Carasco, LATMOS (tholins material)' [one of the sample material provided, but not described as a matter]

*sample*_is_generic	boolean	S3 [!!_m]	Sampl	F	--	Flag telling if the sample is 'generic': virtual sample representing a series of samples BoolEnum: {yes, no} or {true, false} *Definition:* A 'generic sample' is a virtual sample synthetizing the properties (common or variable) of the whole series of samples which have been used to generate a spectrum product (absorption coefficient, optical constants, …) *Note:* - used in particular for absorption coefficients or optical constants spectra, ie. when a simple (only one layer and mostly one material) virtual sample is used to represent a series of very similar samples either with just different thicknesses or recorded over different wavelength ranges, ... - When using a "generic sample" for a series of samples the parameter that changes should be left blanc (e.g. the different layer thicknesses + uncertainties) and their values or range of values should be noted in "*layer*_comments". - When the spectrum is a compilation of different wavelength ranges, the variables "*instrument*_spectral_range_min/_max" (list) should be used to specify its full valid spectral range. "*spectrum*_analysis" should be used to explain how the whole spectrum has been assembled.

sample_original_samples	***List [L1b]***	[O]				£: original samples of a generic sample
*sample*_original_sample_uid [*]	varchar(255)	S1i [$o_m]	Sampl Sampl L1b	F	--	LINK to the existing UID of the original sample (if present in the database) used to create this virtual generic sample *Constraint:* only when *"sample*_is_generic" = {yes, true} *Recommendation:* Strongly recommended when already exist in the database. *Ex:* a series of samples with different thicknesses used to make an optical constant spectrum
*sample*_previous_sample_uid [*]	varchar(255)	S1i [£o_m]	Sampl Sampl	F	--	Link to the existing UID of the previous sample (if present in the database) that leaded to this one by some processing 'during' the experiment *Condition:* compulsory only when "*sample*_parent_sample_uid" = Φ *Constraint:* only when *"sample*_is_generic" = {no, false} *Recommendation:* Compulsory when exist *Notes*: - the processing(s) during the experiment that induce significant composition, phase or texture sample changes could be irradiation, chemical reaction, adsorption … - when these changes in the sample are small it is possible to use a single sample, but giving the values that slightly change in the relevant "*sample*_xxx_comments" - when these changes in the sample are unknown it is possible, as a first step of description, to use a single sample, but keeping blanc all values that change and giving the known information in the relevant "*sample*_xxx_comments" *Ex:* a sample irradiated during an experiment produce a sample from the previous unirradiated sample.
*sample*_parent_sample_uid [*]	varchar(255)	S1i [£o_mc]	Sampl Sampl	F	--	Link to the existing UID of the parent of the sample (present in the database) used to create this one by some processing(s) 'before' (or just prior) the

current experiment

Condition: compulsory to provide (when exist in the database) only the parent of the first sample of the experiment

- ⇨ calculated recursively for all samples of the experiment linked with "*spectrum*_chronologically_ordered"='yes' or using "*sample*_previous_sample_uid", when it exist

Constraint: only when *"sample*_is_generic" = {no, false}

Notes:

- this parent sample can be the initial sample of the last experiment that created this one by some processing during or after the last experiment
- Not for a 'generic sample'. In the case of 'generic sample' (for high level spectral products: absorption coefficient, optical constants, …) the 'set of samples' used to produce it are not truly 'parent samples' as defined above. However they generic sample is linked to them through the 'parent spectra' of the optical constants spectrum ("*spectrum*_parent_spectra/spectrum_uid") and their associated sample ("*spectrum*_sample_uid").

Ex: a granular sample sieved to a specific grain size range gives a daughter sample from the parent unsieved sample.

Sample: Earth body		[!o]						*Note:* special case for natural terrestrial sample (at least one "*material*_origin"= 'natural terrestrial'), but without matter
*sample*_body_uid [*] [-xml] [*matter*_body_uid]	varchar(255)	S1/S1s [!!o_m]	Mineral Body	F	F	--	--	Link to the existing UID of Earth from which the natural sample originates *Condition:* absolute mandatory when "*sample*_geolocation_place" ≠ Ø OR when "*sample*_geolocation_region" ≠ Ø OR when "*sample*_geolocation_country" ≠ Ø OR when "*sample*_geolocation_coordinate_latitude" ≠ Ø ➔ Calculated: "*sample*_body_uid" = 'BODY_planet_Earth' *Constraint:* "*sample*_body_uid" = {Ø, BODY_planet_Earth}

							Note: - can only be void or with the UID of Earth 'BODY_planet_Earth' - calculated but can be also put manually in the xml
*sample*_body_terrain_type [*matter*_body_terrain_type]	openum(text)	S2 [!o_m]	Sampl Miner	F	F	--	--	Type of geological/geophysical terrain on Earth where the natural sample is/was situated. OpenEnum: {mineral surface, icy surface, organic surface, liquid surface, mixed surface types, mineral subsurface, icy subsurface, organic subsurface, liquid subsurface, mixed subsurface types, atmosphere, other, unknown} *Condition:* mandatory and only when "*sample*_body_uid" = 'BODY_planet_Earth' *Definitions: see "matter_solid*_body_terrain_type*"*
*sample*_body_coordinate_system [*matter*_body_coordinate_system]	openum(text)	S3 [!!o_m]	Sampl	F		--	Coordinate system on Earth of the geographic location of the natural sample OpenEnum: {WGS84, …} *Condition:* absolute mandatory and only when "*sample*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_body_coordinate_system" *Notes*: - currently only 'WGS84' system for Earth
Natural solid matter: geolocation		[!o]					*Note:* special case for natural terrestrial sample (at least one "*material*_origin"= 'natural terrestrial'), but without matter
*sample*_geolocation_place [*matter*_geolocation_place]	varchar(255)	S1b [!o_m]	Sampl Miner	F	F	--	--	Geologic source and geographic location on Earth of the natural sample (geologic type, place and area names) *Condition:* mandatory when *sample*_geolocation_region" or "*sample*_geolocation_country_code" or "*sample*_geolocation_type" ≠ Ø *Notes:* - only and compulsory for natural terrestrial sample when a 'natural terrestrial' material is described but without 'natural terrestrial' matter

						(which should contain a geolocation) - if the sample contain a 'natural terrestrial' material' and a 'natural terrestrial' matter then check if this material is of importance - not used for laboratory, commercial and simulated matters *Ex:* - 'east side of Ploskaya Mt, Western Keivy Massif, Kola Peninsula' (Earth) - 'volcanic flow 1 km SW from crater rim, Etna volcano' (Earth)
*sample*_geolocation_region [*matter*_geolocation_region]	varchar(255)	S1b [!o_m]	Sampl	F	--	Region, state, province or county (administrative location) on Earth of the natural sample *Condition:* mandatory when *sample*_geolocation_place" or "*sample*_geolocation_country_code" or "*sample*_geolocation_type" ≠ Ø *Notes:* see "*sample*_geolocation_place" *Ex:* - 'Murmanskaja Oblast', 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi' (Earth)
*sample*_geolocation_country_code [*matter*_geolocation_country_code]	enum(text)	S1b [!o_m]	Sampl	F	--	2-digit code of the country of the geographic location on Earth of the natural sample Enum: {CH, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory when *sample*_geolocation_region" or "*sample*_geolocation_place" or "*sample*_geolocation_type" ≠ Ø *Definitions:* see "*laboratory*_address_country_code" *Notes:* see "*sample*_geolocation_place"
*sample*_geolocation_type [*matter*_geolocation_type]	enum(text)	U [!!o_m]	Sampl	F	--	Type of geographic location of the natural sample Enum: {point, line, box, polygon}

						Condition: absolute mandatory and only when "*sample*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: see "*experiment*_geolocation_type"
sample_geolocation_coordinates [*sample/matter_geolocation_coordinates*]	**List [L0]**	[!o]				£: Geolocation on Earth of the natural sample *Condition*: absolute mandatory when "*sample*_geolocation_type" ≠ Ø *Conditions:* on the number of long/lat couple: see *"experiment*_geolocation_coordinates" *Note DB*: will be stored in shapefile format ?
*sample*_geolocation_coordinate_latitude [*matter*_geolocation_coordinate_latitude]	float	S3 [!!o_m]	Sampl L0	F	deg	Latitude of the geographic location on Earth of the natural sample *Format*: in N 'decimal degrees' in "*sample*_body_coordinate_system" *Condition:* absolute mandatory when "*sample*_geolocation_coordinate_longitude" ≠ Ø
*sample*_geolocation_coordinate_longitude [*matter*_geolocation_coordinate_longitude]	float	S3 [!!o_m]	Sampl L0	F	deg	Longitude of the geographic location on Earth of the natural sample *Format*: in E 'decimal degrees' (in the E direction only) in "*sample*_body_coordinate_system" *Condition:* absolute mandatory when "*sample*_geolocation_coordinate_latitude" ≠ Ø
*sample*_geolocation_coordinate_altitude [*matter*_geolocation_coordinate_altitude]	float	S3 [m]	Sampl L0	F	m	Altitude of the geographic location on Earth of the natural sample *Format*: in 'meter' in "*sample*_body_coordinate_system" *Notes*: - from the WGS84 reference ellipsoid (planetographic coordinates)
*sample*_geolocation_comments [*matter*_geolocation_comments]	blob	U [m]	Sampl	F	--	Any additional information or comments about the geolocation of this sample *Ex:* 'sample collected within 100m of this point', 'very approximate

						coordinates (+/- 0.1°)'…
Sample physical characteristics						
sample_images	***List [L2]***	[O]				£: Pictures of the sample
*sample*_image_filename	varchar(255)	U [m]	Sampl L2	F	--	File name(s) (with extension) of the picture(s) of the sample *Image formats:* .png, .jpg, (.gif) *Note:* these files can include pictures of the sample but also of the different materials and layers. Sample images maybe also composition maps or any maps of sample properties. *Note:* this file will be imported in the database
*sample*_image_caption	varchar(255)	U [m]	Sampl L2	F	--	Caption(s) or comment(s) on the picture(s) of the sample
*sample*_surface_roughness	varchar(255)	U [m]	Sampl	F	--	Qualitative surface roughness of the top layer of the sample
*sample*_size_unit	enum(text)	U [!!_m]	Sampl	F	--	Unit for the sample and layers dimensions: thicknesses, sample diameter (linear), surface (square) and volume (cubic) Enum: {nm, micron, mm, cm, m} *Note:* all sizes data will be stored in 'm' *Note:* used for "*sample*_thickness/_error", "*sample*_diameter", "*sample*_volume", "*layer*_thickness/_error"
*sample*_thickness	float	U [cm]	Sampl	F	var.	Sample thickness *Unit:* in "*sample*_size_unit" • converted in 'm' unit in the database but provided to user in "*sample*_size_unit"

						Exception: 'infinite' (or 'INFINITE', 'Infinite') is the special value to deal with infinite thickness (simulation, ...) ➔ Calculated from the sum of the layer thicknesses ("*layer*_thickness") only if no value is given *Note:* Sometimes for multilayer samples the knowledge and accuracy of the total sample thickness is much better than the ones of the individual layers: it then best to give it here. Otherwise always provide the thickness information in "*layer*_thickness". *Note:* For "generic samples" with varying sample thickness the list of thicknesses covered by the generic sample should be given in "*sample*_comments" or "*layer*_comments"
*sample*_thickness_error	float	U [cm]	Sampl	F	var.	Absolute uncertainty on sample thickness *Unit:* in "*sample*_size_unit" • converted in 'm' unit in the database but provided to user in "*sample*_size_unit" ➔ Calculated from the sum of the "*layer*_thickness_error" of all layers only if no value is given *Note:* except special cases (see"sample_thickness") always provide the thickness error information in '*layer*_thickness_error'. *Note:* For "generic samples" with varying sample thickness the list of errors of the thicknesses covered by the generic sample may be given in "*sample*_comments" or "*layer*_comments"
*sample*_diameter	float	U [m]	Sampl	F	var.	Sample diameter or minimum lateral dimension *Unit:* in "*sample*_size_unit" • converted in 'm' unit in the database but provided to user in "*sample*_size_unit"
*sample*_volume	float	U [m]	Sampl	F	var.	Sample volume *Unit:* in cubic "*sample*_size_unit": nm^3, μm^3, mm^3, cm^3 or m^3

						• converted in ‘m^3’ unit in the database but provided to user in “*sample*_size_unit”^3
*sample*_mass	float	U [cm]	Sampl	F	g	Total mass of the sample • stored in the database and provided to user in ‘g’ unit ➔ Calculated from the sum of layer masses ("*layer*_mass") only if no value is given *Note:* For “generic samples” the list of masses could be given in “*layer*_comments”
*sample*_mass_error	float	U [cm]	Sampl	F	g	Absolute uncertainty on total mass of the sample • stored in the database and provided to user in ‘g’ unit ➔ Calculated from the sum of layer mass errors ("*layer*_mass_error") only if no value is given *Note:* For “generic samples” the list of mass errors may be given in “layer_comments”
*sample*_comments	blob	U [m]	Sampl	F	--	Experimentalist comments about this sample (ex: origin, shape, size, …). *Note:* For "generic samples" it should tell the variable parameter(s), such as thicknesses, or masses.
Sample substrate						
*sample*_substrate_material	varchar(255) CS	U [!_m]	Sampl	F	--	name or composition of sample substrate materials *Note:* put ‘NULL’ if no substrate *Ex:* ‘MgF2’, ‘Saphire’, ‘Si’, … *Ex:* for meteorites (for FIB, or ultra-microtomed samples): ‘TEM grid’, ‘gold foil’, ‘glass slide’, ‘diamond’, ‘Teflon’, ‘epoxy resin’, ‘ZnS’, ‘KBr’, ‘Ge’, …
*sample*_substrate_comments	varchar(255)	U	Sampl	F	--	Additional information on substrate *Note:* Number, type, configuration, thickness of windows, surface cleaning

		[m]					and treatment, or cell configuration (closed cell, simulation chamber, window separation, …) *Ex:* '2 windows 2mm thick parallel in closed cell' *Ex:* 'below (sample substrate): aluminum plate, above: saphire window without sample contact'

Sample environment parameters

Note: For environment variables affecting the composition and phase of the sample it is compulsory to define a new sample (with processing of parent sample) (see "*experiment*_variables_sample").

For the other sample changes (T, P, compaction/sintering, sputtering, textural/structural evolutions without phase change, minor chemical evolutions, …) it is possible to change some of the environment variables (parameters marked 'V') during an experiment but it is necessary to provide at least some comments in "*sample*_changes" explaining which changes are observed/expected.

sample_parameters_environment							£: temperature, pressure, fluid, stress and irradiation parameters
*sample*_time_unit	enum(text)	U [!o_m] [V: m]	Sampl	(V)	--		Unit of time of the experiment (except for "irradiation") Enum: {s, min, h, d} Condition: Mandatory only when "sample_temperature_time" or " sample_pressure_time" or " sample_fluid_time" has a value *Note DB:* all time data will be stored in 's' *Note:* used for "*sample*_temperature_time/_error", "*sample*_temperature_max_time", "*sample*_pressure_time/_error", "*sample*_pressure_max_time", "*sample*_fluid_time/_error" **Variable: during an experiment ("Spectrum")** *Note:* better to keep the same for the whole experiment
Sample parameters environment: Temperature							This bloc describes the temperature conditions of the sample

*sample*_temperature		[!!_m] [V: O]				
*sample*_temperature_unit	enum(text)	U [!!_m] [V: m]	Sampl	(V)	--	Unit of temperature Enum: {K, C, F} *Note DB:* all temperature data will be stored in 'K' *Note:* used for "*sample*_temperature_value/_error", "*sample*_temperature_max/_error", "*sample*_fluid_temperature/_error" , "*layer*_formation_temperature" **Variable: during an experiment ("Spectrum")** *Note:* better to keep the same for the whole experiment
*sample*_temperature_value	float	S3 [!!_m] [V: m]	Sampl	**V+**	var.	Effective temperature of the sample after sample formation *Unit:* in "*sample*_temperature_unit" • converted in 'K' unit in the database and provided to user in 'K' **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_temperature_error	float	U [!_m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on effective temperature of the sample after sample formation *Unit:* in "*sample*_temperature_unit" • converted in 'K' unit in the database and provided to user in 'K' **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_temperature_time	float	U [m] [V: m]	Sampl	V	var.	Total duration of the stage the sample was kept at this temperature after sample formation *Unit:* in "*sample*_time_unit" • converted in 's' unit in the database but provided to user in "*sample*_time_unit"

						Variable: during an experiment ("Spectrum") *Note:* before (and during) spectrum recording *Note:* this time can be estimated either at beginning or at mid-time of spectrum recording (tell which one in comments).
*sample*_temperature_time_error	float	U [m] [V: m]	Sampl	V	var.	Absolute uncertainty on total duration of the stage at this temperature after sample formation *Unit:* in "*sample*_time_unit" • converted in 's' unit in the database but provided to user in "*sample*_time_unit" **Variable: during an experiment ("Spectrum")** *Note:* before (and during) spectrum recording
*sample*_temperature_max	float	S3 [!_m] [V: m]	Sampl	V	var.	Maximum temperature reached by the sample after sample formation *Unit:* in "*sample*_temperature_unit" • converted in 'K' unit in the database and provided to user in 'K' *Note:* this maximum temperature is the highest that the sample reached during one of the steps of processing of the final sample (annealing, …) but before the experiment (max of "sample_processing_temperature" of the processing steps). It can be just the final temperature after sample formation. **Variable: during an experiment ("Spectrum")** *Note*: before spectrum recording *Note:* this maximum temperature is the highest that has been reached either before the experiment or during one previous spectrum measurement of the experiment (max of "*sample*_temperature_value" of the previous spectra) including the current one, or possibly between 2 spectrum measurements (heating step then cooling before recording) of this experiment.
*sample*_temperature_max_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on maximum temperature reached by the sample after sample formation *Unit:* in "*sample*_temperature_unit"

							• converted in ‘K’ unit in the database and provided to user in ‘K’ **Variable: during an experiment (“Spectrum”)** *Note*: before spectrum recording
*sample*_temperature_max_time	float		U [m] [V: m]	Sampl	V	var.	Total duration of the stage at maximum temperature after sample formation *Unit:* in “*sample*_time_unit” • converted in ‘s’ unit in the database but provided to user in “*sample*_time_unit” **Variable: during an experiment (“Spectrum”)** *Note*: before spectrum recording *Note:* if the maximum temperature is the current temperature, then this time can be estimated either at beginning or at mid-time of spectrum recording (tell in comments).
*sample*_temperature_comments	blob		U [m] [V: m]	Sampl	V+ Aj	--	Comments about the temperature environment of the sample after sample formation. . *Ex:* Errors on T max time, … **Variable: during an experiment (“Spectrum”)** *Note:* for additional information before and during spectrum recording
Sample parameters environment: Fluid temperature and pressure							This bloc describes the fluid environment (gas or liquid) in contact with the sample, mainly to define the condition of vacuum/room, for adsorption studies, for chemical reactions, … *Note*: The temperature conditions of the sample are in the previous bloc and mechanical pressure conditions on the sample are in the next bloc.
sample_fluid			[!_m] [V: O]				*Condition:* Mandatory when “*sample*_fluid_type” = {atomic gas, plasma, molecular gas, molecular liquid, liquid solution, ambient air, purged air}

*sample*_fluid_type	enum(text)	S2 [!_m] [V: m]	Sampl	V	--	Type of fluid (plasma, gas, or liquid) in contact with the sample after sample formation Enum: {atomic gas, plasma, molecular gas, molecular liquid, liquid solution, ambient air, purged air, vacuum, other} *Definitions:* - '*atomic gas'*: gas made of atoms (in particular rare gases) - '*plasma*: electrically neutral medium of unbound positive and negative species (i.e. the overall charge of a plasma is roughly zero). - '*molecular gas'*: gas made of molecules - '*molecular liquid'*: liquid made of molecules - '*liquid solution'*: liquid made of several species, one being the solvent of the others - '*ambient air'*: air with H_2O and CO_2 - '*purged air'*: air with H_2O and CO_2 removed, as in purged spectrometers. - '*vacuum'*: primary or secondary vacuum - 'other': when type is none of the above. Give information in "*sample*_fluid_comments" *Notes:* – 'ambient air' and 'vacuum' are used to tell that measurement condition of the sample was in air or under vacuum (whatever level). – 'purgend air' corresponds to typical conditions in a purged instrument (air with H_2O and/or CO_2 removed) **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_fluid_temperature	float	S3 [!o_m] [V: !o_m]	Sampl	V	var.	Temperature of the fluid (gas or liquid) in contact with the sample after sample formation *Condition:* Mandatory when "*sample*_fluid_type" = {atomic gas, plasma, molecular gas, molecular liquid, liquid solution, ambient air, purged air} *Unit:* in "*sample*_temperature_unit" • converted in 'K' unit in the database and provided to user in 'K'

						Variable: during an experiment (“Spectrum”) *Condition:* same as above *Note:* during spectrum recording
*sample*_fluid_temperature_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on the temperature of the fluid (gas or liquid) in contact with the sample after sample formation *Unit:* in “*sample*_temperature_unit” • converted in ‘K’ unit in the database and provided to user in ‘K’ **Variable: during an experiment (“Spectrum”)** *Note:* during spectrum recording
*sample*_fluid_pressure_unit	enum(text)	U [!o_m] [V: m]	Sampl	(V)	--	Unit of pressure for the fluid Enum: {Pa, hPa, MPa, GPa, mbar, bar, atm, torr} *Condition:* Mandatory when “*sample*_fluid_pressure” ≠ Ø *Condition:* Compulsory when “*layer*_formation_fluid_pressure” ≠ Ø *Note DB:* all pressure data will be stored in ‘Pa’ *Note:* used for “*sample*_fluid_pressure/_error” **Variable: during an experiment (“Spectrum”)** *Note:* better to keep the same pressure unit for the whole experiment
*sample*_fluid_pressure	float	S3 [!_m] [V: m]	Sampl	V	var.	Total pressure of the fluid (gas or liquid) in contact with the sample after sample formation *Unit:* in “*sample*_fluid_pressure_unit” • converted in ‘Pa’ unit in the database and provided to user in ‘Pa’ *Note:* the partial pressures of each gas species can be obtained by: “fluid_pressure” x ”fluid_mole_fraction” **Variable: during an experiment (“Spectrum”)** *Note:* during spectrum recording

*sample*_fluid_pressure_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on the total pressure of the fluid (gas, or liquid) in contact with the sample after sample formation *Unit:* in "*sample*_fluid_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa' **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
sample_fluid_ph	float	S3 [m] [V: m]	Sampl	V	*no*	pH of the liquid aqueous solution in contact with the sample after sample formation **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
sample_fluid_ph_error	float	U [m] [V: m]	Sampl	V	*no*	Absolute uncertainty on the pH of the liquid aqueous solution in contact with the sample after sample formation **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_fluid_time	float	S [m] [V: m]	Sampl	V	var.	Total duration of the sample-fluid contact at these temperature and pressure before (and during) spectrum recording *Unit:* in "*sample*_time_unit" • converted in 's' unit in the database but provided to user in "*sample*_time_unit" *Note:* this time can be estimated either a beginning or at mid-time of spectrum recording (tell in comments) **Variable: during an experiment ("Spectrum")** *Note:* before (and during) spectrum recording
*sample*_fluid_time_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on the total duration of the sample-fluid contact at these temperature and pressure before (and during) spectrum recording *Unit:* in "*sample*_time_unit"

- converted in ‘s’ unit in the database but provided to user in “*sample*_time_unit”

Variable: during an experiment (“Spectrum”)

Note: before (and during) spectrum recording

Sample parameters environment: Fluid composition

Note: these parameters should be changed during an experiment only if they induce minor chemical composition and phase changes of the sample (but rare cases!)

Note: adsorption experiments use the *‘fluid’* parameters to define the T, P and gas molecules environment but define the adsorbed phase at the constituent/species levels (one sample per T,P,gas conditions because they modifiy the composition of the sample).

Condition: one of the two blocs mandatory when:
“*sample*_fluid_type” = {atomic gas, plasma, molecular gas, molecular liquid, liquid solution}

Variable: during an experiment (“Spectrum”)

Note xml: when fluid composition change, it should be fully redefined

sample_fluid_composition_matter *s*	***List [L3a]***	[£o]				£: Gas or liquid molecules, or fluid matters, in contact with the sample after sample formation *Condition:* bloc compulsory when the fluid is a matter **Variable: during an experiment (“Spectrum”)** *Note:* during spectrum recording
*sample*_fluid_composition_matter_uid [*]	varchar(255)	S2/S1i [!!o_m] [V: !o_m]	Sampl Matter L3a	(V)	--	Link to the existing UID of the fluid matter (gas or liquid) in contact with the sample *Condition:* absolute mandatory when “*sample*_fluid_type” = {atomic gas, plasma, molecular gas, molecular liquid, liquid solution} *AND* when “*sample*_fluid_composition_specie_uid” = Φ *Notes:* - used instead of “specie” for liquid solutions such as acids, bases or

					electrolytes. They are described by “fluid matters” using “liquid phases” - “fluid_matter” also used for well defined gas or liquid mixtures (commercial gas cylinder, …) by creating a specific “fluid matter” - for samples in contact with air, you can use an ‘air matter’ that refer to the ‘O2’,’N2’, H2O’ and’CO2’ molecules. - for samples under vacuum, you can use a ‘vacuum matter’ that refer to typical residual gases **Variable: during an experiment (“Spectrum”)** *Condition:* same as above *Note:* during spectrum recording
*sample*_fluid_composition_matter_mole_fraction [+]	float	U [!o_m] [V: !o_m]	Sampl L3a	(V)	*no*	Mole fraction of the fluid matter in contact with the sample *Condition:* mandatory when bloc *”sample_fluid_composition_matters“* is used *Notes:* - value between 0 and 1. **Variable: during an experiment (“Spectrum”)** *Condition:* same as above *Note:* during spectrum recording
*sample*_fluid_composition_matter_mole_fraction_error [+]	float	U [m] [V: m]	Sampl L3a	(Vc)	*no*	Absolute uncertainty on mole fraction of the fluid matter in contact with the sample **Variable: during an experiment (“Spectrum”)** *Note:* during spectrum recording
sample_fluid_composition_species	***List [L3b]***	[!o]				£: Gas or liquid species in contact with the sample after sample formation **Variable: during an experiment (“Spectrum”)**

						Note: during spectrum recording
*sample*_fluid_composition_specie _uid [*]	varchar(255)	S2/S1i [!!o_m] [V: !o_m]	Sampl Molec L3b	(V)	--	Link to the existing UID of the gas or liquid species in contact with the sample *Condition:* absolute mandatory when "*sample*_fluid_type" = {atomic gas, plasma, molecular gas, molecular liquid, liquid solution} *AND* when "*sample*_fluid_composition_matter_uid" = Φ *Note:* gases and molecular liquids can be fully described by mixtures of molecules, but liquid solution may need to be described by a fluid matter that use a fundamental 'liquid phase' (see "*sample*_fluid_composition_matter_uid") **Variable: during an experiment ("Spectrum")** *Condition:* same as above *Note:* during spectrum recording
*sample*_fluid_composition_specie _mole_fraction [+]	float	U [!o_m] [V: !o_m]	Sampl L3b	(V)	*no*	Mole fraction of the gas or liquid species in contact with the sample *Condition:* mandatory when bloc *"sample_fluid_composition_species"* is used *Notes:* - value between 0 and 1. **Variable: during an experiment ("Spectrum")** *Condition:* same as above *Note:* during spectrum recording
*sample*_fluid_composition_specie _mole_fraction_error [+]	float	U [m] [V: m]	Sampl L3b	(Vc)	*no*	Absolute uncertainty on mole fraction of the gas or liquid species in contact with the sample **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording

*sample*_fluid_comments	blob	U [m] [V: m]	Sampl	Vc Aj	--	Experimentalist comments about the fluid composition and environment of the sample after sample formation. **Variable: during an experiment ("Spectrum")** *Note:* before (and during) spectrum recording *Note:* for additional information during experiment
Sample parameters environment: Mechanical pressure						This bloc describes the mechanical pressure applied to the sample
sample_pressure		[!_m] [V: O]				
*sample*_pressure_unit	enum(text)	U [!o_m] [V: m]	Sampl	(V)	--	Unit of mechanical pressure Enum: {Pa, hPa, MPa, GPa, mbar, bar, atm, torr} *Condition:* Mandatory when "*sample*_pressure_value" or "*sample*_pressure_max" ≠ Ø *Condition:* Compulsory when "*layer*_formation_pressure" ≠ Ø *Note DB:* all pressure data will be stored in 'Pa' *Note:* used for "*sample*_pressure_value/_error", "*sample*_pressure_max/_error", and "*layer*_formation_pressure" **Variable: during an experiment ("Spectrum")** *Note:* better to keep the same pressure unit for the whole experiment
*sample*_pressure_value	float	S3 [m] [V: m]	Sampl	**V+**	var.	Effective mechanical pressure applied to the sample after sample formation *Unit:* in "*sample*_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa' (will be tools to convert in bar and multiple of Pa and bar) *Note:* for samples at ambient pressure => 1 bar (or 10^5Pa). For samples under vacuum: give approximate vacuum level. Use large "pressure_error" when pressure not well known.

						Variable: during an experiment (“Spectrum”) *Note:* during spectrum recording
*sample*_pressure_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on the effective mechanical pressure applied to the sample after sample formation *Unit:* in “*sample*_pressure_unit” • converted in ‘Pa’ unit in the database and provided to user in ‘Pa’ **Variable: during an experiment (“Spectrum”)** *Note:* during spectrum recording
*sample*_pressure_time	float	U [m] [V: m]	Sampl	V	var.	Total duration of the stage this mechanical pressure was applied to the sample after sample formation *Unit:* in “*sample*_time_unit” • converted in ‘s’ unit in the database but provided to user in “*sample*_time_unit” *Note:* this time can be estimated either at beginning or at mid-time of spectrum recording (tell in comments). **Variable: during an experiment (“Spectrum”)** *Note:* before (and during) spectrum recording
*sample*_pressure_time_error	float	U [m] [V: m]	Sampl	V	var.	Absolute uncertainty on total duration of the stage this mechanical pressure was applied to the sample after sample formation *Unit:* in “*sample*_time_unit” • converted in ‘s’ unit in the database but provided to user in “*sample*_time_unit” **Variable: during an experiment (“Spectrum”)** *Note:* before (and during) spectrum recording
*sample*_pressure_max	float	S3 [m] [V:	Sampl	V	var.	Maximum mechanical pressure applied to the sample after sample formation *Unit:* in “*sample*_pressure_unit”

		m]				• converted in ‘Pa’ unit in the database and provided to user in ‘Pa’ *Note:* this maximum pressure is the highest that has been reached either during one step of processing of the sample before the experiment (max of “sample_processing_pressure” of the processing steps) or during one previous spectrum measurements of the experiment (max of “*sample*_pressure_value” of the previous spectra) including the current one, or possibly between 2 spectrum measurements (high pressure step then decreasing before recording) of this experiment. **Variable: during an experiment (“Spectrum”)** *Note:* before spectrum recording
*sample*_pressure_max_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on maximum mechanical pressure applied to the sample after sample formation *Unit:* in “*sample*_pressure_unit” • converted in ‘Pa’ unit in the database and provided to user in ‘Pa’ **Variable: during an experiment (“Spectrum”)** *Note:* before spectrum recording
*sample*_pressure_max_time	float	U [m] [V: m]	Sampl	V	var.	Total duration of the mechanical pressuring or stress stage at maximum pressure after sample formation *Unit:* in “*sample*_time_unit” • converted in ‘s’ unit in the database but provided to user in “*sample*_time_unit” *Note:* if this maximum pressure is the current pressure then this time can be estimated either at beginning or at mid-time of spectrum recording (tell in comments). **Variable: during an experiment (“Spectrum”)** *Note:* before spectrum recording

*sample*_pressure_comments	blob	U [m] [V: m]	Sampl	V+ Aj	--	Comments about the pressure and stress environment of the sample after sample formation. . *Ex:* Errors on P max time, … **Variable: during an experiment ("Spectrum")** *Note:* for additional information before and during spectrum recording

Sample parameters environment: Mechanical stress of the sample

sample_stress		[O] [V: O]				
*sample*_stress_type	enum(text)	S1b [m] [V: m]	Sampl	V	--	Type of stress applied to the sample after sample formation Enum: {normal uniaxial tension, normal uniaxial compression, simple shear, normal biaxial tension, normal biaxial compression, cylindrical normal tension, cylindrical normal compression, isotropic normal tension, isotropic normal compression, combined biaxial, combined triaxial, other, unknown, no} *Definitions:* - '*normal uniaxial tension'*: tension in an unique direction normal to one axis of the material - '*normal uniaxial compression'*: compression in an unique direction normal to one axis of the material - '*simple shear'*: when a material is pulled in opposite directions by forces parallel to the material; - '*normal biaxial tension'*: tension in two directions normal to two axis of the material - '*normal biaxial compression'*: compression in two directions normal to two axis of the material - '*cylindrical normal tension*': stress with cylindrical symmetry. Occur in such parts have rotational or even cylindrical symmetry

						- '*cylindrical normal compression*': stress with cylindrical symmetry. Occur in such parts have rotational or even cylindrical symmetry - '*isotropic normal tension'*: when the material body is under equal tension in all directions - '*isotropic normal compression'*: when the material body is under equal compression in all directions - '*combined biaxial'*: two stresses are applied in 2 directions - '*combined triaxial'*: three stresses are applied in 3 directions - '*other*': other or complex combinations of stress. Describe this combination in "*sample*_pressure_comments" - '*unknown*': unknown stress field - '*no*': no stress applied **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_stress_unit	enum(text)	U [!o_m] [V: m]	Sampl	(V)	--	Unit of stress Enum: {Pa, hPa, MPa, GPa, bar} *Condition:* mandatory when "*sample*_stress_value" ≠ {Ø, NULL} *Note DB:* all pressure data will be stored in 'Pa' *Note:* used for "*sample*_stress_value/_error" **Variable: during an experiment ("Spectrum")** *Note:* better to keep the same for the whole experiment
*sample*_stress_value	float	S3 [!o_m] [V: !o_m]	Sampl	V	var.	Average stress τ applied to the sample (Force / Area) after sample formation *Unit:* in "*sample*_stress_unit" *Condition:* mandatory when "*sample*_stress_type" ≠ Φ **Variable: during an experiment ("Spectrum")** *Condition:* same as above *Note:* during spectrum recording

*sample*_stress_error	float	U [m] [V: m]	Sampl	Vc	var.	Absolute uncertainty on the average stress τ applied to the sample (Force / Area) after sample formation *Unit:* in "*sample*_stress_unit" **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording
*sample*_stress_comments	blob	U [m] [V: m]	Sampl	Vc Aj	--	Experimentalist comments about the stress environment of the sample after sample formation *Ex*: orientation of the force(s) relative to sample geometry, ... **Variable: during an experiment ("Spectrum")** *Note:* during spectrum recording *Note:* for additional information during experiment

Sample parameters environment: irradiation

sample_irradiations	***List [L4]***	[O] [V:£o]				£: Irradiations of the sample after sample formation and before any spectrum recording *Condition:* Optional bloc - Mandatory active below when "*sample*_irradiation_particle_family" ≠ 'NULL' *Note:* one of the following combinaison of KW is necessary to define the fluence (dose): - "irradiation_particle_flux" & "irradiation_time", - "irradiation_particle_fluence" - "irradiation_radiant_flux" & "irradiation_time" - "irradiation_radiant_fluence" **Variable: during an experiment ("Spectrum")** *Condition:* this bloc is compulsory when a Raman or fluorescence instrument is used (see "*instrument*_type") to describe the energy deposited by laser irradiation. However for experiments with irradiation and with Raman measurement, the information on the Raman irradiation should be put in

						"*sample*_irradiation_comments" *Note:* before and/or during spectrum recording. *Note xml:* When an <irradiation> bloc is filled in 'variable', it will be added as a new item to the ones already defined in <sample> in order to provide the full irradiation history of the sample
*sample*_irradiation_source	varchar(255)	U [m] [V: £o_m]	Sampl L4	V	--	Type of source of irradiation or bombardment of the sample Free List: {X generator, VUV lamp, H2 lamp, Hg lamp, Ar lamp, Ar+ laser, Ar+ laser Raman, , Ar+ WaveTrain laser Raman, He-Ne laser Raman, Nd:YAG laser Raman, synchrotron radiation, ions accelerator, particle gun,...} *Note:* wavelengths of Raman lasers - He-Ne laser: 632.8 nm - Ar+ laser: 647.1 nm, 514.5 nm, 457.9 nm - Ar+ laser "WaveTrain": 244nm (=frequency doubled) - Nd:YAG laser: 532 nm **Variable: during an experiment ("Spectrum")** *Condition:* compulsory for Raman and Fluorescence spectroscopies = {xxx laser Raman} *Note:* before and/or during spectrum recording.
*sample*_irradiation_filter	varchar(255)	U [m] [V: m]	Sampl L4	V	--	Any filter (optical, electric, magnetic, …) applied to the irradiation or bombardment source. **Variable: during an experiment ("Spectrum")** *Note:* before and/or during spectrum recording.
*sample*_irradiation_chronology [-xml]: in xml "*Sample*"	enum(text)	U [!o_c] [V:!£o_m]	Sampl L4	V	--	Tell the relative chronology between the irradiation of the sample and spectrum recording Enum: {before spectrum, *(before and during spectrum, during spectrum)*} *Condition: Default* = {before spectrum} when "*sample*_irradiation_particle_family" ≠ 'NULL'

						Definitions: - '*before spectrum'*: after sample preparation but before any spectrum recording. - '*before and during spectrum'*: after sample preparation and during spectrum recording - '*during spectrum'*: only during spectrum recording *Note:* 'before spectrum' is the only value allowed for "*Sample*". It tells that irradiation of the sample occured after sample preparation but before any spectrum recording **Variable: during an experiment ("Spectrum")** Enum: {before spectrum, before and during spectrum, during spectrum} *Conditions:* same as in sample *Condition:* compulsory for Raman and Fluorescence spectroscopies = {during spectrum} *Note:* before and/or during spectrum recording. In particular during one experiment (if limited chemical changes) or during successive experiments (with successive samples, if significant chemical changes) but with same first parent sample. *Note:* For Raman laser irradiation it should be mostly 'during spectrum' as the laser is the measurement source. But if a laser pulse has been already made at the same sample location (with or without measurement) then use 'before and during spectrum'
*sample*_irradiation_time_unit	enum(text)	U [!o_m] [V: !o_m]	Sampl	(V)	--	Unit of time of irradiation Enum: {s, min, h, d} *Condition:* mandatory when "*sample*_irradiation_time" ≠ { Ø, NULL} *Note DB:* all time data will be stored in 's' *Note:* used for "*sample*_irradiation_time" **Variable: during an experiment ("Spectrum")**

						Condition: mandatory when "*sample*_irradiation_time" ≠ { Ø, NULL} *Note:* better to keep the same for the whole experiment
*sample*_irradiation_time	float	U [!o_m] [V: £!o_m]	Sampl L4	V	var.	Total irradiation or bombardment time of the sample after sample formation *Unit:* in "time_unit" • converted in 's' unit in the database but provided to user in "*sample*_irradiation_time_unit" *Condition #1:* mandatory when "*sample*_irradiation_particle_family" ≠ 'NULL' *Condition #2:* Mandatory when "*sample_irradiation_particle_flux*" OR "*sample_irradiation_radiant_flux*" ≠ {Ø, NULL} **Variable: during an experiment ("Spectrum")** *Conditions:* same as in sample *Condition:* Compulsory for Raman and Fluorescence spectroscopies = {photons} Time before end of spectrum recording *Note:* - before and/or during spectrum recording. - if irradiation continue during spectrum recording ("*sample*_irradiation_chronology" = 'before and during spectrum' or 'during spectrum') then this time can be estimated either at beginning or at mid-time of spectrum recording (tell in comments). - for Raman laser irradiation it is the total laser irradiation time at the measurement spot. If measurement spot change then the irradiation time is reset.
*sample*_irradiation_time_error	float	U [m] [V: m]	Sampl L4	Vc	var.	Absolute uncertainty on the total irradiation or bombardment time of the sample after sample formation *Unit:* in "time_unit" • converted in 's' unit in the database but provided to user in "*sample*_time_unit" *Note:* only if "*sample*_irradiation_time" has a value ≠ {Ø, NULL}

						Variable: during an experiment (“Spectrum”) Uncertainty on time before end of spectrum recording *Note:* before and/or during spectrum recording.
Irradiation: Particle						
sample_irradiation_particle						
*sample*_irradiation_particle_family	enum(text)	S1b [££do_m] [V: ££o_m]	Sampl L4	V	--	Family of particle used to irradiate or bombard the sample Enum: {photons, fundamental particles, atoms and molecules, condensed matter} *Default* = ‘NULL’ *Condition:* absolute compulsory to fill this KW when this optional bloc is used. *Note*: It triggers the ‘mandatory’ status of several others KW in the optional bloc. *Definitions:* - ‘*photons’*: any type of photon or electromagnetic wave (from gamma to radio frequencies) - ‘*fundamental particles’*: any type of fundamental particles (except photon): electrons, protons, neutrons, … - *‘atoms and molecules’*: atoms, atomic ions, molecules, molecular ions, radicals, … - ‘*condensed matter’*: any type of liquid or solid matter (molecular or mineral) in form of particles of any size. Include also molecule clusters - ‘*Raman laser’*: particular case of instrument source (laser) for spectral measurements (Raman, fluorescence, …) that can induce changes in the sample **Variable: during an experiment (“Spectrum”)** *Conditions:* same as in sample *Condition:* Compulsory for Raman and Fluorescence spectroscopies =

						{photons} *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_type	enum(text)	S1b [!o_m] [V: £!o_m]	Sampl L4	V	--	Type of irradiation (photons of all energies) or particle bombardment (ions, electrons, …) of the sample Enum: {gamma photons, X photons, VUV photons, UV photons, Vis photons, NIR photons, MIR photons, micro-waves, electrons, protons, neutrons, atoms, atomic ions, molecules, molecular ions, molecule clusters, solid material, liquid material} *Condition:* mandatory when "*sample*_irradiation_particle_family" ≠ 'NULL' *Definitions:* - 'gamma photons': photons in the 0.1-10 pm wavelength range (10-0.1 MeV) - 'X photons': photons in the 0.01-10 nm wavelength range (100-0.12 keV) - 'VUV photons': photons in the 10-200 nm wavelength range (120-6 eV) - 'UV photons': photons in the 200-400 nm wavelength range (6-3 eV) - 'Vis photons': photons in the 400-800 nm wavelength range (3-1.5 eV) - 'NIR photons': photons in the 800-3000 nm wavelength range (1.5-0.4 eV) - 'MIR photons': photons in the 3-50 µm wavelength range (0.4-0.025 eV) - 'micro-waves': photons in the 1-10 mm wavelength range - 'electrons': - 'protons': - 'neutrons': - 'particles': - 'atoms': - 'atomic ions': - 'molecules': - 'molecular ions':

						- ‘molecule clusters’: - ‘solid material’: - ‘liquid material’: **Variable: during an experiment (“Spectrum”)** *Conditions:* same as in sample *Condition:* Compulsory for Raman and Fluorescence spectroscopies = {VUV photons, UV photons, Vis photons, NIR photons, MIR photons} *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_uid [*]	varchar(255)	S2 [!o_m] [V: !o_m]	Sampl Atom Molec L4	V	--	Link to the existing UID of the ion, atom, molecule or molecular ion used to bombard the sample *Condition:* Mandatory when “*sample*_irradiation_particle_type” = {atoms, atomic ions, molecules, molecular ions} **Variable: during an experiment (“Spectrum”)** *Conditions:* same as in sample *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_energy_unit	enum(text)	U [!o_m] [V: !o_m]	Sampl	V	--	Unit of energy of the particles (for irradiation processing) Enum: {J, kJ, eV, keV, MeV, angstrom, nm, micron, cm-1} *Condition:* mandatory when “*sample_irradiation_particle_energy*” ≠ { Ø, NULL} *Constraint: “sample*_irradiation_particle_energy_unit” = {angstrom, nm, micron, cm-1} only when “*sample*_irradiation_particle_family” = {photons} *Note DB:* all irradiation energy data will be stored in ‘J’ *Note:* energy in {angstrom, nm, micron, cm-1} are only for photons, i.e., for “*sample*_irradiation_particle_type“ = {gamma photons, X photons, VUV photons, UV photons, Vis photons, NIR photons, MIR photons} *Note:* used for “*sample_irradiation_particle_energy*”, “*sample_irradiation_radiant_flux*”, “*sample_irradiation_radiant_fluence*”

						Variable: during an experiment (“Spectrum”) *Conditions:* same as in sample *Note:* better to keep the same for the whole experiment
*sample*_irradiation_particle_energy	float	S3 [!o_m] [V: £!o_m]	Sampl L4	V	var.	Energy of the particles (photons, ions, electrons, …) at the sample surface *Unit:* “*sample_irradiation_particle_energy*_unit(•.particle^{-1})” • converted in ‘J.particle^{-1}’ unit in the database but provided to user in “*sample*_irradiation_particle_energy_unit”.particle^{-1} *Condition:* mandatory when “*sample*_irradiation_particle_family” ≠ ‘NULL’ *Note:* give the average irradiation energy when there is a broad energy spectrum. Energy distribution to be described in “*sample_irradiation_particle_energy*_distribution” **Variable: during an experiment (“Spectrum”)** *Conditions:* same as in sample *Condition:* Compulsory for Raman and Fluorescence spectroscopies *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_energy_distribution	vachar(255)	U [m] [V: m]	Sampl L4	V	--	Description of energy distribution of the particles (photons, ions, electrons, …) at the sample surface **Variable: during an experiment (“Spectrum”)** *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_flux	float	S3 [!o_mc] [V: !o_mc]	Sampl L4	V	part/s/m2	Irradiation or bombardment flux in number of particles (photons, ions, electrons, …) per unit time and unit surface of the sample *Unit:* particle • s^{-1} • m^{-2} *Condition #1:* mandatory when “*sample*_irradiation_particle_family” ≠ ‘NULL’ *Condition #2:* Mandatory when “*sample*_irradiation_particle_fluence” = {Ø, NULL} AND when “*sample*_irradiation_radiant_fluence” = {Ø, NULL}

						AND when “*sample*_irradiation_radiant_flux” = {Ø, NULL} OR “*sample*_irradiation_time” = {Ø, NULL} ➔ when “*sample*_irradiation_particle_flux” = ‘Ø’, calculated by: ⇨ “*sample*_irradiation_particle_flux” = “*sample*_irradiation_radiant_flux” / “*sample*_irradiation_particle_energy” **Variable: during an experiment (“Spectrum”)** *Conditions and calculations:* same as in sample *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_flux_error	float	U [m] [V: m]	Sampl L4	Vc	part/s/m2	Absolute uncertainty on the irradiation or bombardment flux in number of particles (photons, ions, electrons, …) per unit time and unit surface of the sample *Unit:* particle • s^{-1} • m^{-2} *Note:* only if “*sample_irradiation_particle_flux*” has a value ≠ {Ø, NULL} **Variable: during an experiment (“Spectrum”)** *Note:* before and/or during spectrum recording.
*sample*_irradiation_particle_fluence	float	S3 [!o_mc] [V: !o_mc]	Sampl L4	V	part/m2	Total particle fluence (dose: in number of particles per unit surface) of irradiation or bombardment received by the sample surface. *Unit:* particle • m^{-2} *Condition #1:* mandatory when “*sample*_irradiation_particle_family” ≠ ‘NULL’ *Condition #2:* Mandatory when “*sample*_irradiation_particle_flux” = {Ø, NULL} OR “*sample*_irradiation_time” = {Ø, NULL} AND when “*sample*_irradiation_radiant_fluence” = {Ø, NULL} AND when “*sample*_irradiation_radiant_flux” = {Ø, NULL} OR “*sample*_irradiation_time” = {Ø, NULL} ➔ when “_particle_flux” and “_time” ≠ {Ø, NULL}, calculated by: ⇨ “*sample*_irradiation_particle_fluence“ = “*sample*_irradiation_particle_flux” * “*sample*_irradiation_time”

					➔ when "_radiant_flux" and "_particle_energy" and "_time" ≠ {Ø, NULL}, calculated by: ⇨ "*sample*_irradiation_particle_fluence" = "*sample*_irradiation_radiant_flux" * "*sample*_irradiation_time" / "*sample*_irradiation_particle_energy" **Variable: during an experiment ("Spectrum")** Dose before end of spectrum recording *Conditions and calculations:* same as in sample *Note:* - before and/or during spectrum recording. - if irradiation continue during spectrum recording then this dose can be estimated either at beginning or at mid-time of spectrum recording (tell in comments). - for Raman laser irradiation it is the total laser irradiation dose at the measurement spot. If measurement spot change then the irradiation dose is reset.
*sample*_irradiation_particle_fluence_error	float	U [o_mc] [V: o_mc]	Sampl L4	Vc	var.	Absolute uncertainty on the total particle fluence (dose) of irradiation or bombardment received by the sample surface. *Unit:* particle • m^{-2} *Note:* only if "*sample_irradiation_particle_fluence*" has a value ≠ {Ø, NULL} ➔ when "_particle_flux_error" and (or) "_time_error" are ≠ {Ø, NULL}, calculated by: ⇨ "*sample_irradiation_particle_fluence*_error" = "*sample_irradiation_particle_fluence*" * ("*sample_irradiation_particle_flux*_error"/ "*sample_irradiation_particle_flux*" + "*sample*_irradiation_time_error"/ "*sample*_irradiation_time") ➔ when "_radiant_flux" and "_particle_energy" and "_time" are ≠ {Ø, NULL}, calculated by: ⇨ "*sample_irradiation_particle_fluence*_error" = "*sample_irradiation_particle_fluence*" *

						("*sample_irradiation_radiant_flux*_error"/ "*sample_irradiation_radiant_flux*" + "*sample*_irradiation_time_error"/ "*sample*_irradiation_time") **Variable: during an experiment ("Spectrum")** Uncertainty on dose before end of spectrum recording *Calculations:* same as in sample *Note:* before and/or during spectrum recording.
Irradiation: Radiance						
sample_irradiation_radiant						
*sample*_irradiation_radiant_flux_unit	enum(text)	U [!o_m]	Sampl	(V)	--	Unit of radiant flux (irradiance) Enum: {J.s-1.m-2, J.s-1.micron-2, eV.s-1.m-2, eV.s-1.micron-2, keV.s-1.m-2, MeV.s-1.m-2, erg.s-1.m-2, erg.s-1.micron-2} *Condition:* mandatory when "*sample*_irradiation_radiant_flux" ≠ { Ø, NULL} • all radiant flux per unit surface data will be stored in 'J.s^{-1}.m^{-2}' (W.m^{-2}) *Notes:* used for "*sample*_irradiation_radiant_flux/_error" - 1 J.s^{-1}.m^{-2} = 1 W.m^{-2} = 10^{-12} J.s^{-1}.µm^{-2} - 1 eV = 1.60218×10^{-19} J - 1 erg = 10−7 J = 0.62415 MeV = 6.2415×10^{11} eV **Variable: during an experiment ("Spectrum")** - *Note:* better to keep the same for the whole experiment
*sample*_irradiation_radiant_flux	float	S3 [!o_mc] [V: £o_mc]	Sampl L4	V	var.	Radiant flux (irradiance: energy per unit time and unit surface) of irradiation or bombardment of the sample surface *Unit:* "*sample*_irradiation_radiant_flux_unit" • converted in the database and provided to user in 'J.s^{-1}.m^{-2}' (W.m^{-2}) unit *Condition #1:* mandatory when "*sample*_irradiation_particle_family" ≠ 'NULL'

						Condition #2: Mandatory when "*sample*_irradiation_radiant_fluence" = {Ø, NULL} AND when "*sample*_irradiation_particle_fluence" = {Ø, NULL} AND when "*sample*_irradiation_particle_flux" = {Ø, NULL} OR "*sample*_irradiation_time" = {Ø, NULL} ➔ when "*sample*_irradiation_radiant_flux" = 'Ø', calculated by: ⇨ "*sample*_irradiation_radiant_flux" = "*sample*_irradiation_particle_flux" * "*sample*_irradiation_particle_energy" **Variable: during an experiment ("Spectrum")** *Condition:* Compulsory for Raman and Fluorescence spectroscopies OR "*sample*_irradiation_radiant_fluence" *Note:* before and/or during spectrum recording.
*sample*_irradiation_radiant_flux_error	float	U [m] [V: m]	Sampl L4	Vc	var.	Absolute uncertainty on the radiant flux (irradiance) of irradiation or bombardment of the sample surface *Unit:* "*sample*_irradiation_radiant_flux_unit" • converted in the database and provided to user in 'J.s^{-1}.m^{-2}' (W.m^{-2}) unit ➔ when "*sample*_irradiation_radiant_flux_error" = 'Ø', calculated by: "*sample*_irradiation_radiant_flux_error" = "*sample*_irradiation_radiant_flux" * "*sample*_irradiation_particle_energy" * "*sample*_irradiation_particle_flux_error" / "*sample*_irradiation_particle_flux" *Note:* only if "*sample*_irradiation_radiant_flux" has a value ≠ {Ø, NULL} **Variable: during an experiment ("Spectrum")** *Note:* before and/or during spectrum recording.
*sample*_irradiation_radiant_fluence	float	S3 [!o_mc]	Sampl L4	V	var.	Total radiant fluence (radiant dose or radiant exposure: energy per unit surface) of irradiation or bombardment received by the sample surface.

		[V: £o_mc]			*Unit:* "radiant_flux_unit" • s : i.e. {J.m-2, eV.m-2, keV.m-2, MeV.m-2, erg.m-2} • converted in the database and provided to user in 'J.m^{-2}' unit *Condition #1:* Mandatory when "*sample*_irradiation_particle_family" ≠ 'NULL' *Condition #2:* Mandatory when "*sample*_irradiation_radiant_flux" = {Ø, NULL} OR "*sample*_irradiation_time" = {Ø, NULL} AND when "*sample*_irradiation_particle_fluence" = {Ø, NULL} AND when "*sample*_irradiation_particle_flux" = {Ø, NULL} OR "*sample*_irradiation_time" = {Ø, NULL} ➔ when "_radiant_flux" and "_time" ≠ {Ø, NULL}, calculated by: ⇨ "*sample*_irradiation_radiant_fluence" = "*sample*_irradiation_radiant_flux" * "*sample*_irradiation_time" ➔ when "_particle_flux" and "_particle_energy" and "_time" ≠ {Ø, NULL}, calculated by: ⇨ "*sample*_irradiation_radiant_fluence" = "*sample*_irradiation_particle_flux" * "*sample*_irradiation_particle_energy" * "*sample*_irradiation_time" **Variable: during an experiment ("Spectrum")** *Condition:* Compulsory for Raman and Fluorescence spectroscopies OR "*sample*_irradiation_radiant_fluence" *Note:* - before and/or during spectrum recording. - if irradiation continue during spectrum recording then this energy dose can be estimated either at beginning or at mid-time of spectrum recording (tell in comments). - for Raman laser irradiation it is the total laser irradiation energy dose at the measurement spot. If measurement spot change then the irradiation energy dose is reset.
*sample*_irradiation_radiant_fluence_error	float	U [mc]	Sampl L4	Vc	var. Absolute uncertainty on the total radiant fluence (radiant dose or radiant exposure) of irradiation or bombardment received by the sample surface. *Unit:* "radiant_flux_unit" • s : i.e. {J.m-2, eV.m-2, keV.m-2, MeV.m-2, erg.m-

		[V: mc]					2} • converted in the database and provided to user in 'J.m^{-2}' unit *Note:* only if "*sample_irradiation_radiant_fluence*" has a value ≠ {Ø, NULL} ⇨ when "_radiant_flux_error" and (or) "_time_error" are ≠ {Ø, NULL}, calculated by: ⇨ "*sample*_irradiation_radiant_fluence_error" = "*sample*_irradiation_radiant_*fluence*" * ("*sample*_irradiation_radiant_flux_error"/ "*sample*_irradiation_radiant_flux" + "*sample*_irradiation_time_error"/ "*sample*_irradiation_time") ➔ when "_particle_flux" and "_particle_energy" and "_time" are ≠ {Ø, NULL}, calculated by: ⇨ "*sample*_irradiation_radiant_fluence_error" = "*sample*_irradiation_radiant_fluence" * ("*sample*_irradiation_particle_flux_error"/ "*sample*_irradiation_particle_flux" + "*sample*_irradiation_time_error"/ "*sample*_irradiation_time") **Variable: during an experiment ("Spectrum")** Uncertainty on energy dose before end of spectrum recording *Note:* before and/or during spectrum recording.
*sample*_irradiation_comments	blob	U [m] [V: m]	Sampl L4	V Aj	--	Experimentalist comments about the irradiation conditions of the sample during spectrum recording. **Variable: during an experiment ("Spectrum")** *Notes:* - for additional information of irradiation before and/or during spectrum recording. - for experiments with irradiation and with Raman measurement, provide here the information on Raman irradiation: "source", "particle_energy", "radiant_flux" & "time", or "radiant_fluence"	

Sample documentation						
sample_documentations	***List [L5a]***	[O]				£: Documentations about the sample
*sample*_documentation_name [*matter*_documentation_name]	varchar(255)	U [m]	Sampl L5a	F	--	Name of the documentation describing the sample *Note:* this name will appear as the documentation title in the database *Ex:* 'Elemental composition of the smectite sample'
*sample*_documentation_filename [*matter*_documentation_filename]	varchar(255)	U [m]	Sampl L5a	F	--	File name (with extension) of the documentation describing the sample *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database. *Note xml*: this file should be zipped with the xml file
Sample publications						
sample_publications	***List [L5b]***	[O]				£: Publications describing the sample and its processings
*sample*_publication_uid [*] [*matter*_publication_uid]	varchar(255)	S2 [m]	Sampl Publi L5b	F	--	Link to the existing UID of the publication(s) describing the sample and its processings *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'sample'
Sample layers organization						
*sample*_layers_number [+][-xml]	int(10)	S2 [!_c]	Sampl	F	*no*	Number of layers added to make the sample ⇨ calculated from "*sample*_layer_index" list
*sample*_layer_addition [+]	varchar(255)	U [!o_m]	Sampl	F	--	Any information on how the layers are added one over the other at the material level in the sample. *Condition:* Mandatory when "*sample*_layers_number" > '1' *Ex:* 'plane parallel', 'irregularly in thickness'...

sample_layers	***List [L6]***	[!!]				£: Layers constituting the sample.
*sample*_layer_index [*§][-xml]	int(11) [Internal Links]	B [!_g]	Sampl Layer L6	F	--	Internal link to the ID of the layer(s) constituting the sample. *Note:* determined automatically during import
sample_precursor_materials *[matter_precursor_materials]*	***List [L7]***	[O]				£: Precursors of the sample.
*sample*_precursor_material_index [*§][-xml] ¬ Same structure as "*materials*" but without the "material arrangement and abundance" bloc	int(11) [Internal Links]	B [!_g]	Sampl PreMater L7	F	--	Internal link to the ID of the precursor(s) of the sample. *Note:* a precursor material is a "*simple material"* described through the material/constituent(s) and specie(s) structure. When the precursor material is a "*matter*" then no need to describe it here because it can be linked directly as a matter (with its "*matter*_uid") in the processings with "*matter*_processing_precursor_matter_uid" *Note xml:* in practice the description of the precursor material(s) is done directly under the "*sample*" structure without providing the ID link *Note:* determined automatically during import
sample_processings	***List [L8]***	[O]				£: Processings of the sample.
*sample*_processing_index [*§][-xml]	int(11) [Internal Links]	B [!_g]	Sampl Process L8	F	--	Internal link to the ID of the processing(s) of the sample. *Note:* determined automatically during import

10.4 Layer Table

Root of the table: ***layer***

Data type: in 'Sample'

Key-word	Type	Level	Table	Exp	Unit	Description
Layer import mode and index						
*layer*_import_mode	enum(text)	P [!!_m]	Layer	(V)	--	Mode of import of the "Layer" metadata Enum: {first import, inherited, ignore, draft, no change, correction} *Default* = 'first import' *Definitions:* see "*sample*_import_mode"
*layer*_index [**][-xml]	int(10)	B [!!_g]	Layer	F	--	Automatic random but unique number (ID) given to new layer
*layer*_uid [**] [-xml]	varchar(255)	S0/S1s [!!_cm]	Layer	F	--	Unique identifier code (UID) given to the layer table (automatically created) *Note:* This code name should start with 'LAYER_' and be very accurately formatted in order to be simple and unique *Ex:* It should be of the style 'LAYER_n_AB_yyyymmdd_123...' where 'n' is '*layer*_order', 'AB' is the initials of people preparing the import, 'yyyymmdd' is the full date of the day, and '123...' is alphanumeric (only with '_'), and with no more than 6 characters. ⇨ calculated from '*sample*_uid' and '*layer*_order' *Note:* except when "*layer*_import_mode" = 'use existing' where it is necessary to fill it manualy with the used layer. *Ex:* "*sample*_uid" = 'SAMPLE_BS_20120912_001' => "*layer*_uid" for layer #1 = 'LAYER_1_BS_20120912_001'

Layer name and organization in sample

*layer*_name	varchar(255)	S0/S1s [m]	Layer	F	--	Name of layer given by the experimentalist *Note:* - It should contain explicit info on the layer and constituting materials: name and some typical properties of the layer (type, thickness, formation, …). - It is used as the title of the layer in the sample structure bloc of the SSHADE interface - mostly useful when there are several layers to distinguish them (include what makes the difference) - when only one layer, it can be the same as sample name
*layer*_order	int(10)	U [!!_m]	Layer	F	*no*	Position of the layer into the sample (bottom to top: from 1 to N) *Note:* the order of the layers is defined as the first layer being in contact of the substrate if there is a single substrate. For samples between 2 substrates (closed cell windows, anvil cells, …) we consider that the top of the sample is the side that receive the measurement light, and the first layer (bottom) is thus the last layer that receive light.
*layer*_type	enum(text)	S0/S0s [!_m]	Layer	F	--	Type of layer Enum: {granular, compact raw, compact, pellet, single grain, grains, aerosols, clusters, fluid, various, other, unknown} *Definitions:* • a '*compact*' layer is a layer with mostly closed porosity or no porosity, i.e. fluids cannot penetrate them, or only weakly. A compact solid has generaly a compacity larger than 80-90%. • A '*granular*' layer is made of individual grains in close contact but more or less aggregated and sintered • '*grain(s)*' and '*aerosols*' are individual or only partly aggregated particles (small aggregats) - '*granular'*: layer constituted of individual grains, in simple contact or

with various degree of sintering (open porosity)
- '*compact raw*': raw piece of compact material of any type of shape
- '*compact'*: compact layer with (roughly) flat faces (closed porosity, if any)
- *'pellet'*: special type of compact layer (few mm thick) specifically made of a transparent material (KBr, …) as a "matrix sample holder" of dispersed solid inclusions.
- '*single grain'*: one single individual grain
- *'grains':* only a few grains, individual or aggregated
- '*aerosols'*: layer constituted of individual or aggregated grains in fluid (or vacuum), without contact
- '*clusters'*: layer constituted of molecular or atomic clusters in vacuum (or fluid), without contact
- '*fluid'*: layer of gas or liquid (that can interpenetrate other non-compact layers)
- *'various'*: used in generic samples when the different samples have different types of layers (*Ex:* 'compact film' and 'compact slab')
- '*other'*: not a type described in the list, will be defined in "comments"
- '*unknown'*: unknown layer type

Note: a '*compact*' raw piece, film or slab is a layer with mostly closed porosity or no porosity, i.e. fluids cannot penetrate them, or only weakly. A compact solid has generaly a compacity larger than 80-90%.

Layer physical characteristics in sample

*layer*_thickness	float	U [!o_m]	Layer	F	var.	Layer thickness *Unit:* in "*sample*_size_unit" • converted in 'm' unit in the database but provided to user in "*sample*_size_unit" *Condition:* Mandatory when "*sample*_is_generic" = 'false' *Exception*: 'infinite' (or 'INFINITE', 'Infinite') is the special value to deal with infinite thickness (simulation, ...)	

*layer*_thickness_error	float	U [!o_m]	Layer	F	var.	Absolute uncertainty on layer thickness *Unit:* in "*sample*_size_unit" • converted in 'm' unit in the database but provided to user in "*sample*_size_unit" *Condition:* Mandatory when "*sample*_is_generic" = 'false' *Note:* only if "*layer*_thickness" has a value ≠ {Ø, NULL}
*layer*_mass	float	U [cm]	Layer	F	g	Total mass of the layer • stored in the database and provided to user in 'g' unit ➔ Calculated from the sum of material masses ("*material*_mass") only if no value is given
*layer*_mass_error	float	U [cm]	Layer	F	g	Absolute uncertainty on total mass of the layer • stored in the database and provided to user in 'g' unit ➔ Calculated from the sum of material mass errors ("*material*_mass_error") only if no value is given
*layer*_texture [*layer/matter*_texture]	enum(text)	S1/S1s [!_m]	Layer	F	--	Macroscopic texture of the layer (at scale above material grains): OpenEnum: {muddy, earthy, pulverulent, loose fine grained, loose coarse grained, loose granular, sintered granular, cemented granular, mixed granular, compact, compact glassy, compact poor grained, compact fine grained, compact coarse grained, compact lamellar, compact fibrous, compact crystal, compact mixed, single grain, individual grains, aggregated grains, isolated aerosols, aggregated aerosols, clusters, liquid, gaseous, other, unknown} *Definitions:* Type = 'granular': - '*muddy*': wet earthy or pulverulent powder - '*earthy*': Dull, clay-like texture (< 2 µm) with no visible crystalline affinities - '*pulverulent*': very fines grains (< 50 µm) without, or with very weak aggregation

- *'loose fine grained'* fine grains (< 1 mm) without, or with very weak mechanical links between grains (large open porosity)
- *'loose coarse grained'* coarse grains (> 1 mm) without, or with very weak mechanical links between grains (large open porosity)
- '*loose granular'*: undefined grain sizes, without, or with very weak mechanical links between grains (large open porosity)
- '*sintered granular'*: grains moderately to strongly linked together without another material between them (open porosity)
- '*cemented granular'*: grains with a material (itself or another) linking them to form a quasi-compact medium
- *'mixed granular'*: mixture of two or more of the above texture

Type = "compact": 'compact raw', 'compact' or 'pellet':

- *'compact'*: simply compact (no knowledge about granularity)
- '*compact glassy'*: compact layer without visible grains (looking vitreous or amorphous)
- '*compact poor grained'*: compact layer with very fine grains (< 50 µm)
- '*compact fine grained'*: compact layer with fine grains (< 1 mm)
- '*compact coarse grained'*: compact layer with coarse grains (> 1 mm)
- '*compact lamellar'*: distinctly foliated (2D) fine-grained forms.
- '*compact fibrous'*: distinctly fibrous (1D) fine-grained forms.
- *'compact crystal':* compact layer with a single, or a few, monocrystal(s)
- '*compact mixed*': at least 2 different compact textures are present

Type = 'single grain':

- *'single grain'*: a single individual grain (its texture will be described in '*material*_grain_texture')

Type = 'grains':

- *'individual grains':* a few isolated grains
- *'aggregated grains':* a few aggregated grains

Type = 'aerosols':

- '*isolated aerosols'*: individual aerosols particles in suspension in fluid
- '*aggregated aerosols'*: aggregated aerosols particles in suspension in fluid (gas, liquid, ...)

Type = 'clusters':

- '*clusters'*: molecular or atomic clusters in jet or vacuum

						Type = ‘fluid’: - ‘*liquid’*: liquid - ‘*gaseous’*: gas Type = other types: - ‘*other’*: not one described in the list, will be defined in “comments” - ‘*unknown’*: unknown layer texture *Note:* a molecular film, a molecular slab or a rock are considered here as one type of ‘compact’ layer
*layer*_porosity_type [*layer/matter*_porosity_type]	enum(text)	S1/S2s [!_m]	Layer	F	--	Type of porosity of the layer (at scale above material grains) OpenEnum: {particulate, porous, open pores, closed pores, without pores, other, unknown} *Definitions:* - *‘particulate’*: discontinuous layer with only little matter (mostly ‘porosity’!), such as individual or aggregated particules, grains or aerosols - ‘*porous’*: non-consolidated or consolidated layer with porosity, but of mixed or unknown type (closed and/or open) - *‘open pores’*: non-consolidated or consolidated layer with mostly open porosity, i.e. fluids can penetrate them. - *‘closed pores’*: consolidated layer with mostly closed porosity, i.e. fluids cannot penetrate them, or only weakly. - *‘without pores’*: consolidated layer with mostly no porosity, i.e. fluids cannot be included in them, or only weakly. Also for liquids without bubble. - ‘*other’*: not one of the cases described above, will be defined in “comments” - ‘*unknown’*: unknown layer texture *Note:* a molecular film, a molecular slab or a rock are considered here as one type of ‘compact’ layer
*layer*_compacity [*layer/matter*_compacity]	float	U [m]	Layer	F	*no*	Compacity of the layer (fraction of solid material volume per unit layer volume)

						Note: compacity = (1 – porosity)
*layer*_compacity_error [*layer/matter*_compacity_error]	float	U [m]	Layer	F	*no*	Absolute uncertainty on the compacity of the layer *Note:* compacity_error = porosity error
*layer*_density [*layer/matter*_density]	float	U [m]	Layer	F	g/cm3	Density of the layer • stored in the database and provided to user in 'g/cm^3' unit
*layer*_density_error [*layer/matter*_density_error]	float	U [m]	Layer	F	g/cm3	Absolute uncertainty on the density of the layer • stored in the database and provided to user in 'g/cm^3' unit
*layer*_comments	blob	U [m]	Layer	F	--	Experimentalist comments about this layer *Ex:* for pellet fabrication, for grain squeezing in diamond cell, for aerosols,... homogeneity of the layer thickness, … List of thicknesses, masses and errors for "generic_sample", …

Layer formation conditions

*layer*_formation_mode	varchar(255)	S1/S1bs [!_m]	Layer	F	--	Mode of formation of the layer FreeList: {processing of parent sample, single gas deposition, gas mixture deposition, gases codeposition, EBPVD, CVD, PECVD, ion-beam sputtering, gas flow sputtering, fractionated sublimation, crystal growth from liquid, crystal growth from fluid, solid-solid phase transition, aerosols in flux, aggregates in jet, liquid condensation, natural deposition, manual deposition, pressing grains, pressing granular material, pressing compact material, mechanical slabing, laser slabing, simulated surface, simulated aerosols,...} *Definitions:* - *'processing of parent sample':* processing a sample already formed - '*gas deposition*': gas phase molecules condensing on a substrate (single gas, gas mixture, co-deposition, …) - '*EBPVD*: Electron Beam Physical Vapor Deposition: form of physical vapor deposition in which a target anode is bombarded with an electron

beam that causes atoms from the target to transform into the gaseous phase and precipitate into a thin layer of solid on the anode.

- *'ion-beam sputtering'* PVD (IBS-PVD)
- *'gas flow sputtering'* PVD (GFS ??-PVD)
  cf. http://en.wikipedia.org/wiki/Sputter_deposition#Ion-beam_sputtering
- '*CVD'*: Chemical Vapor Deposition: one or more volatile precursors, which react and/or decompose on the substrate surface to produce the desired deposit
- '*PECVD'*: Plasma-Enhanced Chemical Vapor Deposition: CVD process that utilize plasma to enhance chemical reaction rates of the precursors
- *'ion-beam sputtering*': sputtering of an initial sample by a beam of energetic ions
- '*gas flow sputtering'*: sputtering of an initial sample by a flux of gas
- '*fractionated sublimation*': formation by differential sublimation of a multiphase mixture, such as ice-dust.
- '*crystal growth from fluid'*: crystal growth from fluid phase (liquid or gas)
- *'solid-solid phase transition'*: solid phase obtained by reversible or irreversible phase transition of another phase
  Ex: beta-N_2 to alpha-N_2 transition, Ia H_2O to Ih H_2O, …
- '*aerosols in flux'*:
- '*aggregates in jet'*: aggregates formed in jet expansion
- '*liquid condensation'*: liquid layer grown by gas condensation
- '*natural deposition'*: as deposited in nature (e.g. snow)
- '*manual deposition'*: deposited by hand
- '*pressing grains'*: grain(s) pressed between windows generaly leading ot its/their crushing
- '*pressing granular material'*: pellet formed by pressing granular material(s) under mechanical pressure
- '*pressing compact material'*: compact material deformed under mechanical pressure
- '*mechanical slabing'*: formation of a slab or a thin section by cutting (saw, microtome, …), grinding, and/or polishing a compact material by

						mechanical tools - '*laser slabing'*: formation of a slab or a thin section by laser cutting - *simulated surface'*: numerical simulation of granular or compact layer - *simulated aerosols'*: numerical simulation of aerosol layer - *multiple'*: when several different formation modes are used: mostly for generic samples *Note:* We also describe in "*layer*_formation" the formation of materials (from material precursors) that occurs during layer formation. Formation and processings of materials that are formed prior layer formation are described in "*material*" processings
*layer*_formation_rate	varchar(255)	U [m]	Layer	F	(var.)	Formation rate of the layer and its uncertainty *Unit:* preferentially in "*sample*_size_unit" / "*sample*_time_unit", but need to specify the unit after the rate value and its error *Note:* mostly useful in case of gas deposition or crystal growth formation modes of the layer *Ex*: '18.2 +/- 0.5 µm/s'
*layer*_formation_temperature	float	S2l [!_m]	Layer	F	var.	Formation temperature of the layer (for synthetic samples) *Unit:* in "*sample*_temperature_unit" • converted in 'K' unit in the database and provided to user in 'K' *Note:* This formation temperature duplicates (but in 'float' format in order to make it searchable) the value given in "*sample_processing*_process" when *"sample/matter_processing*_chronology" = 'during layer formation'
*layer*_formation_temperature_error	float	U [m]	Layer	F	var.	Absolute uncertainty on the formation temperature of the layer (for synthetic samples) *Unit:* in "*sample*_temperature_unit • converted in 'K' unit in the database and provided to user in 'K'
*layer*_formation_pressure	float	S2l [m]	Layer	F	var.	Mechanical pressure applied on the layer during formation

						Unit: in "*sample*_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa' *Note:* This formation pressure duplicates (but in 'float' format in order to make it searchable) the value given in "*sample_processing*_process" when *"sample/matter_processing*_chronology" = 'during layer formation'
*layer*_formation_pressure_error	float	U [m]	Layer	F	var.	Absolute uncertainty on the mechanical pressure applied on the layer during formation *Unit:* in "*sample*_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa'
*layer*_formation_fluid_pressure	float	S3 [m]	Layer	F	var.	Pressure of the fluid surrounding the layer during formation *Unit:* in "*sample*_fluid_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa' *Note:* This formation fluid pressure duplicates (but in 'float' format in order to make it searchable) the value given in "*sample_processing*_process" when *"sample/matter_processing*_chronology" = 'during layer formation'
*layer*_formation_fluid_pressure_error	float	U [m]	Layer	F	var.	Absolute uncertainty on the pressure of the fluid surrounding the layer during formation *Unit:* in "*sample*_fluid_pressure_unit" • converted in 'Pa' unit in the database and provided to user in 'Pa'
*layer*_formation_comments	blob	U [m]	Layer	F	--	Experimentalist additional information about the formation stage of this layer *Ex:* type of gas (pure, mixture, co-deposited, …), position of deposition tubes, details on PVD and CVD deposition processes, type of fluid (gas, liquid), method of sqeezing grain (diamond cell, …), …, variations and error in the formation rate number, …

Layer materials mixing

*layer*_materials_number [+][-xml]	int(10)	S2 [!_c]	Layer	F	*no*	Number of different materials mixed in the layer ➔ Calculated from "*layer*_materials" list
*layer*_materials_mixing [+]	enum(text)	S1/S2 [!_m]	Layer	F	--	Mode of mixing of the material grains in the layer Enum: {single material, homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, spatial distribution} *Definitions:* - '*single material'*: a single material (no mixing) - '*homogeneous mixing'*: well mixed solid materials with homogeneous grain abundances in the volume of the resulting material - '*heterogeneous mixing'*: incomplete mixing of solid materials with heterogeneous grain abundances in the volume of the resulting material - '*grains in fluid'*: solid material(s) in suspension in a fluid material (liquid, gas) with possible volumic inhomogeneity (sedimentation, …) - '*fluid in porous solid'*: fluid material (liquid, gas) in porous solid material(s) with possible volumic inhomogeneity - '*spatial distribution'*: spatial distribution of grain abundances. The different materials (grains) are not fully mixed in the volume but are distributed spatially (as 'patches') over the layer surface. *Note:* When matter(s) is used in the layer, "*layer*_materials_mixing" should take into account "*matter*_materials_mixing" (should be mostly '*single material'* or '*homogeneous mixing', grains in fluid'*, '*fluid in porous solid'*), especially when the matter(s) is constituted of several materials *Note:* it is also possible to mix a solid with a liquid, or a gas, in a layer either as 'grains in fluid' or as 'fluid in porous solid' *Note:* for particules in pellets: 'homogeneous mixing' with "*layer*_texture" = 'compact poor grained'
layer_matters	***List [L1]***	[!]				£: Matters constituting the layer
*layer*_matter_index [*$][-xml]	varchar(255) [Internal link]	B [!_g]	Layer Mater	F	--	Internal link to the ID of the different matters constituting the layer *Note:* with "*material*_is_precursor" = 'false'

			L1			*Note:* these matters are those constituting the layer in the sample before measurement, i.e. the eventual layer and sample processings should not have modified their composition and state. *Note:* ID determined automatically during import *Note xml:* in practice the description of the matters(s) are done directly under "layer" without ID link
layer_materials	***List [L2]***	[!]				£: Materials constituting the layer
*layer*_material_index [*$][-xml]	varchar(255) [Internal link]	B [!_g]	Layer Mater L2	F	--	Internal link to the ID of the different materials constituting the layer *Note:* with "*material*_is_precursor" = 'false' *Note:* these materials are those constituting the layer in the sample before measurement, i.e. the final materials after all the listed layer and sample processings. *Note:* ID determined automatically during import *Note xml:* in practice the description of the material(s) are done directly under "layer" without ID link

10.5 Matter Table

Root of the table: ***matter***

Data type: in 'Sample'

Key-word	Type	Level	Table	Exp	Unit	Description
Matter index		[!!O]				*Condition:* absolute mandatory when "*material*_uid" = Ø
*matter*_uid [*]	varchar(255)	S0/S1/S1i [!!o_m]	Matter MatXxx	F	--	Link to the existing UID of the matter *Notes:* - Only for unaltered 'fluid matter', 'solid matter' (including mineral matter), 'carbonaceous matter', and 'extraterrestrial matter'. - Processed matters and the others materials are described with the full material/constituent/species structure (Material table) - When a matter is processed before, during or after formation of the layer, in such a way that the initial matter composition or structure is significantly altered, then the matter should be listed as a "precursor matter" with '*precursor_matter*_uid' inside sample processing(s) structure, and the final composition/structure of its altered material(s) should be given within the sample description with the full material(s)/constituent(s)/specie(s) structure.
Matter arrangement and abundance in the layer						
*matter*_arrangement	varchar(256)	U [m]	Matter	F	--	Relative arrangement of the material grains of the matter within the layer *Note:* - related to "*layer*_materials_mixing" who describes the mode of mixing (of the grains) of the different materials in the layer. - mostly useful for materials with "*layer*_materials_mixing"='spatial distribution'. An image showing the spatial heterogeneity can be provided in "*sample*_images"

varchar(256) U Matter F --
[m]

						Ex: 'gradient of abundances of olivine and pyroxene along one axis of the sample', 'spatial distribution of abundances of olivine and pyroxene given in "*sample*_image"='map-abundances_olivine-pyroxene-materials.jpg' *Note:* For matters "*sample_matter*_arrangement" replaces "*matter_materials*_arrangement" in all the materials of the matter, but should take it/them into account when filled.
*matter*_mass [+]	float	U [!o_m]	Matter	F	g	Total mass of the matter in the layer *Condition:* mandatory for one of "*material*_mass" or "*material*_mass_fraction" • stored in the database and provided to user in 'g' unit
*matter*_mass_error [+]	float	U [!o_m]	Matter	F	g	Absolute uncertainty on total mass of the matter in the layer *Condition:* mandatory when "*matter*_mass" ≠ {Ø, NULL} • stored in the database and provided to user in 'g' unit
*matter*_mass_fraction [+]	float	U [!o_mc]	Matter L1	F	*no*	Mass fraction of the matter in the layer *Condition:* mandatory for one of "*material*_mass" or "*material*_mass_fraction" ➔ if no value is given, then calculated from the material masses ("*material*_mass") and matter masses ("*matter*_mass") of all the materials and matters in layer. ⇨ *"matter*_mass_fraction" = *"matter*_mass" / [$\sum_{layer}$("*material*_mass") + $\sum_{layer}$("*matter*_mass")] *Note:* value between 0 and 1. *Note:* a warning will be issued during import if the mass fraction of one matter is not present or cannot be calculated
*matter*_mass_fraction_error [+]	float	U [!o_mc]	Matter	F	*no*	Absolute uncertainty in mass fraction of the matter in the layer *Condition:* mandatory when "*matter*_mass_fraction" ≠ {Ø, NULL}

						➔ if no value is given, then calculated from material masses errors (“*material*_mass_error”) and matter mass errors (“*matter*_mass_error”) of all the materials and matters in layer. ⇨ *“matter*_mass_fraction_error” = “*matter*_mass_fraction” * [“*matter*_mass_error” / ” *material*_mass” + ($\sum_{layer}$ (“*material*_mass_error”) + $\sum_{layer}$ (“*matter*_mass_error”)) / ($\sum_{layer}$ (“*material*_mass”) + $\sum_{layer}$ (“*matter*_mass”))]
matter_material_masses [-xml]	***List [L1]***	[O_c]				£: Masses of all the matter’s materials in the layer
*matter*_material_uid [*] [-xml]	varchar(255)	S0m/S1/S1i [o_c]	Matter Mater L1	F	--	Link to the existing UID of the material in the matter
*matter*_material_mass [-xml]	float	U [o_c]	Matter L1	F	g	Mass of the matter’s material in the layer *Condition:* calculated when “*matter*_mass” ≠ Ø • stored in the database and provided to user in ‘g’ unit ⇨ *“matter*_material_mass” = “*matter_xxx*_material_mass_fraction” * “*matter*_mass” *Note:* determine the mass in the layer of each of the materials of the matter using the “*matter_xxx*_material_mass_fraction” of the materials in the matter (mineral, carbonaceous, …) and the “*matter*_mass” of the matter in the layer.
*matter*_material_mass_error [-xml]	float	U [o_c]	Matter L1	F	g	Absolute uncertainty on the mass of the matter’s material in the layer *Condition:* calculated when “*matter*_mass” ≠ Ø AND “*matter*_mass_error” ≠ Ø • stored in the database and provided to user in ‘g’ unit ⇨ *“matter*_material_mass_error” = *“matter*_material_mass” * (“*matter_xxx*_material_mass_fraction_error” / “*matter_xxx*_material_mass_fraction” + “*matter*_mass_error” /

						"*matter*_mass") *Note:* determine the error of the mass in the layer of each of these materials of the matter using the "*matter_xxx*_material_mass_fraction" and "_error" of the materials in the matter (mineral, carbonaceous, …) and the "*matter*_mass_error" of the matter in the layer.
*matter*_material_mass_fraction [-xml]	float	U [!o_c]	Matter L1	F	*no*	Mass fraction of the matter's material in the layer *Condition:* when "*matter*_mass_fraction" ≠ Ø • stored in the database and provided to user in 'g' unit ➔ calculated by: ⇨ *"matter*_material_mass_fraction" = "*matter_xxx*_material_mass_fraction" * "*matter*_mass_fraction" *Note:* value between 0 and 1. *Note:* determine the mass fraction in the layer of each of the materials of the matter using the "*matter_xxx*_material_mass_fraction" of the materials in the matter (mineral, carbonaceous, …) and the "*matter*_mass_fraction" of the matter in the layer.
*matter*_material_mass_fraction_error [-xml]	float	U [!o_c]	Matter L1	F	*no*	Absolute uncertainty on the mass fraction of the matter's material in the layer *Condition:* when "*matter*_mass_fraction" ≠ Ø AND "*matter*_mass_fraction_error" ≠ Ø • stored in the database and provided to user in 'g' unit ➔ calculated by: ⇨ *"matter*_material_mass_fraction_error" = *"matter*_material_mass_fraction" * ("*matter_xxx*_material_mass_fraction_error" / "*matter_xxx*_material_mass_fraction" + "*matter*_mass_fraction_error" / "*matter*_mass_fraction") *Note:* determine the error of the mass fraction in the layer of each of these materials of the matter using the "*matter_xxx*_material_mass_fraction" and

						"_error" of the materials in the matter (mineral, carbonaceous, …) and the "*matter*_mass_fraction" and "_error" of the matter in the layer.
*matter*_abundance_comments	blob	U [m]	Matter	F	--	Additional information or comments about the abundance of this matter *Note*: other type of comments can possibly be added as it will be the only place to put comments on the matter *Ex:* …
*matter*_additional_comments	blob	U [m]	Mater	F	--	Experimentalist additional information or comments about this matter *Note*: used in particular to describe small changes relative to the matter description, but that did not need creation of a derived matter. *Ex:* matter storage conditions, changes in density by slight compression, …

10.6 Material Table

Root of the table: ***material***

Data type: in 'Sample'

Note: not for precursor materials

Key-word	Type	Level	Table	Exp	Unit	Description
Material import mode and index		[!!O]				*Condition:* absolute mandatory when "*matter*_uid" = Ø
*material*_import_mode	enum(text)	P [!!_m]	Mater	(V)	--	Mode of import of the "Material" metadata Enum: {first import, inherited, use existing, ignore, draft, no change, correction} *For precursor_material:* Enum: {first import, inherited, ignore, draft, no change, correction} *Implied conditions*: when "*material*_import_mode" = 'use existing', only "*material*_uid", and the KWs of "material arrangement and abundance in the layer" are needed. *Definitions:* see "*sample*_import_mode"
*material*_index [**][-xml]	int(10)	B [!!_g]	Mater	F	--	Automatic random but unique number (ID) given to new material
*material*_uid [**]	varchar(255)	S0/S1 [!!_m]	Mater	F	--	Unique identifier code (UID) given to the material table (to be created) *Important note:* when "*material*_import_mode" = 'use existing', this UID is then the "*material*_uid" of an existing material already in the database *Nomenclature:* This UID should start with 'MATERIAL_' both for sample or matter materials, and be very accurately formatted in order to be simple and unique It should be of the style 'MATERIAL_AB_yyyymmdd_123...' where 'AB' are the initials of the person preparing the import, 'yyyymmdd' is the full date of

						the day, and '123...' should be at the end and alphanumeric (only with '_'), with no more than 6 characters. *Ex:* 'MATERIAL_BS_20181006_059', 'MATERIAL_OB_20000101_01' 'MATERIAL_KD_20170712_X50A' *Notes:* - The post-fix '123...' may just be an incremental order number for that day, or may give a short description of the varying parameter of the material. *Ex:* 'MATERIAL_KD_20170712_X50A'
*material*_relevance [-xml dans precursor]	enum(text)	S1b [!_m]	Const	F	--	Relevance of the material in the layar Enum: {main - major, main - minor, impurity, product, precursor, unknown} *Definitions:* - '*main - major'*: essential material of the sample/layer before the beginning of an experiment (and prior any processing of the sample) *Note*: 'major' refers both to a 'major abundance contribution' of a material and to a 'major spectroscopic contribution' of a minor abundance material - '*main - minor'*: minor material of the sample/layer before the beginning of an experiment (and prior any processing of the sample) *Note*: 'minor' refers to a material with both a 'minor abundance contribution' and a 'minor spectroscopic contribution'. - *'impurity'*: material not wanted in the nominal composition of the sample/layer but present in samples or matters. - *'product'*: material produced in the sample/layer subjected to a processing during the experiment - *'precursor'*: precursor material used for synthetic sample/layer formation, or pre-processing of natural matters. *Note*: they are flagged 'precursor' only in the precursor material description. If some amount of this material remain in the sample after formation they are thus flagged 'main - minor' or 'impurity' in the sample description, depending if they are wanted or unwanted,

- *'unknown'*: if origin of the material is not clear: 'impurity' or 'product' ?

Note: complex materials in synthetic samples are set as 'product' only if they are formed during the experiment.

Precursor material

Enum: {precursor}

Default = {precursor} when "*material*_is_precursor" = {yes, true}

Material type

*material*_is_precursor [-xml]	boolean	S0 [!!_g]	Mater	F	--	Flag telling if the material is a 'precursor material'

BoolEnum: {yes, no} or {true, false}

Definition:

- *Precursor material* ('*yes*' or *'true'*): material used to prepare the final material of a sample or of a matter through a series of processings.
- *Normal material ('no'* or *'false'):* material that is part of a final sample or a matter.

Note xml: set automatically depending where it is situated in the xml: "materials" or "precursor_materials"

Precursor material

➔ Calculated:

⇨ will be set automatically to 'yes' or 'true'

Material arrangement and abundance in the layer

Condition: also needed when "*material*_import_mode" = 'use existing'

Note: not for precursor materials

Note: When the abundance info is fully known at the species or constituent level, then give it at the lowest possible level. The values (and errors) at the material level will then be calculated during import where values are missing (but filled values are kept). Provide abundances (absolute and/or fractional) for materials only

when values are known only at this level or more accurately than the sum of the lower levels.

*material*_arrangement	varchar(256)	U [m]	Mater	F	varchar(256)	Relative arrangement of the material grains within the layer *Note:* related to "*layer*_materials_mixing" who describes the mode of mixing (of the grains) of the different materials in the layer. *Note:* mostly useful for materials with "*layer*_materials_mixing"='heterogeneous spatial mixing' or 'spatial distribution'. An image showing the spatial heterogeneity can be provided in "*sample*_images" *Ex:* 'gradient of abundances of olivine and pyroxene along one axis of the sample', 'spatial distribution of abundances of olivine and pyroxene given in "*sample*_image"='map-abundances_olivine-pyroxene-materials'
*material*_mass [+]	float	U [!o_mc]	Mater	F	g	Total mass of the material in the layer *Condition:* mandatory for one of "*material*_mass" or "*material*_mass_fraction" • stored in the database and provided to user in 'g' unit ➔ if no value is given, then calculated from the constituent masses ("*constituent*_mass") of all the constituents in the material: ⇨ *"material*_mass" = $\sum_{material}$("*constituent*_mass")
*material*_mass_error [+]	float	U [!o_mc]	Mater	F	g	Absolute uncertainty on total mass of the material in the layer *Condition:* mandatory when "*material*_mass" ≠ {Ø, NULL} • stored in the database and provided to user in 'g' unit ➔ if no value is given, then calculated from the constituent mass errors ("*constituent*_mass_error") of all the constituents in the material: ⇨ *"material*_mass_error" = $\sum_{material}$ ("*constituent*_mass_error")
*material*_mass_fraction [+]	float	U [!o_mc]	Mater	F	*no*	Mass fraction of the material in the layer *Condition:* mandatory for one of "*material*_mass" or

						"*material*_mass_fraction" ➔ if no value is given, then calculated from the material masses ("*material*_mass") of all the materials in layer. ⇨ *"material*_mass_fraction" = *"material*_mass" / $\sum_{layer}$("*material*_mass") *Note:* value between 0 and 1. *Note:* a warning will be issued during import if the mass fraction of one material is not present or cannot be calculated
*material*_mass_fraction_error [+]	float	U [!o_mc]	Mater	F	*no*	Absolute uncertainty in mass fraction of the material in the layer *Condition:* mandatory when "*material*_mass_fraction" ≠ {Ø, NULL} ➔ if no value is given, then calculated from material masses errors ("*material*_mass_error") of all the materials in layer ⇨ *"material*_mass_fraction_error" = "*material*_mass_fraction" * ["*material*_mass_error" / " *material*_mass" + $\sum_{layer}$ (" *material*_mass_error") / $\sum_{layer}$("*material*_mass")] *Note:* only if "*material*_mass_fraction" has a value ≠ {Ø, NULL}
*material*_abundance_comments	blob	U [m]	Mater	F	--	Additional information or comments about the abundance of this material *Note*: other type of comments can possibly be added, especially when import mode ='use existing' as it will be the only place to put comments *Ex:* …
*material*_additional_comments	blob	U [m]	Mater	F	--	Experimentalist additional comments about this material when used as 'use existing' *Note*: used in particular to describe small changes relative to the initial material description, but that did not need creation of a new material *Ex:* small adsorption , changes in density by slight compression, , …

Note: **When "*material*_import_mode"='use existing'**: all Key Words below should not be used

Note: for precursor materials all this information can alternatively be described more simply (text) in *"processing*_process*"*

Material name and reference

*material*_name	varchar(255)	S0/S0 [!!_m]	Mater	F	--	Material name *Note:* - It should contain explicit info on the material: name and some properties of the material (grain size, …). - It is used as the title of the material in the sample structure bloc of the SSHADE interface
*material*_family [*matter*_family]	enum(text)	S0/S1s [!_m]	Mater	F	--	Family of the material Enum: {fluid, solid, mineral, carbonaceous, extraterrestrial, mixed, other, unknown} *Definitions:* - '*solid'*: synthetic material made of different types of synthetic solids - '*mineral'*: material made primarily of natural minerals - '*carbonaceous'*: material made primarily of natural or synthetic carbonaceous materials - '*extraterrestrial'*: material made primarily of extraterrestrial materials collected on Earth - '*fluid'*: fluid material - '*mixed'*: mixture of at least two of the above - '*other*': any other type of material - '*unknown*': unknown material! *Note:* this list is equivalent to the "matter_family" list (except {mixed, other, unknown})
*material*_local_reference_code	varchar(255)	S1/S1b [m]	Mater	F	--	Possible reference code given to the material after its preparation

Material origin

*material*_origin [*matter*_origin]	enum(text)	S0/S0 [!!_m]	Mater	F	--	General origin of the material. Enum: {natural terrestrial, extraterrestrial, planetary, laboratory, commercial, simulated} *Definitions:* - *'natural terrestrial'*: natural material colleted on Earth - *'extraterrestrial'*: extraterrestrial material collected on Earth (meteorite, micrometeorite, IDP). - *'planetary'* extraterrestrial material (planetary soil, rock or grains, …) collected on or around planetary bodies (planets, satellites, comets, asteroids, …) and in the interplanetary space. - *'laboratory'*: non-natural material experimentally synthesized in a laboratory (well or relatively well-known synthesis process) - *'commercial'*: non-natural material synthesized by a chemical company (less or no knowledge on the synthesis process). May be partly natural or obtained from a natural material. - *'simulated'*: fictive material defined for a numerical simulation

Material grain size distribution and texture

Note: for a matter these parameters may be already decribed at the global scale in *matter*_grain_sizes (_grain_size_method, _grain_texture, _bulk_density/_error)

*material*_grain_size_unit	enum(text)	U [£o_m]	Sampl	F	--	Unit for the material grain sizes (diameter) Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*material*_grain_size_min" OR "*material*_grain_size_min" OR "*material*_grain_size_max" has a value *Note DB:* all grain sizes data will be stored in 'm' *Note:* used for "*material*_grain_size_min/_max"

*material*_grain_size_method	blob	U [m]	Mater	F	--	Description of the definition of the grain size (particle diameter) used, of the methods used for grain size selection and of grain size (median/width or min/max) determination *Definitions:* particle diameter definition can be of several types: - Dv (volume): Diameter of a sphere having the same volume as the particle - Ds (surface): Diameter of a sphere having the same external surface area as the particle - Dsv (surface-volume): Diameter of a sphere having the same ratio of external surface area to volume as the particle - Dp (projected area): Diameter of a sphere having the same projected area as the particle in random orientation (for convex particle Dp = Ds) - D_A (sieve): width of the minimum square aperture through wich the particle will pass *Ex:* 'sieving by 2 stainless steel sieves with 50 and 100 µm meshs'
material_grain_sizes	***List [L1]***	[O]				£: Size distribution of the material grains *Note*: there are several choices to describe them depending on which information is available.
*material*_grain_size_median [*material/matter*_grain_size_median]	float	S3 [m]	Mater L1	F	var.	Median size (diameter) of material grains *Unit:* in "*material*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*material*_grain_size_unit" *Note*: mostly used when only one median size is known for the material grains
*material*_grain_size_width [*material/matter*_grain_size_width]	float	U [m]	Mater L1	F	var.	Full width at half maximum of the size distribution (diameter) of material grains *Unit:* in "*material*_grain_size_unit" • converted in 'm' unit in the database but provided to user in "*material*_grain_size_unit"

						Note: mostly used mostly when only one median size and its distribution width is known for the material grains
*material*_grain_size_min	float	S3 [m]	Mater L1	F	var.	Smallest size (diameter) of material grains of this size range *Unit:* in "*material_grain_size_unit*" • converted in 'm' unit in the database but provided to user in "*material*_grain_size_unit"
*material*_grain_size_max	float	S3 [m]	Mater L1	F	var.	Largest size (diameter) of material grains of this size range *Unit:* in "*material_grain_size_unit*" • converted in 'm' unit in the database but provided to user in "*material_grain_size_unit*"
*material*_grain_size_fraction	float	U [m]	Mater L1	F	*no*	Mass fraction of material grains comprised between size min and size max (diameter) *Note:* value between 0 and 1.
*material*_grain_size_fraction_error	float	U [m]	Mater L1	F	*no*	Absolute uncertainty on the mass fraction of material grains comprised between size min and size max (diameter)
*material*_grain_size_shape	enum(text)	S1b/S2 [m]	Mater L1	F	--	Shape of the individual material grains of this size range : Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions:* Simple shapes: - '*amorphous*': no crystalline form or imitative shape - '*irregular*': occurs as irregular, anhedral crystals - '*equant*': shape tends to be convex equidimensional (e.g. feldspars). - '*reniform*': "kidney like" in shape (e.g.. hematite). - '*globular*': spherical, or nearly so, rounded forms (e.g. wavellite). - '*spherical*': spherical, rounded aggregates.

						- '*flakes'*: flat, thin crystals or aggregates. - '*platy'*: sheet forms (e.g. micas). - '*tabular*': book shape (plagioclase) - '*lathlike'*: flat elongate grains (plagioclase) - '*columnar'*: forms columns - '*acicular'*: needle-like crystals. - '*capillary'*: very slender and long, like a thread or hair (e.g. millerite). Crystalline shapes: - '*cubic'*: cubic shaped crystals. - '*cylindrical'*: shaped like a cylinder. - '*hexagonal'*: six-sided crystal shape in cross-section or habit. - '*octahedral'*: octahedral shaped crystals. - '*prismatic'*: crystals shaped like slender prisms. - '*pyramidal'*: crystals are shaped like pyramids. - '*rhombohedral'*: rhombohedral crystals. Complex shapes: - '*nuggets'*: irregular lumps - '*botryoidal'*: "grape-like" rounded forms (e.g.. malachite). - '*dendritic'*: branching "tree-like" growths of great complexity - '*spheres aggregate'*: made of aggregated spheres. - '*aggregate'*: made of aggregated particles or clustered molecules Other: - '*fluid'*: for liquid, gas and adsorbed - '*other'*: not one described in the list, will be defined in "comments" - '*unknown'*: unknown shape *Note:* for rocks, meteorites, … the material shape is that of the individual grains of each species constituting the rock. The shape of the rock itself is defined in the matter Note: cf.: https://en.wikipedia.org/wiki/Crystal_habit
*material*_grain_size_distribution [*material/matter*_grain_size_distribution]	blob	U [m]	Mater	F	--	Description and parameters of the size distribution of the material grains *Note:* it can provide the shape of the distribution (normal/Gaussian, log-normal, bimodal, …) as well as several parameters such as:

- the modal size (maximum abundance)
- the mean size (center of gravity of the distribution)
- the interquartile range (=D_{75}-D_{25})
- the interpercentile range (=D_{90}-D_{10})
- the coefficient of uniformity (Cu=D_{60}/D_{10})
- the coefficient of curvature (Cc=$D_{30}^2/(D_{10}.D_{60})$)
- …

*material*_grain_texture	openum(text)	S1b/S2 [m]	Mater	F	--	Description of the global texture of the grains OpenEnum: {clay-like, silt-like, compact, compact with defects, compact with bubbles, compact porous, compact microporous, lamellar, fibrous, compact mixed, complex, molecular layer, cluster, liquid, gaseous, other, unknown, …} *Definitions:* - '*clay-like'*: clay-like texture (< 2µm), aggregates with no visible individual particles - '*silt-like'*: very fine particles (2-50 µm) invisible to barely visible individual particles - '*compact'*: fine (> 50µm) and coarse (> 1 mm) compact grain/particle without bubbles, or open/closed porosity - '*compact with defects'*: compact grain/particle with presence or cracks, voids, … - '*compact with bubbles'*: compact grain/particle with isolated bubbles (closed porosity) - '*compact porous'*: compact grain/particle with visible open porosity - '*compact microporous'*: compact grain/particle with invisible open microporosity - '*lamellar'*: compact grain/particle with foliated texture - '*fibrous'*: compact grain/particle with fibrous texture - '*compact mixed'*: compact grain/particle with more than one simple texture described above (describe it in "*material*_comments") - '*complex'*: grain/particle with texture too complex or variable within grains to be described by a single of the above words (explain in "*material*_comments") - '*molecular layer'*: for 'adsorbed' and 'interlayer'

						- *'cluster'*: atomic or molecular cluster - '*liquid'*: for liquids - '*gaseous'*: for gases - '*other'*: texture, or mix of textures, that cannot be described by one of above words (describe it in "*material*_comments") - '*unknown'*: when texture is unknown
*material*_grain_compacity [*material/matter*_grain_compacity]	float	U [m]	Mater	F	*no*	Compacity of the grains of the material (fraction of solid volume per grain volume unit) *Notes:* - compacity = (1 – porosity) - it is the compacity of an individual grain, including the prosity inside the grain (beetween the crystals), but excluding the 'layer porosity' between the grains
*material*_grain_compacity_error [*material/matter*_grain_compacity _error]	float	U [m]	Mater	F	*no*	Absolute uncertainty on the compacity of the grains of the material
*material*_grain_density	float	U [m]	Mater	F	g/cm^3	Density of the grains • stored in the database and provided to user in 'g/cm^3' unit
*material*_grain_density_error	float	U [m]	Mater	F	g/cm^3	Absolute uncertainty on the density of the grains • stored in the database and provided to user in 'g/cm^3' unit
*material*_comments	blob	U [m]	Mater	F	--	Experimentalist additional information or comments about this material *Ex:* various material characterizations …

Material references

material_publications	***List [L3]***	[O]				£: Publications describing the material and its eventual formation/processing
*material*_publication_uid [*] ----	varchar(255)	S2m [m]	Mater Publi L3	F	--	Link to the existing UID of the publication(s) describing the material and its eventual formation/processing. *Note:* these papers should be in the bibliography database, with "*publication*_content" = 'material-matter'

Material constituents organization

*material*_constituents_number [+][-xml]	int(10)	U [!!_c]	Mater	F	*no*	Number of different constituents of the material grains ⇨ calculated from the "*material*_constituents_index" and "*material*_basic_constituents_index" list
*material*_constituents_mixing [+]	openum(text)	S1b/S2 [!_m]	Mater	F	--	Describe how the constituents are mixed at the sub-grain level in the material grains OpenEnum: {single phase, multi-phases, endmembers polyphase, matrix with inclusions, grains with inclusions, filled agglomerate, coated grains, concentric zoning, sector zoning, layer zoning, interlayering, foam, emulsion, colloidal solution, complex mixing, adsorbate-adsorbent, other, unknown, ...} *Definitions:* Compact phases: - '*single phase'*: only one constituent in the grains (but possibly several crystals). Also for liquid solutions. - '*multi-phases'*: limited number of phases coexisting in the grains without specific organization. Also used for adsorption on a multi-phase adsorbent. - '*endmembers polyphase'*: intimate mixing (at microscopic level) of endmember phases within a solid solution phase (equivalent to a single solid solution of intermediate composition) - '*matrix with inclusions'*: mix of phases with a matrix-inclusions organization: individual phase(s) isolated in a continuous matrix. - '*grains with inclusions'*: the grains are mostly one single phase but with small inclusions of another phase (solid, liquid, or gas) fully

embedded inside the grains

Aggregates and agglomerates:

- '*filled agglomerate'*: aggregate or agglomerate of one phase (or more) with their pores filled by another phase

Coated grains:

- '*coated grains'*: the grains have their core made of one phase and an external shell of another phase (the coating)

Zoning in compact materials:

- '*concentric zoning'*: concentric organization of several phases inside grains
- '*sector zoning'*: sector organization of several phases inside grains
- '*layer zoning'*: layered organization of several phases inside grains
- '*interlayering*': crystalline structures in which two or more constituents (layer types) are vertically stacked at the scale of a few atomic layers in the direction parallel to c*
    - *Note*: mostly in interstratified clay minerals
    - *ref*: http://clay.uga.edu/courses/8550/CM13.html

Colloid systems (particles 1 nm - 1 µm) or suspensions (above 1 µm):

- '*foam*': gas dispersed in a continuous liquid or solid phase
- '*emulsion*': liquid dispersed in a continuous liquid or solid phase
- '*colloidal solution'*: (or 'sol') solid dispersed in a continuous liquid or solid phase

Others:

- '*complex mixing'*: complex mixture of phases (numerous or indicernable and/or very heterogeneous) without clear topologic organization or too complex to be described.
- '*adsorbate-adsorbent'*: sorbed phase constituent(s), i.e. 'adsorbate' ("*constituent*_arrangement" = 'sorbed phase') 'mixed' with an '(ad)sorbate' constituent. This also includes interlayer adsorption. When there are several adsorbents, then use 'multi-phases'.

    Note: The relation 'adsorbent/adsorbate' will be given by "*constituent*_sorption_constituents" in the adsorbed phase constituent description.
- '*other'*: when type of mixing cannot be described by one of above words (explain in "*material*_comments")

- ‘*unknown’*: when type of mixing is impossible to observe

material_basic_constituents	***List [L4]***	[!!]				£: Basic constituents composing the material grains.
*material*_basic_constituent_index [*§] [-xml]	int(11) [Internal Links]	B [!!_g]	Mater BConst L4	F	--	ID of the basic constituent(s) composing the material grains. *Note:* determined automatically during import *Note xml:* in practice the description of the basic constituents(s) are done directly under “material” without ID link
material_constituents	***List [L5]***	[!!]				£: Constituents composing the material grains.
*material*_constituent_index [*§] [-xml]	int(11) [Internal Links]	B [!!_g]	Mater Const L5	F	--	ID of the constituent(s) composing the material grains. *Note:* determined automatically during import *Note xml:* in practice the description of the constituents(s) are done directly under “material” without ID link

10.7 Basic constituent Table

Root of the table: ***basic_constituent***

Data type: in ‘Sample’

Condition: not when a matter is used (“*material*_is_a_matter” = ‘true’)

Condition: if the constituent is a “basic constituent” (i.e. that can be described by one of the “fundamental solid, mineral or liquid” phases) then use this “Basic constituent” table. If not (constituent defined manually), then use the "Constituent" table.

Key-word	Type	Level	Table	Exp	Unit	Description
Basic constituent index						
*basic_constituent*_import_mode	enum(text)	P [!!_m]	BConst	(V)	--	Mode of import of the actual “Basic constituent” metadata Enum: {first import, inherited, use existing, ignore, draft, no change, correction} *Definitions:* see ”*sample*_import_mode”
*basic_constituent*_index [**][-xml]	int(10)	B [!!_g]	BConst	F	--	Automatic random but unique number (ID) given to new actual basic constituent
*basic_constituent*_uid [**]	varchar(255)	S0c/S1 [!!_m]	BConst	F	--	Unique identifier code (UID) given to the actual basic constituent table (to be created) *Nomenclature:* This code name should start with ‘CONST_’ and be very accurately formatted in order to be simple and unique It should be of the style ‘CONST_AB_yyyymmdd_123...’ where ‘AB’ is initial of people preparing the import, ‘yyyymmdd’ is the full date of the day, and ‘123...’ should be at the end and alphanumeric (only with '_'), with no more than 6 characters. *Ex:* ‘CONST_BS_20181006_059’, ‘CONST_OB_20000101_01’, ‘CONST_KD_20170712_X50A’

Notes:

- The post-fix '123...' may just be an incremental order number for that day, or may give a short description of the varying parameter of the constituent.
  Ex: 'CONST _KD_20170712_X50A'

Important note:

- when "*basic_constituent*_import_mode" = 'use existing', this UID is then the "*basic_constituent*_uid" of an existing constituent already in the database

*basic_constituent*_relevance	enum(text)	S1b [!!_m]	BConst	F	--	Relevance of the basic constituent in the material Enum: {main – major, main - minor, impurity, product, precursor, unknown} *Definitions:* cf. *"constituent*_relevance" **Precursor material** Enum: {precursor} *Default* = {precursor} when "*material*_is_precursor" = {yes, true}

Basic constituent arrangement and abundance in the material

General condition: mandatory to give one of the following "*basic_constituent*_mass", "*basic_constituent*_mass_fraction", "*basic_constituent*_mole" or "*basic_constituent*_mole_fraction"

Note: abundances (mass or mole / absolute or fractional) should be given homogeneously for all basic constituents and constituents (next table)

*basic_constituent*_arrangement	enum(text)	S2 [!_m]	BConst	F	--	Relative arrangement of the constituent within the material grains OpenEnum: {single phase, homogeneous in multi-phases, heterogeneous in multi-phases, endmember in polyphase, matrix, inclusion, bubble, suspended particles, medium of suspension, in aggregate, in agglomerate, pore filling, coated core, coating shell, concentric zone, sector zone, layer zone, mixed-layer, complex intimate mix, sorbed phase, other, unknown, …} *Definitions:* see "*constituent*_arrangement"

						Notes: see "*constituent*_arrangement"
*basic_constituent*_mass	float	U [!o_mc]	BConst	F	g	Total mass of the basic constituent in the material *Condition:* see general condition • stored in the database and provided to user in 'g' unit ➔ calculated from "*basic_constituent*_mole" when it is provided (need the molar masses of the species of the actual basic constituent => in "molecule species" table: "*molecule*_molar_mass") for "*solid*_specie_family" = 'molecule' and for "*liquid*_molecule": - "mass" = "mole" * "*molecule*_molar_mass" for "*solid*_specie_family" = 'element': - "mass" = "mole" * "*atom*_molar_mass"
*basic_constituent*_mass_error	float	U [!o_mc]	BConst	F	g	Absolute uncertainty on the total mass of the basic constituent in the material *Condition:* mandatory when "*basic_constituent*_mass" ≠ {Ø, NULL} • stored in the database and provided to user in 'g' unit ➔ calculated from "*basic_constituent*_mole_error" when it is provided for "*solid*_specie_family" = 'molecule' and for "*liquid*_molecule": - "mass_error" = "mole_error" * "*molecule*_molar_mass" for "*solid*_specie_family" = 'element': - "mass_error" = "mole_error" * "*atom*_molar_mass" *Note:* - when the unit of "*basic_constituent*_mole_error" is mol/g or mol/kg (liquid solutions) it is best to set "*basic_constituent*_mass_error" = 'NULL' to remove the calculated value
*basic_constituent*_mass_fraction	float	U [!o_mc]	BConst	F	*no*	Mass fraction of the constituent in the material *Condition:* see general condition ➔ if no value is given, then calculated from the constituent and basic constituent masses ("*basic_constituent*_mass") of all the constituents in the material:

						⇨ “ mass_fraction” = “ mass” / $\sum_{material}$(“mass”) ➔ otherwise calculated from “*basic_constituent*_mole_fraction” when provided for all constituents (mainly for atomic and molecular constituents: need the molar masses of all species in the constituent => in “*molecule species*” table: “*molecule*_molar_mass” of each “*solid/liquid*_species_uid”) ⇨ “mass_fraction” = mole_fraction * *molecule*_molar_mass / Σi(mole_fraction(i) * *molecule*_molar_mass(i)) *Note:* value between 0 and 1. *Note:* a warning will be issued during import if the mass fraction of one constituent is not present or cannot be calculated
*basic_constituent*_mass_fraction_error	float	U [!o_mc]	BConst	F	*no*	Absolute uncertainty on the mass fraction of the constituent in the material. *Condition:* mandatory when “*basic_constituent*_mass_fraction” ≠ {Ø, NULL} ➔ if no value is given, then calculated from constituent and basic constituent masses errors (“*basic_constituent*_mass_error”) of all the constituents in the material: ⇨ “mass_fraction_error” = “mass_fraction” * [“mass_error” / ” mass” + $\sum_{material}$ (“mass_error”) / $\sum_{material}$(“mass”)]

Abundances in mole

Note: abundances in mole should be used only in specific conditions:

Conditions: compulsory to be used only if all constituents of the material are “fundamental solids” of “*solid*_family” = {molecular solid, ionic solid}, or “fundamental liquids” ("*liquid*_family" = {molecular liquid, atomic liquid, ionic liquid, metallic liquid}), but neither “fundamental minerals” ("mineral_family" = {mineral}), nor “custom constituents”, and if these basic constituents can be expressed homogeneously either all in “mole” or all in “mole fraction”.

*basic_constituent*_mole	float	U [!o_mc]	BConst	F	*mol*	Total mole of the basic constituent in the material *Condition:* see general condition *Units*: in ‘mol’ *Note*: number of moles of fundamental constituent formula, as defined by the “*solid*_specie_number_min” or “*liquid*_specie_mole_fraction” values

*basic_constituent*_mole_error	float	U [!o_mc]	BConst	F	*mol*	Absolute uncertainty on the total mole of the basic constituent in the material *Condition:* mandatory when "*constituent*_mole" ≠ {Ø, NULL} *Units*: in 'mol'
*basic_constituent*_mole_fraction	float	U [!o_mc]	BConst	F	*no*	Mole fraction of the basic constituent in the material *Condition:* see general condition ➔ if no value is given, then calculated from the basic constituent moles ("*basic_constituent*_mole") of all the constituents in the material: ⇨ *"constituent*_mole_fraction" = *"constituent*_mole" / $\sum_{material}$("*constituent*_mole") *Note:* value between 0 and 1. *Note:* a warning will be issued during import if the mole fraction of one constituent is not present or cannot be calculated
*basic_constituent*_mole_fraction_error	float	U [!o_mc]	BConst	F	*no*	Absolute uncertainty on the mole fraction of the basic constituent in the material. *Condition:* mandatory when "*basic_constituent*_mole_fraction" ≠ {Ø, NULL} ➔ if no value is given, then calculated from basic constituent moles errors ("*basic_constituent*_mole_error") of all the constituents in the material: ⇨ *"constituent*_mole_fraction_error" = "c*onstituent*_mole_fraction" * ["*constituent*_mole_error" / "*constituent*_mole" + $\sum_{material}$ ("c*onstituent*_mole_error") / $\sum_{material}$("c*onstituent*_mole")]
*basic_constituent*_abundance_comments	blob	U [m]	BConst	F	--	Additional information or comments about the abundance of this constituent in the material. *Ex:* …

Condition: **When "*basic_constituent*_import_mode"='use existing'**: All Key Words below should not be used (they are already described)

Basic constituent name and index

*basic_constituent*_name	varchar(255)	S0c/S1 [!!o_m]	BConst	F	--	Name of the actual basic constituent *Note:* - It may contain explicit info on the fundamental constituent or its variant: species name, specific abundance, and some properties of the constituent (phase, …), origin, …. - It is used as the title of the constituent page on the SSHADE interface *Ex:* 'San Carlo Olivine', 'Synthetic fayalite 3% Mg', Water ice Ih with 0.1% CO2', …
*basic_constituent*_fundamental_phase_uid [*]	varchar(255)	S0c/S1 [!!_m]	BConst Solid Miner Solut	F	--	Link to the existing UID of the fundamental 'solid', 'mineral', or 'liquid' phase *Notes:* - Only for fundamental 'solid', 'mineral', and 'liquid' phases. - The others constituents are described with the full constituent/species structure ("Constituent" table) - When a sample is processed before, during or after formation of the layer, in such a way that the initial fundamental constituent composition or structure is altered, then it is necessary to define if the fundamental constituent is still relevant (minor changes in composition or structure, to be defined with the variable parameters) or if a new description with the constituent(s)/specie(s) structure is necessary when the changes are significant.

Fundamental constituent variable parameters

Condition: OPTIONAL block but COMPULSORY to change what is better known or different from the linked fundamental solid/mineral/liquid.

Note: The variable parameters are mostly used to provide more accurate composition of the actual solid/mineral/liquid: for variable solids/minerals/liquids or solid/mineral liquid/hydration series, or when solid/mineral (sub-)groups are used for ill-defined solids/minerals. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental solids/minerals for describing some related amorphous solids/minerals.

*basic_constituent*_solid_variables		[O]	BConst Solid	VS		£: solid variable parameters *Note:* mostly used to provide more accurate composition of the actual solid: for variable solids or solid solution/hydration series, or when solid (sub-

						)groups are used for ill-defined solids. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental solids for describing some related amorphous solids
*basic_constituent*_solid_variables		[O]	BConst Miner	VMi		£: mineral variable parameters *Note:* mostly used to provide more accurate composition of the actual mineral: for variable or solution/hydration series minerals, or when mineral (sub-)groups are used for ill-defined minerals. Also for adding replacement or impurity elements. Also used for changing structural info of equivalent crystalline fundamental minerals for describing some related amorphous minerals.
*basic_constituent*_liquid_variables		[O]	BConst Solut	VL		£: liquid variable parameters *Note:* mostly used to provide the accurate composition of the actual liquid
Constituent texture						
*basic_constituent*_crystal_size_unit [*sample/matter*_crystal_size_unit]	enum(text)	U [£o_m]	Const	F	--	Unit for the basic constituent crystal sizes (diameter) Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*basic_constituent*_crystal_size_median" OR "*basic_constituent*_crystal_size_min" OR "*basic_constituent*_crystal_size_max" has a value *Note DB:* all crystal sizes data will be stored in 'm' *Note:* used for "*basic_constituent*_crystal_size_median/_width/_min/_max"
*basic_constituent*_crystal_size_method [*constituent*_crystal_size_method]	blob	U [m]	BConst	F	--	Description of the crystal size (mean/width or min/max) definition, and of the method of determination of the crystal size distribution *Ex:* 'SEM microscope measurement of section'
basic_constituent_crystal_sizes	***List [L1]***	[O]				£: Size distribution of the basic constituent crystals

*basic_constituent*_crystal_size_median [*constituent*_crystal_size_median]	float	S3 [m]	Const L1	F	var.	Median size (diameter) of basic constituent crystals *Unit:* in "*basic_constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*basic_constituent*_crystal_size_unit" *Note*: mostly used when only one median size is known for the constituent
*basic_constituent*_crystal_size_width [*constituent*_crystal_size_width]	float	U [m]	BConst L1	F	var.	Full width at half maximum of the size distribution (diameter) of basic constituent crystals *Unit:* in "*basic_constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*basic_constituent*_crystal_size_unit" *Note*: mostly used when only one median size and its distribution is known for the constituent crystals
*basic_constituent*_crystal_size_min [*constituent*_crystal_size_min]	float	S3 [m]	BConst L1	F	var.	Smallest size (diameter) of basic constituent crystals of this size range *Unit:* in "*basic_constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*basic_constituent*_crystal_size_unit"
*basic_constituent*_crystal_size_max [*constituent*_crystal_size_max]	float	S3 [m]	BConst L1	F	var.	Largest size (diameter) of basic constituent crystals of this size range *Unit:* in "*basic_constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*basic_constituent*_crystal_size_unit"
*basic_constituent*_crystal_size_fraction [*constituent*_crystal_size_fraction]	float	U [m]	BConst L1	F	*no*	Mass fraction of basic constituent crystals comprised between size min and size max (diameter) *Note:* value between 0 and 1
*basic_constituent*_crystal_size_fraction_error [*constituent*_crystal_size_fraction	float	U [m]	BConst L1	F	*no*	Absolute uncertainty on the mass fraction of basic constituent crystals comprised between size min and size max (diameter)

_error]

*basic_constituent*_crystal_size_shape [*constituent*_crystal_size_shape]	enum(text)	S2 [m]	BConst L1	F	--	Dominant shape of the basic constituent crystals of this size range Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions: see "material*_grain_size_shape*"*
*basic_constituent*_crystal_size_distribution [*constituent*_crystal_size_distribution]	blob	U [m]	BConst	F	--	Description and parameters of the size distribution of the basic constituent crystals *Note:* see "*material*_grain_size_distribution"
*basic_constituent*_texture	enum(text)	S2 [m]	BConst	F	--	Internal texture of the basic constituent crystals Enum: {monocrystalline, polycrystalline, cryptocrystalline, nanocrystalline, metamict, amorphous, glassy, polymeric, macromolecular, complex, liquid, other, unknown} *Definitions & notes: see "constituent*_crystal_texture*"*
*basic_constituent*_comments	blob	U [m]	BConst	F	--	Additional information on basic constituent, in particular for coating of grains: coating thickness

10.8 Constituent Table

Root of the table: ***constituent***

Data type: in 'Sample'

Condition: not when a matter is used ("*material*_is_a_matter" = 'true')

Key-word	Type	Level	Table	Exp	Unit	Description
Constituent import mode and indexes						
*constituent*_import_mode	enum(text)	P [!!_m]	Const	(V)	--	Mode of import of the "Constituent" metadata Enum: {first import, inherited, use existing, ignore, draft, no change, correction} *Implied conditions*: when "*constituent*_import_mode" = 'use existing', only "*constituent*_uid", "*constituent*_arrangement", "*constituent*_sorption_constituent_uid" (if needed) and the mandatory KWs of "Constituent abundance in the material" stay mandatory below *Definitions:* see "*sample*_import_mode"
*constituent*_index [**][-xml]	int(10)	B [!!_g]	Const	F	--	Automatic random but unique number (ID) given to new constituent
*constituent*_uid [**]	varchar(255)	S0c/S1 [!!_m]	Const	F	--	Unique identifier code (UID) given to the constituent table (to be created) *Nomenclature:* This code name should start with 'CONST_' and be very accurately formatted in order to be simple and unique *Note:* It should be of the style 'CONST_AB_yyyymmdd_123...' where 'AB' is initial of people preparing the import, 'yyyymmdd' is full date of the day, and '123...' should be at the end and alphanumeric (only with '_'), with no more than 6 characters. *Ex:* 'CONST_BS_20181006_059', 'CONST_OB_20000101_01', 'CONST

						_KD_20170712_X50A’ *Notes:* - the post-fix ‘123...’ may just be an incremental order number for that day, or may give a short description of the varying parameter of the constituent. *Ex:* ‘CONST _KD_20170712_X50A’ *Important note:* - when “*constituent*_import_mode” = ‘use existing’, this UID is then the “*constituent*_uid” of an existing constituent already in the database
*constituent*_relevance [*constituent*_relevance]	enum(text)	S1b [!!_m]	Const	F	--	Relevance of the constituent in the material Enum: {main - major, main - minor, impurity, product, precursor, unknown} *Definitions:* - ‘*main - major’*: essential constituent of the material before the beginning of an experiment (and prior any processing of the sample) *Note*: ‘major’ refers both to a ‘major abundance contribution’ of a constituent and to a ‘major spectroscopic contribution’ of a minor abundance constituent - ‘*main - minor’*: minor constituent of the material before the beginning of an experiment (and prior any processing of the sample) *Note*: ‘minor’ refers to a constituent with both a ‘minor abundance contribution’ and a ‘minor spectroscopic contribution’. - *‘impurity’*: constituent not wanted in the nominal composition of the material but present in synthetic materials or others matters. - *‘product’*: constituent produced in the sample subjected to a processing during the experiment - *‘precursor’*: precursor constituents used for synthetic material formation, or pre-processing of natural matters. *Note*: they are flagged ‘precursor’ only in the precursor material description. If some amount of the constituent remain in the sample after formation they are thus flagged ‘main - minor’ or ‘impurity’ in the sample description, depending if they are wanted or unwanted,

- *'unknown'*: if origin of the constituent is not clear: 'impurity' or 'product' ?

Note: constituents of complex materials in synthetic samples are set as 'product' only if they are formed during the experiment.

Precursor material

Enum: {precursor}

Default = {precursor} when "*material*_is_precursor" = {yes, true}

Constituent arrangement and abundance in the material

Condition: also needed when "*constituent*_import_mode" = 'use existing'
Condition: mandatory to give one of the following "*constituent*_mass", or "*constituent*_mass_fraction"

Notes:
- when the abundance info is fully known at the species level, then give it at the species level. The values (and errors) at the constituent level will thus be calculated during import where the fields values are missing.
- provide below abundances for constituents only when values are known only at this level or more accurately than the sum of the species abundances.
- abundances (absolute or fractional) should be given homogeneously for all constituents and basic constituents (previous table)

*constituent*_arrangement	enum(text)	S2 [!_m]	Const	F	--	Relative arrangement of the constituent within the material grains OpenEnum: {single phase, homogeneous in multi-phases, heterogeneous in multi-phases, endmember in polyphase, matrix, inclusion, bubble, suspended particles, medium of suspension, in aggregate, in agglomerate, pore filling, coated core, coating shell, concentric zone, sector zone, layer zone, mixed-layer, complex intimate mix, sorbed phase, other, unknown, …} *Condition:* also mandatory when "*constituent*_import_mode" = 'use existing' *Definitions:* Compact mono- and poly-phases: - '*single phase'*: single constituent of a grain (include crypto-polymineral) - '*homogeneous in multi-phases'*: homogeneous arrangement of the constituent in compact multi-phases grains. Include adsorbat with

another constituent adsorbed or as an interlayer phase.
- '*heterogeneous in multi-phases'*: heterogeneous arrangement of the constituent in compact multi-phases grains
- '*endmember in polyphase'*: endmember phase intimately mixed (at microscopic level) within a solid solution phase (equivalent to a single solid solution of intermediate composition)
- '*matrix*': matrix containing inclusions, bubbles, veinules (layer zone), …
- '*inclusion*': solid inclusion in grains (in polymineral, …)
- '*bubble*': liquid or gas inclusion in grains

Colloid systems (foams, emulsions, colloidal solutions) and suspensions:
- '*suspended particles'*: solid or liquid (or gas) particles dispersed in a continuous phase (the medium of suspension). Particles have between 1 nm and 1 µm for colloid systems and above 1 µm for suspension.
- '*medium of suspension'*: solid, liquid or gaseous medium in which the particles are suspended

Aggregates and agglomerates:
- '*in aggregate':* constituent part of an aggregate of particles (same or different phase) i.e. particles in close contact without sintering
- '*in agglomerate':* constituent part of an agglomerate of particles (same or different phases), i.e. particles in close contact with sintering
- '*pore filling'*: pore-filling phase forming "bridges" between aggregate or agglomerate particle of another phase thereby binding them together.

Coated grains:
- '*coated core'*: internal core of coated grains
- '*coating shell'*: external coating shell surrounding coated grains

Zoning in compact materials:
- '*concentric zone'*: concentric zone(s) of concentric zoned grains
- '*sector zone'*: sector zone(s) of sector zoned grains
- '*layer zone'*: layer(s) of layer zoned grains
- '*mixed-layer'*: layer in an interlayered material with crystalline structure in which two or more constituents (mixed-layers) are vertically stacked at the scale of a few atomic layers in the direction parallel to c*

- *Note*: mostly in interstratified clay minerals
- *ref*: http://clay.uga.edu/courses/8550/CM13.html

Others:

- '*complex intimate mix'*: complex heterogeneous arrangement of a constituent in a complex mixture of phases (numerous or indicernable and/or very heterogeneous) without clear topologic organization
- '*sorbed phase*': adsorbed or interlayer phase on/in another constituent
- '*other'*: when arrangement of constituent cannot be described by one of above words (explain in "*constituent*_comments")
- '*unknown'*: when arrangement of constituent is unknown

Note:
- For gases and liquids (without particles), and for molecular and inorganic solids, minerals, and complex matters (organic, carbonaceous, mineral) with mono-constituent: 'single phase'
- For gases and liquids (with particles): 'homogeneous in multi-phases', bubble'
- For molecular, ionic, covalent solids, minerals, and complex matters with multi-constituents: 'homogeneous in multi-phases', 'heterogeneous in multi-phases', 'in aggregate', 'in agglomerate', 'concentric zone', 'sector zone', 'layer zone', 'inclusion'
- For grains with coating: 'coating core', 'coated shell'
- For constituents in complex mixture of several molecular, organic, inorganic and/or mineral phases: 'complex intimate mix'
- For molecular species adsorbed on, or in interlayer in other solid constituent(s): 'sorbed phase'.

Note: the constituent(s) (adsorbat) on which the *sorbed phase* is sorbed is/are described in (an)other material(s) which is/are linked below with its sorbed constituent by the list "*constituent*_adsorption_constituents"

Note: "*constituent*_arrangement" depends on "*material*_constituents_mixing" which describes how the constituents are mixed at material level

*constituent*_mass	float	U [!o_mc]	Const	F	g	Total mass of the constituent in the material *Condition:* mandatory for one of "constituent_mass" or

						"constituent_mass_fraction" • stored in the database and provided to user in 'g' unit ➔ if no value is given, then calculated from the species masses ("*species*_mass") of all the species in the constituent: ⇨ *"constituent*_mass" = $\sum_{constituent}$(*"species*_mass") *Note:* For sorbed species (surface adsorption or insertion) this total mass allows to determine the mass fraction of sorbed species ("*constituent*_sorption_mass_fraction") relative to the constituent(s) of other material(s) on/in which it is sorbed
*constituent*_mass_error	float	U [!o_mc]	Const	F	g	Absolute uncertainty on the total mass of the constituent in the material *Condition:* mandatory when "*constituent*_mass" ≠ {Ø, NULL} • stored in the database and provided to user in 'g' unit ➔ if no value is given, then calculated from the species mass errors ("*species*_mass_error") of all the species in the constituent: ⇨ *"constituent*_mass_error" = $\sum_{constituent}$(*"species*_mass_error")
*constituent*_mass_fraction	float	U [!o_mc]	Const	F	*no*	Mass fraction of the constituent in the material *Condition:* mandatory for one of "constituent_mass" or "constituent_mass_fraction" ➔ if no value is given, then calculated from the constituent masses ("*constituent*_mass") of all the constituents in the material: ⇨ *"constituent*_mass_fraction" = *"constituent*_mass" / $\sum_{material}$("*constituent*_mass") *Note:* value between 0 and 1. *Note:* a warning will be issued during import if the mass fraction of one constituent is not present or cannot be calculated *Note:* For sorbed species this mass fraction is relative to a possible other sorbed phase (another constituent/species mixed with this one) of the specific material describing the sorbed phase(s), but not relative to the adsorbat abundance (wich belong to another material): see

						"*constituent*_sorption_mass_fraction"
*constituent*_mass_fraction_error	float	U [!o_mc]	Const	F	*no*	Absolute uncertainty on the mass fraction of the constituent in the material. *Condition:* mandatory when "*constituent*_mass_fraction" ≠ {Ø, NULL} ➔ if no value is given, then calculated from constituent masses errors ("*constituent*_mass_error") of all the constituents in the material: ⇨ "*constituent*_mass_fraction_error" = "*constituent*_mass_fraction" * ["*constituent*_mass_error" / "*constituent*_mass" + $\sum_{material}$ ("*constituent*_mass_error") / $\sum_{material}$("*constituent*_mass")]

Constituent sorption

						Condition: also needed when "*constituent*_import_mode" = 'use existing'
constituent_sorption_constituents	***List [L1]***	[!!o]				£: constituents on which this constituent is sorbed *Condition:* absolute Mandatory when "*constituent*_arrangement" = 'sorbed phase'
*constituent*_sorption_constituent_uid [*]	varchar	S1i [!!o_m]	Const Const L1	F	--	Link to the existing UID of the constituent on which this constituent is sorbed. *Condition:* Only for sorbed phases: Absolute Mandatory when "*constituent*_arrangement" = 'sorbed phase'. *Note:* Do not fill when condition is not met. *Note:* these adsorbate constituents should be among the other constituents(s) of this material.
*constituent*_sorption_mass_fraction	float	U [!o_mc]	Const	F	*no*	Mass fraction of the sorbed phase (molecular species) relative to the total mass of the constituent(s) on/in which it is sorbed *Condition:* Only for sorbed phases: Mandatory when "*constituent*_arrangement" = 'sorbed phase'. ➔ if no value is given, then calculated (sorbed/sorbent) from "*constituent*_mass" of this sorbed constituent and the "*constituent*_mass" of all

						constituents given by "*constituent*_sorption_constituent_uid" ⇨ *"constituent*_sorption_mass_fraction » = "*constituent*_mass" / $\sum_{adsorbat}$("*constituent*_mass") *Note:* value between 0 and 1
*constituent*_sorption_mass_fraction_error	float	U [!o_mc]	Const	F	*no*	Absolute uncertainty on the mass fraction of the sorbed phase (molecular species) relative to the mass of the constituent(s) on/in which it is sorbed *Condition:* only and mandatory when "*constituent*_sorption_mass_fraction" ≠ {Ø, NULL} ➔ if no value is given, then calculated from "*constituent*_mass_error" of this sorbed constituent and the "*constituent*_mass_error" of all constituents given by "*constituent*_sorption_constituent_uid" ⇨ *"constituent*_sorption_mass_fraction_error" = *"constituent*_mass_error" / *"constituent*_mass" + $\sum_{adsorbat}$("*constituent*_mass_error") / $\sum_{adsorbat}$("*constituent*_mass") *Note:* the 'adsorbat' are all constituents listed in *"constituent*_sorption_constituent_uid"
*constituent*_abundance_comments	blob	U [m]	Const	F	--	Additional information or comments about the abundance of this constituent in the material, or adsorbed on another constituent *Note*: other type of comments can possibly be added, especially when import mode ='use existing' as it will be the only place to put comments *Ex:* …

Condition: **When "*constituent*_import_mode" = 'use existing'**: All Key Words below should not be used (they are already described)

Constituent name and family

*constituent*_name	varchar(255)	S0c/S1 [!!_m]	Const	F	--	Constituent name *Note:* - It should contain explicit info on the constituent: species name and some properties of the constituent (phase, …).

- It is used as the title of the constituent in the sample structure bloc of the SSHADE interface

*constituent*_family [*constituent/phase*_family]	enum(text)	S1 [!!_m]	Const	F	--	Family (or major class) of the constituent Enum: {molecular solid, covalent network solid, ionic solid, metallic solid, molecular and covalent solid, molecular and ionic solid, covalent and ionic solid, complex solid, mineral, molecular liquid, atomic liquid, ionic liquid, metallic liquid, molecular and atomic liquid, molecular and ionic liquid, atomic and ionic liquid, liquid solution, complex liquid, adsorbed, clusters, gas, complex mix, other, unknown} [to be changed in v0.9.0a] *Definitions:* Solids: - '*molecular solid*': Solid made up of atoms or molecules held together by London dispersion forces, dipole-dipole forces, or hydrogen bonds. - '*covalent network solid*': solid made up of atoms connected by covalent bonds; the intermolecular forces are covalent bonds as well. - '*ionic solid*': Solid made up of positive and negative ions and held together by electrostatic attractions. - '*metallic solid*': solid made up of metal atoms that are held together by metallic bonds. - 'molecular and covalent solid': solid made up of atoms or molecules held together by both molecular and covalent bonds. - 'molecular and ionic solid: solid made up of atoms or molecules held together by both molecular and ionic bonds. - 'covalent and ionic solid': solid made up of atoms or molecules held together by both ionic and covalent bonds. - 'complex solid': solid made up of atoms or molecules held together by several of bonds: molecular, covalent, ionic or metallic bonds - '*mineral*': single naturally occurring mineral phase (include natural salts, and native elements) Liquids: - '*molecular liquid*': single molecular liquid phase (possibly with mixture of molecules)

- '*atomic liquid*': single covalent liquid phase
- '*ionic liquid*': single ionic liquid phase
- '*metallic liquid*': single metallic liquid phase (also called 'ion-electronic liquid')
- 'molecular and covalent liquid': liquid made up of atoms or molecules held together by both molecular and covalent bonds.
- 'molecular and ionic liquid: liquid made up of atoms or molecules held together by both molecular and ionic bonds.
- 'covalent and ionic liquid': liquid made up of atoms or molecules held together by both ionic and covalent bonds.
- 'complex liquid': liquid made up of atoms or molecules held together by several of bonds: molecular, covalent, ionic or metallic bonds
- '*liquid solution*': homogeneous mixture in a single phase of several liquids from the above families, or a gas or a solid dissolved in a liquid

  Note: In such a mixture, the solute is the substance dissolved in another substance, known as the solvent. The solvent does the dissolving limited by the solubility (for gaz and solid in liquid), or by the miscibility for liquid in a liquid.
  Reference: http://en.wikipedia.org/wiki/Solution)

Notes:
- 'colloid systems', i.e., a phase (the suspended particles of size between 1 nm and 1 µm) dispersed in a continuous phase (the medium of suspension) and 'suspension', i.e. a phase (the suspended particles of size above 1 µm) dispersed in a continuous phase (the medium of suspension), will be considered as a material constituted of two (or more) constituents.
- Types of 'colloid systems': foam (gas dispersed in liquid or solid), aerosols (liquid or solid dispersed in gas) , emulsion (liquid dispersed in liquid or solid), sol (colloidal solution: solid dispersed in liquid or solid).

  Reference: http://molphys.univ.kiev.ua/?p=204&lang=en

Adsorbed and gas:
- *'adsorbed*': phase (possibly with mixture of species) adsorbed on, or in interlayer in other solids
- '*clusters'*: free clusters (possibly with mixture of species)

- ‘*gas’*: gas phase (possibly with mixture of species)
- ‘*complex mix’*: complex mixture of solid and/or liquid phases (atomic, molecular, ionic, covalent, and/or metallic, mineral)

Others:

- ‘*other’*: when family of constituent cannot be described by one of above words (explain in “*constituent*_comments”)
- ‘*unknown’*: when family of constituent is unknown

Note: The ‘complex mix’ allows to represent with a single constituent a complex mixture of constituent types too numerous or too complex to be described separately.

*constituent*_class	enum(text)	S1 [!_m]	Const	F	--	Class of solid composing the constituent.
						
						Enum: {non polar molecular solid, polar molecular solid, hydrogen bonded molecular solid, mixed molecular solid, chain covalent network solid, sheet covalent network solid, tridimentional covalent network solid, glass, acid salt, alkali salt, normal salt, mixed salt, true metal, pseudometal (semi-conductor), native element, non-silicate mineral, silicate mineral, organic mineral, non polar molecular liquid, polar molecular liquid, hydrogen bonded molecular liquid, molecular liquid solution, atomic liquid, atomic liquid solution, ionic liquid, ionic liquid solution, metallic liquid, metallic liquid solution, mixed liquid solution, atomic adsorbed, molecular adsorbed, atomic clusters, molecular clusters, atomic gas, molecular gas, complex mix, other, unknown}
						
						Definitions:
						- For molecular, covalent network, ionic and metallic solids:
						  - see “*solid*_class”
						- For minerals:
						  - see “*mineral*_class”
						- For liquids:
						  - see “*liquid*_class”
						- For adsorbed species (molecules/radicals/ions/atoms):
						  - ‘*atomic adsorbed phase’*: natural or isotopic atomic species adsorbed on a solid, in its (micro)porosity or in its porous structure
						  - ‘*molecular adsorbed phase’*: natural or isotopic molecular sspecies adsorbed on a solid, in its (micro)porosity or in its porous structure

						- For clusters: - '*atomic clusters'*: pure or mixed atomic species (or any isotopic mixture) in clusters - '*molecular clusters'*: pure or mixed molecular species (or any isotopic mixture) in clusters - For gases: - '*atomic gas'*: pure or mixed atomic species (or any isotopic mixture) in gas phase - '*molecular gas'*: pure or mixed molecular species (or any isotopic mixture) in gas phase - Complex mixtures and others compounds: - '*complex mix'*: complex mixture of compounds too numerous, too intermixed or at a scale difficult to separate them - '*other'*: compounds which cannot be described by one of the above words (include some mixtures such as atomic+molecular clusters) (describe in "*constituent*_comments") - '*unknown'*: unknown compound *Note:* - These classes correspond to the classes defined in "solid", "mineral" and "liquid" fundamental constituents. See their respective "_class"
*constituent*_compound_type [*phase*_compound_type]	enum(text)	S0c/S0 [!_m]	Const	F	--	Type of solid compound composing the constituent. It tells how the species are mixed at the molecular level OpenEnum: {elemental solid, elemental mineral, noble gas solid, carbon allotrope, organic molecular solid, organic mineral, inorganic molecular solid, clathrate, clathrate hydrate, hydrate, homopolymer, copolymer, molecular solid solution, solid molecular mixture, oxide, hydroxyde, oxide-hydroxide, non-oxide ceramic, antimonate, antimonite, arsenate, arsenite, borate, bromide, carbonate, chlorate, chloride, chlorite, chromate, cyanate, cyanide, fluoride, fulminate, halide, iodate, iodide, molybdate, nitrate, nitrite, perchlorate, phosphate, phosphite, selenate, selenide, selenite, sulfate, sulfide, sulfite, sulfosalt, tellurate, tellurite, tungstate, vanadate, vanadium oxysalt, organic salt, silicate, cyclosilicate, inosilicate, nesosilicate, phyllosilicate, sorosilicate, tectosilicate, metal, metallic alloy, semi-conductor, complex mineral mix,

solid oligomers, homopolymer, copolymer, Insoluble Organic Matter, Soluble Organic Matter, complex macromolecular mixture, complex organic-mineral mix, liquid, liquid solution, physically adsorbed phase, chemically adsorbed phase, interlayer phase, clusters, gas, gas mixture, other compound, other complex mix, unknown, …}

Definitions:

- For molecular, ionic, covalent network and metallic solids:
  - see "*solid*_compound_type"
- For minerals:
  - see "*mineral*_compound_type"
  - '*complex mineral mix'*: complex mixture of minerals too numerous, too intermixed or at a scale difficult to separate them
- For organic solids:
  - '*solid oligomers*': Solid of molecules made of a small number of monomer units, up to a few dozen.
  - '*homopolymer*' & '*copolymer*': see "*solid*_compound_type"
- For complex organic matters:
  - '*Insoluble Organic Matter'* (IOM): insoluble mixture of macromolecules composed of various and non-repeating structural units.
  - '*Soluble Organic Matter'* (SOM): soluble mixture of macromolecules composed of various and non-repeating structural units.
  - '*complex macromolecular mixture'* (IOM+SOM): mixture of soluble and insoluble macromolecules composed of various and non-repeating structural units.
- For complex organic+mineral matter:
  - '*complex organic-mineral mix'*: complex mixture of organic solids/matter and minerals too numerous, too intermixed or at a scale difficult to separate them
- For liquids
  - see "*liquid*_compound_type"
- For adsorbed molecular or atomic species (molecules/radicals/ions/atoms):
  - '*physically adsorbed phase'*: natural or isotopic atomic or molecular species physically adsorbed on a solid, in its (micro)porosity or in its porous structure (as in zeolites).

- ‘*chemically adsorbed phase’*: natural or isotopic atomic or molecular sspecies chemically adsorbed on a solid, in its (micro)porosity or in its porous structure

- For interlayer atomic species (atoms/ions) or molecular species (molecules/radicals/ions) in solids:
  - ‘*interlayer phase’*: natural or isotopic atomic or molecular species adsorbed in the interlayer space of a solid

    Note: ‘interlayer phase’ is only for atomic and molecular species not part of the solid structure.

    Ex: mostly clay minerals
- For atomic and molecular clusters:
  - ‘*clusters’*: Van der Walls aggregates of 2 to 100 000 atoms or molecules
- For gases:
  - ‘*gas’*: pure gas
  - ‘*gas mixture’*: mixed species (or any non-terrestrial isotopic mixture) in gas phase
- Others compounds and complex mixtures
  - ‘*other compound’*: compounds which cannot be described by one of the above words (include some mixtures such as atomic+molecular clusters) (describe in “*constituent*_comments”)
  - ‘*other complex mix’*: complex mixture of compounds too numerous, too intermixed or at a scale difficult to separate them (describe in “*constituent*_comments”)
  - ‘*unknown’*: unknown compound

Constituent chemical composition

*constituent*_formula [*phase*_formula]	varchar(255)	U [m]	Const	F	--	Developed structural (empirical) chemical formula of the constituent *Syntax:* Latex format *Notations:* see “*solid*_formula” *Note:* of use only when not using a fundamental species

*constituent*_chemical_formula [*phase*_chemical_formula]	CS-varchar(255)	S1 [m]	Const	F	--	Developed global chemical and structural formula of the constituent *Notations:* see "*solid*_chemical_formula" *Notes:* - of use only when not using a fundamental species - contain ionic information.
*constituent*_hydration [*phase*_hydration]	boolean	S0c/S2 [m]	Const	F	--	Flag telling if the constituent contains structural H_2O BoolEnum: {yes, no} or {true, false}
*constituent*_hydration_number [*phase*_hydration_number]	varchar(255)	S2c/S3 [!o_m]	Const	F	*var.*	Number or amount (or range) of H_2O in the constituent structure *Condition*: mandatory when "*constituent*_hydration" = 'true' • *Unit:* can be expressed in any unit, to be specified *Notes:* - exclude adsorbed water - put 'n' if there is hydration but the number is unknown *Ex:* '2', '4 - 6', '0 - 2', 'n', '4.5 mol/kg', 25 g/kg, …
constituent_chemical_functions	***List [L2]***	[£]				£: List of different chemical functions present in the constituent, except those already in the molecular "species" *Condition*: compulsory if exist
*constituent*_chemical_function_uid [*] [*phase*_chemical_function_uid]	varchar(255)	S2c [!o_m]	Const ChemFL2	F	--	Link to the existing UID of the chemical function present in the constituent *Condition*: mandatory if bloc used: *"constituent*_chemical_function_number" ≠ Ø *Note*: If the constituent is described in terms of molecular species with "*constituent*_specie_uid" their chemical functions (already implicitely taken into account) should not be listed here
*constituent*_chemical_function_number [+]	varchar(255)	S2c [m]	Const	F	*var.*	Amount or range of amount of the chemical function present in the constituent

[*phase*_chemical_function_number]			L2				• *Unit:* can be expressed in any unit, to be specified *Ex*: 10^{18}mol/mol ➔ Calculated: ➔ For solids described with molecular species ("*constituent*_specie_family"={molecule, chemical function}): for each 'function_i' of all 'molecule_j' or ''function_j' of "*constituent*_specie_uid" excepted those with "*constituent*_specie_relevance" = {impurity, unknown} it is: *Condition*: when all "*constituent*_specie_number_min" ≠ {Ø, NULL} ⇨ *See "solid*_chemical_function_number" *Condition*: else when all "*constituent*_specie_mole_fraction" ≠ {Ø, NULL} ⇨ *See "liquid*_chemical_function_number" *Notes*: - in constituent when the amount of species is given in mole, mass or mass fraction (not in number or mole fraction) and when it cannot be converted in mole fraction, it is no possible to determine a mole fraction of functions from the species present in the constituent. - in such a case only the type of function will be listed, without number
constituent_chemical_bonds	***List [L3]***	[£]					£: Chemical bond(s) of the constituent, except those already in the molecular "species" *Condition*: compulsory if exist
*constituent*_chemical_bond_uid [*] [*phase*_chemical_bond_uid]	varchar(255)	S2c/S1i [!o_m]	Const ChemB L3	F	--		Link to the existing UID of the chemical bonds of the constituent *Condition*: mandatory if bloc used: *"constituent*_chemical_bond_number" ≠ Ø *Note*: – If you describe the constituent in terms of molecular species in "*constituent*_specie_uid" you should not list here their chemical functions (already implicitely taken into account) – these bonds are only the molecular bonds between atoms

– for isotopic substituted constituent made of at least one purely isotopic atom the bonds are the isotopic bonds using the pure isotopic atom(s) and only the main isotope of the others

*constituent*_chemical_bond_number [+] [*phase*_chemical_bond_number]	varchar(255)	S2c [m]	Const L3	F	*var.*	Amount, or minimum amount, of this bond composing the constituent • *Unit:* can be expressed in any unit, to be specified *Note:* this number can be an absolute one (tell relative to what: per molecule, unit mole, unit mass, …) or a relative value (ratio, fraction, …) ➔ Calculation of 'n_min(bond_i)' for display: ➔ For constituents described with molecular species ("*constituent*_specie_family"={molecule, chemical function}): for each 'bond_i' of all 'specie_j' of "*constituent*_specie_uid" excepted those with "*constituent*_specie_relevance" = {impurity, unknown} it is: *Condition*: when all "*constituent*_specie_number_min" ≠ {Ø, NULL} ⇨ *See "solid*_chemical_bond_number" *Condition*: else when all "*constituent*_specie_mole_fraction" ≠ {Ø, NULL} ⇨ *See "liquid*_chemical_bond_number" *Condition*: else no calculation *Notes*: - "*constituent*_specie_mole_fraction" will be calculated when all "*constituent*_specie_mole" are given, so "*constituent*_chemical_bond_number" will be also calculated in this case

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Constituent molecular and atomic composition

*constituent*_elemental_formula [-xml] [*phase*_elemental_formula]	CS-varchar(255)	S0c/S1 [!o_c]	Const	F	--	Empirical elemental formula of the constituent ➔ Calculated: ➔ For solids described with atomic or molecular species for each 'atom_i' of "*constituent*_specie_uid" (atom) or of "*molecule*_atom_uid" of

all ‘molecule_j’ of “*constituent*_specie_uid” excepted those with “*constituent*_specie_relevance” = {impurity, unknown} it is:

Condition: when all “*constituent*_specie_number_min” ≠ {Ø, NULL}

- n(atom_i) = $\sum_{specie_j}$ (“_specie_number_min(specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)

Condition: when also a “*constituent*_specie_number_max” ≠ {Ø, NULL}

- n_min(atom_i) = $\sum_{specie_j}$ ((“_specie_number_min(specie_j) * “*specie*_atom_number(specie_j,atom_i)”)
- n_max(atom_i) = $\sum_{specie_j}$ ((“_specie_number_max(specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)

  with “*specie*_atom_number(atom_i)” = “*molecule*_atom_number(atom_i)” for a molecule and “*specie*_atom_number(atom_i)” = 1 for an atom or element
- n_min or n_max(atom_i) is set to ‘n’ when one instance of the element (element or molecule containing this element) has “*constituent*_specie_number_min/_max” = ‘n’

Note: for each type of atom it is the sum over all the molecules of the constituent of the product of the number of molecules in the constituent by the number of this atom in the molecule, plus possibly the number of elements or atoms of this type not included in molecules. If there are isotopes the isotopic atoms are counted separately

Condition: else when all “*constituent*_specie_mole_fraction” ≠ {Ø, NULL}

- n(atom_i) = [$\sum_{specie_j}$ (“_specie_mole_fraction (specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)] / $\sum_{atom_i}$ [$\sum_{specie_j}$ (“_specie_mole_fraction (specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)]

Condition: when also a “*constituent*_specie_mole_fraction_error” ≠ {Ø, NULL}

- n_min(atom_i) = [$\sum_{specie_j}$ ((“_specie_mole_fraction (specie_j)” - “_specie_mole_fraction_error (specie_j)”) *

“*specie*_atom_number(specie_j,atom_i)”)] / $\sum_{atom_i}$ [$\sum_{specie_j}$ (“_specie_mole_fraction (specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)]

- n_max(atom_i) = [$\sum_{specie_j}$ ((“_specie_mole_fraction (specie_j)” + “_specie_mole_fraction_error (specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”)] / $\sum_{atom_i}$ [$\sum_{specie_j}$ (“_specie_mole_fraction (specie_j)” * “*specie*_atom_number(specie_j,atom_i)”)]

Condition: else when all “*constituent*_specie_mass_fraction” ≠ {Ø, NULL}

- n(atom_i) = [$\sum_{specie_j}$ ((“_specie_mass_fraction (specie_j)” / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”)] / $\sum_{atom_i}$ [$\sum_{specie_j}$ ((“_specie_mass_fraction (specie_j)” / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”)]

  with “*specie*_molar_mass(specie_j)” = “*molecule*_molar_mass(specie_j)” for a molecule and “*specie*_molar_mass(specie_j)” = “*atom*_molar_mass(specie_j)” for an atom or element

Condition: when also a “*constituent*_specie_mass_fraction_error” ≠ {Ø, NULL}

- n_min(atom_i) = [$\sum_{specie_j}$ (((“_specie_mass_fraction (specie_j)” - “_specie_mass_fraction_error (specie_j)”) / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”))] / $\sum_{atom_i}$ [$\sum_{specie_j}$ ((“_specie_mass_fraction (specie_j)” / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”)]
- n_max(atom_i) = [$\sum_{specie_j}$ (((“_specie_mass_fraction (specie_j)” + “_specie_mass_fraction_error (specie_j)”) / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”))] / $\sum_{atom_i}$ [$\sum_{specie_j}$ (“_specie_mass_fraction (specie_j)” / “*specie*_molar_mass(specie_j)”) * “*specie*_atom_number(specie_j,atom_i)”)]

Notations:

- suite of the atomic elements followed by the total number (possibly decimal) or range of their occurrence. Isotope can be added before each atom. This atom information is separated by a 'space'
  Ex: 'C2.5 O0.4 N0.7 H7.3',
  Ex: '13C0.3-0.4 12C0.9 16O1.5 17O0.001 18O2.3'
- put ions between parentheses
  Ex: '(Fe2+) (Fe3+)2 O4'
- when there is only one occurrence of the atom the '1' should be omitted
- for variable elements in solid solutions: need to put the atom between brackets ( ) followed by an occurrence of '_atom_number_min'-'_atom_number_max'
  Ex: '(N)1.9-2 (C)0-0.05 (H)0-0.2' for CH4 in solution in N2
  Ex: '(Fe)0.1-1 (Mg)0-0.9 Si O4'
- the maximum is set to 'n' when one instance of the element (element or molecule containing this element) has "*solid*_specie_number_max" = 'n'
  Ex: 'Cn Hn' for polyethylene
- for solids with non-natural isotopic abundance (isotopic substitution), non-natural atoms will have their atomic mass preceding the atom symbol. D can be used for 2H.
  Ex: 'Ca2 (Fe2+)3 Al4 28Si1.4 30Si4.6 O24 H1.4 D0.6'

Notes: use only ascii symbols

*constituent*_isotope_mixture_type [*phase*_isotope_mixture_type]	enum(text)	S1 [!!_m]	Const	F	--	Type of isotopic mixture of the constituent Enum: {pure isotope, partly substituted, terrestrial abundance, specific abundance, unknown} *Definitions:* – '*pure isotope*': when all molecules/atoms of the constituent are pure isotopes (only one isotopic species for each type of molecule or atom) *Ex:* $^{14}ND_3$:$D_2{}^{16}O$ – '*partly substituted*': when at least one, but not all, molecule/atom of the

						constituent is fully (i.e. pure isotopic species) or partly substituted *Ex:* NH_3:$D_2{}^{16}O$, ND_3:$D_2{}^{16}O$, … – '*terrestrial abundance*': when all molecules/atoms of the constituent are in terrestrial isotopic abundance – '*specific abundance*': when at least one molecule/atom of the constituent has a specific isotopic abundance *Ex:* (50% NH_3 + 50% ND_3):H2O *Note*: define the effective type of isotopic mixture of the constituent
*constituent*_species_mole_fraction_unit	enum(text) [od_m]	U	Const	F	--	Unit for the molar fraction or concentration of the species in the liquid constituent Enum: {mol/mol, mol/g, mol/kg, mol/l} *Default*: 'mol/mol' *Constraint:* only when "*constituent*_phase_type" = {amorphous, glassy, mesophase, supercooled liquid, liquid, supercritical fluid} *Note*: - the 'mol/g', 'mol/kg' and 'mol/l' units are used only in liquid solutions and allow to express the concentration of solutes relative to a solvent - in liquid solutions, the solvent mole fraction should be expressed in the same unit as the solutes - used only for "*constituent*_specie_mole_fraction" and "*constituent*_specie_mole_fraction_error"
constituent_species	***List [L4]*** [!]					£: List of different species present in the constituent *Notes:* – For pure isotopes (atom, molecule), for natural or synthetic isotopic mixtures in terrestrial abundance (idem) or for substituted molecular mixtures (molecule), i.e. with one pure isotopic atom and the others in terrestrial abundance: it is necessary to link to the single corresponding fundamental species existing in the database (if not present: request it) using "*constituent*_specie_atom_uid/_molecule_uid" – For non-standard natural or synthetic isotopic mixtures it is necessary

						to build your own mixture using several fundamental pure isotopic species (at least the most abundant), i.e. several times this '*constituent*_specie' structure.
*constituent*_specie_family	enum(text)	S1 [!!_m]	Const L4	F	--	General family of the species composing the constituent. Enum: {atom, element, molecule, chemical function, unknown} *Definitions:* - '*atom*': atoms and ions - '*element*': atoms and ions as part of molecules, solids, minerals or liquids. - '*molecule*': molecules, molecular ions and radicals - '*chemical function'*: only for anionic radicals (as in minerals) - '*unknown*': for complex organic or mineral matters with unknown composition, neither in terms of molecular, nor atomic species. *Note*: 'unknown' is used to overpass the absolute mandatory and the following mandatories. *Notes:* – complex constituents of complex organic or mineral matters mostly refer to the "*atom*" table to describe their elemental composition ('element')
*constituent*_specie_uid [*]	varchar(255)	S0c/S1/ S1i [!!o_m]	Const Atom Molec L4	F	--	Link to the existing UID of the atomic or molecular species composing the constituent *Condition:* absolute mandatory when "*constituent*_specie_family" = {atom, element, molecule, chemical function} *Notes:* – will be "*atom*_uid" (atomic, element) or "*molecule*_uid" depending on "*constituent*_specie_family". – for complex solids (organic or mineral matters, …) this value refers to '*atom*_uid' – complex constituents can also use the"*constituent_chemical_functions*" bloc to describe in parallel (or solely) their functional groups ('chemical function') and/or "*constituent_chemical_bonds*" bloc to

describe their bonds (‘chemical bond’), if known.

Species abundance in constituent

*constituent*_specie_mole [+]	float	U [!o_m]	Const L4	F	*mol*	Number of moles of the species in the constituent *Condition #1:* mandatory for one of “*constituent*_specie_mole”, “_mole_fraction”, “_mass”, “_mass_fraction”, or “_number_min” AND *Condition #2:* when “*constituent*_specie_family” = {atom, element, molecule} • *Units*: in ‘mol’ *Notes*: - generally available only for fully atomic or molecular constituents. - for adsorbed and interlayer species, it is the number of moles of the species in the adsorbed or interlayer phase (not including the adsorbat, which belong to another material/constituent)
*constituent*_specie_mole_error [+]	float	U [!o_m]	Const L4	F	*mol*	Uncertainty on number of moles of the species in the constituent *Condition:* mandatory when “*constituent*_specie_mole” ≠ {Ø, NULL} *Units*: see “*constituent*_specie_mole”
*constituent*_specie_mole_fraction [+]	float	U [!o_mc]	Const L4	F	*var*	Mole fraction or concentration of the species in the constituent *Condition #1:* mandatory for one of “*constituent*_specie_mole”, “_mole_fraction”, “_mass”, “_mass_fraction”, or “_number_min” AND *Condition #2:* when “*constituent*_specie_family” = {atom, element, molecule} *Condition*: calculated only when all “*constituent*_specie_mole” ≠ {Ø, NULL} ➔ calculated from “*constituent*_specie_mole” when available for all species of the constituent ⇨ “_specie_mole_fraction(specie_j)” = “_specie_mole(specie_j)” / Σi (“_specie_mole(specie_i)”) or

						Condition: calculated only when all "*constituent*_specie_number_min" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_number_min" when available for all species of the constituent ⇨ "_specie_mole_fraction(specie_j)" = "_specie_number_min(specie_j)" / Σi ("_specie_number_min(specie_i)") • *Units*: in "*constituent*_species_mole_fraction_unit" *Notes*: - value between 0 and 1 - generally available only for fully atomic or molecular constituents. - for adsorbed and interlayer species, it is the mole fraction of the species in the adsorbed or interlayer phase (not including the adsorbat, which belong to another material/constituent)
*constituent*_specie_mole_fraction_error [+]	float	U [!o_m]	Const L4	F	*var*	Absolute uncertainty on mole fraction or concentration of the species in the constituent *Condition:* only when "*constituent*_specie_mole_fraction" ≠ {Ø, NULL} *Condition*: calculated only when all "*constituent*_specie_mole" and "*constituent*_specie_mole_error" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mole_error" ⇨ "_specie_mole_fraction_error(specie_j)" = "_specie_mole_fraction(specie_j)" * ["_mole_error(specie_j)" / "_mole(specie_j)" + Σi ("_mole_error(specie_i)") / Σi ("_mole(specie_i)")] *Condition*: calculated only when all "*constituent*_specie_number_min" and "*constituent*_specie_number_max" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_number_min/_max" ⇨ "_specie_mole_fraction_error(specie_j)" = "_specie_mole_fraction(specie_j)" * [("_number_max(specie_j)" - "_number_min(specie_j)") / ("_number_max(specie_j)" + "_number_min(specie_j)") + Σi ("_number_max(specie_j)" -

						"_number_min(specie_j)") / Σi ("_number_max(specie_j)" + "_number_min(specie_j)")] • *Units*: see "*constituent*_species_mole_fraction"
*constituent*_specie_mass [+]	float	U [!o_mc]	Const L4	F	g	Mass of the species in the constituent *Condition #1:* mandatory for one of "*constituent*_specie_mole", "_mole_fraction", "_mass", "_mass_fraction", or "_number_min" AND *Condition #2:* when "*constituent*_specie_family" = {atom, element, molecule} *Condition*: calculated only when "*constituent*_specie_mole" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mole" when it is provided (need the molar masses => in "molecule and atom species" tables: "*molecule/atom*_molar_mass") ⇨ "_specie_mass(specie_j)" = "_specie_mole(specie_j)" * "*specie*_molar_mass(specie_j)" with "*specie*_molar_mass(specie_j)" = "*molecule*_molar_mass(specie_j)" for a molecule and "*specie*_molar_mass(specie_j)" = "*atom*_molar_mass(specie_j)" for an atom or element *Notes:* - for adsorbed and interlayer species, it is the mass of the species in the adsorbed or interlayer phase (not including the adsorbat, which belong to another material/constituent)
*constituent*_specie_mass_error [+]	float	U [!o_mc]	Const L4	F	g	Absolute uncertainty on mass of the species in the constituent *Condition:* only when "*constituent*_specie_mass" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mole_error" when it is provided ⇨ "_specie_mass_error(specie_j)" = "_specie_mole_error(specie_j)" * "*specie*_molar_mass(specie_j)" *Note*: see "*constituent*_specie_mass"

*constituent*_specie_mass_fraction [+]	float	U [!o_mc]	Const L4	F	*no*	Mass fraction of the species in the constituent *Condition #1:* mandatory for one of "*constituent*_specie_mole", "_mole_fraction", "_mass", "_mass_fraction", or "_number_min" AND *Condition #2:* when "*constituent*_specie_family" = {atom, element, molecule} *Condition*: calculated only when all "*constituent*_specie_mass" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mass" when available for all species of the constituent ⇨ "_specie_mass_fraction(specie_j)" = "_specie_mass(specie_j)" / Σi ("_specie_mass(specie_i)") *Condition*: calculated only when all "*constituent*_specie_mole_fraction" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mole_fraction" when provided for all species of the constituent (need the molar masses of all species in the constituent => in "*molecule* and *atom species*" tables: "*molecule/atom*_molar_mass" of each "*constituent*_specie_uid") ⇨ "_specie_mass_fraction(specie_j)" = "_specie_mole_fraction(specie_j)" * "*specie*_molar_mass(specie_j) / Σi ("_specie_mole_fraction(specie_i)" * "*specie*_molar_mass(specie_i)") with "*specie*_molar_mass(specie_j)" = "*molecule*_molar_mass(specie_j)" for a molecule and "*specie*_molar_mass(specie_j)" = "*atom*_molar_mass(specie_j)" for an atom or element ➔ not calculated when "*constituent*_species_mole_fraction_unit" = {mol/g, mol/kg, mol/l} *Note*: - the calculation with "*constituent*_specie_mole_fraction_unit" = {mol/g, mol/kg, mol/l} is not made as it is not useful - when "*constituent*_specie_number_min" is provided for all species of the constituent, then the "*constituent*_specie_mole_fraction" are first calculated and then the "*constituent*_specie_mass_fraction" are

						calculated from the "*constituent*_specie_mole_fraction" *Notes:* - value between 0 and 1 - for adsorbed and interlayer species, it is the mass fraction of the species in the adsorbed or interlayer phase (not including the adsorbat, which belong to another material/constituent) - a warning will be issued during import if the mass fraction of one species is not present or cannot be calculated
*constituent*_specie_mass_fraction_error [+]	float	U [!o_mc]	Const L4	F	*no*	Absolute uncertainty on mass fraction of the species in the constituent *Condition:* only when "*constituent*_specie_mass_fraction" ≠ {Ø, NULL} *Condition*: calculated only when all "*constituent*_specie_mole_fraction" and "*constituent*_specie_mole_fraction_error" ≠ {Ø, NULL} ➔ calculated from "*constituent*_specie_mole_fraction_error" for atomic and molecular constituents ⇨ "_specie_mass_fraction_error(specie_j)" = "_specie_mass_fraction(specie_j)" * ["_mole_fraction_error(specie_j)" / "_mole_fraction(specie_j)" + Σi ("_mole_fraction_error(specie_i)") / Σi ("_mole_fraction(specie_i)")] ➔ not calculated when "*constituent*_species_mole_fraction_unit" = {mol/g, mol/kg, mol/l}
*constituent*_specie_number_min [+]	float or 'n'	S2 [!o_m]	Const L4	F	--	Nominal or minimum total number of the molecular/atomic species in the constituent formula *Condition #1:* mandatory for one of "*constituent*_specie_mole", "_mole_fraction", "_mass", "_mass_fraction", or "_number_min" AND *Condition #2:* when "*constituent*_specie_family" = {atom, element, molecule} *Notes*: - generally available only for fully atomic or molecular constituents. - If only a range of number is known then give a minimum value here and a maximum value in "*constituent*_specie_number_max"

						- If the number is known within an uncertainty (±) then "number_min" = 'nominal number' – 'error' - for adsorbed and interlayer species, it is the number of moles of the species in the adsorbed or interlayer phase (not including the adsorbat, which belong to another material/constituent)
*constituent*_specie_number_max [+]	float or 'n'	S2 [m]	Const L4	F	--	Maximum total number of the molecular/atomic species in the constituent formula *Notes*: - do not fill for well defined constituent - If the number is known within an uncertainty (±) then "number_max" = 'nominal number' + 'error' - If undefined then put 'n'

Species state in constituent

*constituent*_specie_state	enum(text)	S1 [!_m]	Const L4	F	--	State of the species inside the compound composing the constituent OpenEnum: {constituent element, constituent cation, constituent anion, constituent mer, constituent molecular, anionic radical, pure, mixed, matrix, monomers, dimers, multimers, solute, solvent, liquid solution, solid solution, clathrate network, clathrate guest, hydration, hydrated, in complex, physically adsorbed, chemically adsorbed, interlayer physically adsorbed, other, unknown, …} *Definitions:* - For complex compounds, and for atoms in minerals, and covalent and metallic compounds which can only be described by elemental composition: - '*constituent element*': for elements (neutral atoms) constituting the constituent, i.e. for elemental composition - '*constituent cation'*: for cations (ions or molecular ions) constituting the constituent - '*constituent anion'*: for anions (ions or molecular ions) constituting the constituent - '*constituent mer'*: mer radical as basic building blocks of polymers - 'con*stituent molecular'*: molecule as building block of a solid structure

or of a larger molecule. Did not include the independent molecules in molecular solids (see ‘pure’, ‘mixed’, ‘matrix’)

- ‘anionic radical’: for anions constituting the constituent (mainly for natural and synthetic minerals)
- ‘*pure’*^: only one atomic species forms the compound (also gas and liquid)

- For molecular compounds (also with radicals/ions: *) and in some cases (^) for ions in ionic compounds:
  - ‘*pure’*^: only one molecular species forms the compound (also gas and liquid)
  - ‘*mixed’**^: more than one type of molecular/atomic species form the compound but the species state cannot be described more specifically with one of the next attributes (also gas, liquid and clusters)
  - ‘*matrix’*^: the species largely dominates the solid compound (mole fraction > 99%)
  - ‘*monomers’**^: the molecular species is fully isolated in minor abundance in the compound (generally when mole fraction < 0.1 %), or in clusters. Also used for precursor monomers of polymers
  - ‘*dimers’**^: the molecular species occurs as isolated pairs of species (generally when mole fraction < 1 %), or in clusters.
  - ‘*multimers’**^: isolated small group of molecular species and with limited size: 3 to 5 monomers (generally when mole fraction < 5 %), or in clusters.

    Note: the “ cases above can be special cases of ‘solute’
  - ‘*solute’*^: molecular/atomic species diluted in a liquid or solid solution (or atom in alloy)

    Note: in solid solutions the solute species can be in substitutional or interstitial sites of the solvent crystal structure
  - ‘*solvent’*^: molecular/atomic species that dilute the solute in a liquid or solid solution (or main element of the alloy)

    Note: in case of complete miscibility (similar crystallographic structures) it is sometimes difficult to define who is the solvent and who is the solute: so we will define a ‘solvent’ and its ‘solute(s)’ only when a mole fraction is < 0.1, and use ‘solid solution’ for the intermediate cases.

- *'liquid solution'*: for liquid solutions when mole fractions is 0.1 < f < 0.9 (solute ~ solvent).
- *'solid solution'*: for mineral or solid solutions when mole fractions is 0.1 < f < 0.9 (solute ~ solvent).
- '*clathrate network'*: host molecule forming the clathrate structure (*Ex:* H_2O for clathrate hydrate)
- '*clathrate guest'*: guest molecule occupying the cages of the clathrate structure
- '*hydration'*: H_2O molecules in solid stoichiometric hydrate
- '*hydrated'**^: species that form with water a solid stoichiometric hydrate

  Note: for liquids, depending on relative amounts and compound formed, H_2O can also be called the 'solvent'

- For molecular (molecules/radicals/ions) or atomic species (atoms/ions) adsorbed at the surface, in (micro)pores or in interlayer of the constituent:
  - '*physically adsorbed'*: physical adsorption at surface and in porosities (macro-, micro-)
  - '*chemically adsorbed'*: chemical adsorption at surface and in porosities (macro-, micro-)
  - '*interlayer physically adsorbed'*: physical adsorption in interlayer spaces of solids (mostly clay minerals)
- For complex organic matter, mineral mixtures and other complex mixtures:
  - '*in complex'*: for elements and chemical functions in complex organic matter.
  - '*unknown'*: unknown state of the species
- Others compounds
  - '*other'*: species state in a compound which cannot be described by one of the above words (describe in "*constituent*_specie_comments")

Note: This state depends on "*constituent*_compound_type" which gives the type of solid compound composing the constituent and tells how the species are mixed at the molecular level

*constituent*_specie_relevance	enum(text)	S1 [!!o_m L4	Const	F	--	Relevance of the species in the constituent Enum: {main, replacement, substituted, impurity, product, precursor,

		]					unknown} *Condition:* absolute mandatory when "*constituent*_specie_family" = {atom, element, molecule} *Definitions:* - '*main'*: essential molecular/atomic species constituting the nominal molecular/atomic composition of the constituent in the sample before the beginning of an experiment (and prior any processing of the sample) - '*replacement'*: common replacement atom not included in the nominal elemental formula of the contituent but present as replacement atoms, *Note*: mostly in solid solutions, … - *'substituted'*: used only for isotopic molecular/atomic species substituting the equivalent "natural molecule/atom" - *'impurity'*: molecular/atomic species not wanted in the nominal composition of the constituent but present in synthetic materials or others matters. - *'product'*: species produced in the constituent of a sample subjected to a processing during the experiment - *'precursor'*: precursor species used for synthetic material formation, or pre-processing of natural matters. *Note*: They are flagged 'precursor' only in the precursor material description. If some species remain in a constituent of the sample after formation they are thus flagged 'main' or 'impurity' in the sample description, depending if they are wanted or unwanted,. - *'unknown'*: if origin of the species is not clear: 'impurity' or 'product'? *Note*: species of complex constituents in synthetic samples are set as 'product' only if they are formed during the experiment.
*constituent*_specie_comments	blob		U [m]	Const L4	F	--	Additional information on the specie state, origin and composition in the constituent

*constituent*_composition_comments	blob	U [m]	Const	F	--	Additional information on the composition and formula of the constituent

Constituent state

*constituent*_phase_name	varchar(255)	S0c/S1 [m]	Const	F	--	Common name of the constituent phase. *Notes:* – name is not normalized but mostly crystal system as defined in the literature, and any information on crystal class, symbol, and spacegroup (Hermann-Mauguin symbol) – for constituents made of one mineral detailed crystallographic information is given in "mineral phase". Just give the crystal system. e.g.: 'alpha-cubic', 'beta-hexagonal', 'orthorhombic', … (mostly for crystalline phase types), 'high density amorphous', 'adsorbed on orthorhombic', …
*constituent*_phase_type	enum(text)	S1 [!_m]	Const	F	--	Type of phase of the constituent (solid, liquid, gas) Enum: {crystalline, semicrystalline, paracrystalline, disordered, quasi-amorphous, amorphous, glassy, mesophase, supercooled liquid, liquid, supercritical fluid, adsorbed, interlayer, adsorbed+interlayer, mono-multimer, cluster, gas, mixed, other, unknown} *Definitions:* - '*crystalline'*: with a well defined crystalline structure - '*semicrystalline'*: partially crystalline, with crystals embedded in an amorphous or glassy matrix - '*paracrystalline*': solid with short and medium range ordering in their lattice (similar to the liquid crystal phases) but lacking crystal-like long-range ordering at least in one direction. Ordering is the regularity in which atoms appear in a predictable lattice, as measured from one point. - *'disordered'*: solid with only irregular and/or local order, mostly for metamict and macromolecular solids - '*quasi-amorphous'*: nanocrystalline solids

- '*amorphous'*: solid lacking the long-range order characteristic of a crystal.
- '*glassy'*: amorphous solid that transforms into a liquid upon heating through the glass transition
- '*mesophase*': for liquid crystal': state of matter intermediate (partly ordered orientation) between solid (ordered position and orientation) and liquid (disordered)
- '*supercooled liquid*': liquid phase under the freezing point
- '*liquid'*: liquid phase
- '*supercritical fluid'*: material at a temperature and pressure above its critical point where distinct liquid and gas phase did not exist
- '*adsorbed'*: phase of adsorbed molecules, or films, at the surface or in pores (macro/meso/micro) of another material
- '*interlayer'*: phase of the interlayer molecular layer (generally H_2O) inside minerals (phylosilicates)
- '*adsorbed+interlayer'*: when it is not possible to distinguish the adsorbed and interlayer phases
- '*mono-multimer'*: Van der Walls aggregates up to 4 molecules
- '*cluster'*: Van der Walls aggregates of 5 to 100 000 molecules
- '*gas'*: gaseous phase
- '*mixed*': a mix of several of the above phase types
- '*other'*: when the phase type of the constituent cannot be described by one of above words (explain in "*constituent*_comments")
- '*unknown'*: when phase type of constituent is unknown

*constituent*_phase_comments [*constituent*_phase_comments]	blob	U [m]	Const	F	--	Any information on the constituent crystal structure (system, class, class symbol, ...) *Note:*

Constituent texture

*constituent*_crystal_size_unit [*sample/matter*_crystal_size_unit]	enum(text)	U [!o_m]	Const	F	--	Unit for the constituent crystal sizes (diameter) Enum: {nm, micron, mm, cm} *Condition:* compulsory when "*constituent*_crystal_size_median" OR

						"*constituent*_crystal_size_min" OR "*constituent*_crystal_size_max" has a value *Note DB:* all crystal sizes data will be stored in 'm' *Note:* used for "*constituent*_crystal_size_median/_width/_min/_max"
*constituent*_crystal_size_method [*constituent*_crystal_size_method]	varchar(255)	U [m]	Const	F	--	Description of the crystal size (min/max) definition, and of the method of determination of the crystal size distribution *Ex:* 'SEM microscope measurement of section'
constituent_crystal_sizes	***List [L6]***	[O]				£: Size distribution of the constituent crystals
*constituent*_crystal_size_median [*constituent*_crystal_size_median]	float	S3 [m]	Const L6	F	var.	Median size (diameter) of constituent crystals *Unit:* in "*constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*constituent*_crystal_size_unit" *Note*: mostly used when only one median size is known for the constituent crystals
*constituent*_crystal_size_width [*constituent*_crystal_size_width]	float	U [m]	Const L6	F	var.	Full width at half maximum of the size distribution (diameter) of constituent crystals *Unit:* in "*constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*constituent*_crystal_size_unit" *Note*: mostly used when only one median size and its distribution is known for the constituent crystals
*constituent*_crystal_size_min [*constituent*_crystal_size_min]	float	S3 [m]	Const L6	F	var.	Smallest size (diameter) of constituent crystals of this size range *Unit:* in "*constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*constituent*_crystal_size_unit"

*constituent*_crystal_size_max [*constituent*_crystal_size_max]	float	S3 [m]	Const L6	F	var.	Largest size (diameter) of constituent crystals of this size range *Unit:* in "*constituent*_crystal_size_unit" • converted in 'm' unit in the database but provided to user in "*constituent*_crystal_size_unit"
*constituent*_crystal_size_fraction [*constituent*_crystal_size_fraction]	float	U [m]	Const L6	F	*no*	Mass fraction of constituent crystals comprised between size min and size max (diameter) *Note:* value between 0 and 1
*constituent*_crystal_size_fraction_error [*constituent*_crystal_size_fraction_error]	float	U [m]	Const L6	F	*no*	Absolute uncertainty on the mass fraction of constituent crystals comprised between size min and size max (diameter)
*constituent*_crystal_size_shape [*constituent*_crystal_size_shape]	enum(text)	S2 [m]	Const L6	F	--	Dominant shape of the constituent crystals of this size range Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown} *Definitions: voir "material*_grain_size_shape*"*
*constituent*_crystal_size_distribution [*constituent*_crystal_size_distribution]	blob	U [m]	Const	F	--	Description and parameters of the size distribution of the constituent crystals *Note:* see "*material*_grain_size_distribution"
*constituent*_texture	enum(text)	S2 [m]	Const	F	--	Internal texture of the constituent crystals Enum: {monocrystalline, polycrystalline, cryptocrystalline, nanocrystalline, metamict, amorphous, glassy, polymeric, macromolecular, complex, liquid, adsorbed layer, cluster, gas, other, unknown} *Definitions:* - '*monocrystalline'*: single crystal or isolated crystals of the constituent

- '*polycrystalline'*: several adjacent crystals of the same constituent
- '*cryptocrystalline'*: crystalline structure with submicroscopic crystals (5nm-1µm?)
- '*nanocrystalline'*: quasi-crystalline (or quasi-amorphous) structure with nano crystallites (0.5-5 nm)
- '*metamict'*: disordered crystalline structure due to some external effects (irradiation, …)

  Ex: metamict structure of zircon minerals submitted to natural alpha radiation
- '*amorphous'*: texture of amorphous solids (without any long range order)
- '*glassy'*: vitreous texture of glassy solids
- '*polymeric'*: texture of polymers. Polymers may consist of both crystalline and amorphous regions, and are characterized by their degree of crystallinity.
- '*macromolecular'*: texture of macromolecular solids
- '*complex'*: complex texture or complex mixture of various textures
- '*liquid'*: for liquid
- '*adsorbed layer'*: for 'adsorbed' atoms or molecules at surface and in (micro)porosity and for mineral 'interlayers'
- '*cluster'*: for atomic and molecular aggregates
- '*gaseous'*: for gas
- '*other'*: when texture of constituent cannot be described by one of above words (describe in "*constituent*_comments")
- '*unknown'*: when texture of constituent is unknown

Notes:

- The compacity of a crystal is considered to be 'unity'. If it is not the case you can note the effective value in "*constituent*_crystal_comments"
- a compact layer or thin film of solid or a mineral slice, are considered here as "polycrystals"

Constituent properties

*constituent*_molar_mass [constituent_molar_mass]	varchar(255)	U [m]	Const	F	g/mol	Molar mass (value with uncertainty) of the constituent • provided in 'g/mol' unit *Notes:* ⇨ Molar mass is frequently called 'molecular weight' ⇨ a mole of solid is a mole of one 'chemical formula unit'. ⇨ Its molar mass is determined from its structural or molecular formula. *ex:* '161.7', '160 +/- 20'
*constituent*_density [constituent_density]	varchar(255)	U [m]	Const	F	g/cm3	Density (value with uncertainty) of the constituent • provided in 'g/cm^3' unit *ex:* '2.37', '2.45 +/- 0.15'

Constituent optical properties

*constituent*_refringence [constituent_refringence]	varchar(255)	U [m]	Const	F	--	Any information on the refringence of the constituent: Note: it can be the type, sign, birefringence, dispersion, ... of the constituent *Ex:* 'isotropic solid'
*constituent*_refraction_index_n [constituent_refraction_index_n]	varchar(255)	U [m]	Const	F	--	Refraction index(es), n, (value or range) of the constituent *Note:* precise the type if not isotropic, and at which wavelength the refraction index is measured *Ex:* '1.125 at 535 nm', '$n_{/alpha} = 1.563 and $n_{/beta} = 1.630 at 636nm'
*constituent*_true_color [constituent_true_color]	varchar(255)	S2 [m]	Const	F	--	Color of the constituent *Note:* *Ex:* 'pale pinkish - green'
*constituent*_diaphaneity [constituent_diaphaneity]	enum(text)	S2 [m]	Const	F	--	Capacity of the constituent to transmit light

						Enum: {transparent, transparent to translucent, transparent to subtranslucent, transparent to opaque, translucent, translucent to subtranslucent, translucent to opaque, subtranslucent to opaque, opaque, various, unknown} *Definitions*: see "*mineral*_diaphaneity"
*constituent*_luster [constituent_luster]	enum(text)	S2 [m]	Const	F	--	Description of how and how much the surface of the constituent reflects light. Enum: {metallic, submetallic, waxy, vitreous, pearly, silky, greasy, resinous, adamantine, earthy, various, unknown} *Definitions*: see "*mineral*_luster"
*constituent*_comments	blob	U [m]	Const	F	--	Additional information on constituent state and compound organization, in particular for coating of grains: coating thickness, phase, and texture

10.9 Precursor Materials

Root of the table: ***precursor_material***

Data type: in 'Sample'

Note: refer to the "*material*" table but with "*material*_is_precursor" = 'true'

Condition: description of precursor materials is optional (can be also simply described with (short) text in the relevant "*processing*") but strongly recommended.

Note: Precursor materials which are not matter(s) are defined here through the "material(s)/constituent(s)/specie(s)" structure. They are used in "processing" through links with their "*precursor_material*_uid". Precursors which are "*matters*" are directly linked in "*processing*".
Their mixing and processing step(s) up to the post-formation processing of the sample before the start of the experiment are described in "*processings*".

Key-word	Type	Level	Table	Exp	Unit	Description
*precursor_material*_index [**][-xml]	int(10)	B [o!!_g]	PreMater L1	F	--	Automatic random but unique number (ID) given to new precursor material used to create the 'sample materials' *Note:* replace *"material*_index" in the material table *Note:* a precursor material is a "*simple material"* described through the material/constituent(s) and specie(s) structure. When the precursor material is a "*matter*" then no need to describe it here because it can be linked directly as a matter (with its "*matter*_uid") in the processings with "*matter*_processing_precursor_material_uid" *Note:* if a material or matter is not processed as a precursor material, or during layer deposition or in the formed layer or in the formed sample (before the start of the experiment), then it is not a '*precursor_material*' but a "*layer*_material" *Note xml:* in practice the description of the precursor material(s) are done directly under "*precursor_material*" in the xml *sample* structure, without ID link *Ex:* a CH4:N2 gas mixture is a single precursor material with a single gaseous

constituent with 2 molecular species, N2 and CH4.

10.10 Processing Table

Root of the table: ***processings***

Data type: in 'Sample'

Condition: optional, but useful at least for the layer(s) deposition step

Notes:

- ⇨ The formation of synthetic samples (or matters) is obtained from (one or) a mixture of precursor materials and/or matters that are subjected to at least one type of processing that affect its chemical composition, phase and/or texture. Natural samples may also be subjected to some pre-processing before the start of the experiment.
- ⇨ Physical and chemical processings can be applied to natural or synthetic precursor matters, to layer under deposition, to an already deposited layer, or to a whole sample (with its layer(s)) before the start of the experiment.
- ⇨ this bloc is like a 'cooking recipe'

Key-word	Type	Level	Table	Exp	Unit	Description
Sample/Matter processings		[O]				£: processings of precursor materials or matters to create the sample (or matter) *Condition:* Optional bloc - Mandatory active below when *"processings*_title" ≠ 'NULL'
*sample/matter_processings*_title	varchar(256)	U [(!!)do_m]	Proces	F	--	Title for the whole processing sequence of the material(s), matter(s) or sample(s). Default = 'NULL' *Condition:* (option trigger) the filling of this KW is 'absolute mandatory' when this optional bloc is used. It triggers the 'mandatory' status of several others KW in the optional bloc. *Ex:* 'irradiation of annealed sulfur produced in a previous experiment (2008/09/25)', 'annealing under vacuum at 100K of freshly deposited

amorphous H2O film'; ...

Sample/Matter processings: precursor sample(s), matter(s) or material(s)

All the material(s), matter(s) or sample(s) that have been used as initial precursors at any step of the processing sequence should be listed below. The precursor material(s) should be described with the "precursor materials" structure, while the precursor matter(s) and sample(s) should already exist in the database.

		[!o]				*Note:* the precursor sample(s), matter(s) or material(s) can be also simply described in *'sample/matter_processing*_process' of the first step.
sample/matter_processings_precursor_samples	***List [L1]***	[!o]				£: Precursor samples processed during the whole processings sequence
*sample/matter_processings*_precursor_sample_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Sampl L1	F	--	Link to the existing UID of the initial precursor sample(s) processed during the whole processings sequence *Note:* the precursor samples should be directly linked here (SAMPLE_, …) instead through their constituting materials **Matters: Not used in processings to create matters**
sample/matter_processings_precursor_matters	***List [L2]***	[!o]				£: Precursor matters processed during the whole processings sequence
*sample/matter_processings*_precursor_matter_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Matter L2	F	--	Link to the existing UID of the initial precursor matter(s) processed during the whole processings sequence *Note:* the precursor matters should be directly linked here (MATMIN_, …) instead through their constituting materials
sample/matter_processings_precursor_materials	***List [L3]***	[!o]				£: Precursor materials processed during the whole processings sequence
*sample/matter_processings*_precursor_material_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Mater L3	F	--	Link to the existing UID of the initial precursor material(s) processed during the whole processings sequence *Note:* all the initial precursor materials (except those included in precursor matters or sample) should be listed and described in *"precursor_materials"*

Sample/Matter processings: produced sample, matter or material(s)

The sample, the matter or all the material(s) that have been formed by the processing sequence should be listed below. The final sample or final matter of the processing sequence is the one described by the “Sample” or “Matter” structure, while the created material(s) should be some of their listed materials.

		[!o]				*Condition*: one of the following 3 blocs
*sample/matter_processings*_product_sample_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Sampl	F	--	Link to the existing UID of the final sample produced by the whole processings sequence *Condition (for Sample):* at least one sample (or material) mandatory when *“processings*_title” ≠ ‘NULL’ *Note:* Used only for final sample created with this processings sequence (not used for matter or when only part of the materials of a sample is created by this processing sequence) **Matters: Not used in processings to create matters**
sample/matter_processings_product_matter_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Mater	F	--	Link to the existing UID of the final matter produced by the whole processings sequence *Condition (for Matter):* at least one matter (or material) mandatory when *“processings*_title” ≠ ‘NULL’ *Note:* **not used in processings to create samples** **Matters:** Used only for final matter created with this processings sequence or when only part of the materials of a matter is created by this processing sequence)
sample/matter_processings_product_materials	***List [L4]***					£: Final materials produced by the whole processings sequence
*sample/matter_processings*_product_material_uid [*]	varchar(255)	U/S1i [!o_m]	Proces Mater L4	F	--	Link to the existing UID of final sample or matter material(s) produced by the whole processings sequence *Condition (for Sample):* at least one material (or sample) mandatory when *“processings*_title” ≠ ‘NULL’ *Condition (for Matter):* at least one material (or matter) mandatory when

*“processings_*title” ≠ ‘NULL’

Notes:

- Used when only part of the materials of a final sample or matter are created with this processings sequence
- When a whole final matter is produced by the processings sequence “*processings*_product_matter_uid” should be given instead of listing here all its“*matter*_materials”

When a whole final sample is produced by the processings sequence “*processings*_product_sample_uid” should be given instead of listing here all its“*sample*_materials”

Sample/Matter processings: steps

sample/matter_processing_steps	***List [L5]***	[!!o]				£: processing steps
*sample/matter_processing*_step_order	int(255)	U [!!o_m]	Proces L5	F	--	Order of occurrence of the processing step *Condition:* absolute mandatory when *“processings*_title” ≠ ‘NULL’
*sample/matter_processing*_chronology [-: for Matter]	enum(text)	U [!!o_m]	Proces L5	F	--	Chronology of the processing step Enum: {before layer formation, during layer formation, after layer formation, after sample formation, on parent sample} *Condition:* absolute mandatory when *“processings*_title” ≠ ‘NULL’ *Note:* only for Sample (not useful for Matter) *Definitions:* These processing steps concern processings performed either: - ‘*before layer formation’*: processing of precursor materials before formation of the layer of the sample (n steps) - ‘*during layer formation’*: processing of precursor materials or of layer during formation of the layer of a sample (mostly 1 step) - ‘*after layer formation’*: processing of layer after its complete deposition but before formation of the next layer of a sample (n steps) - ‘*after sample formation’*: on the whole sample after last layer

formation (before start of any experiment)

- '*on parent sample'*: processings of a alredy exisiting parent sample. This parent sample is given in *"processings*_precursor_sample_uid" and can also be given in *"sample*_parent_sample_uid".

Notes for Sample:

- Order: first the processings of the precursor materials ('before layer formation'), then formation of the layer ('during layer formation'), and then processing of the formed layer ('after layer formation'), and processing of the formed sample ('after sample formation'), if any of each type.
- Processings of a parent sample can describe either the processings on the sample before a new experiment and/or the processing which occurred during the last experiment (described for each spectrum in the previous experiment with "*sample*_temperature_xxx", "_pressure_xxx", "_stress_xxx", "_fluid_xxx", or "_irradiation_xxx")
- The layer(s) formation step(s) can be described in full details using this "*processing*s" table. But alternatively the formation conditions (temperature, pressure, rate and mode of layer formation) can also be described in a synthetic way only with "*layer*_formation_temperature", "_pressure", "_rate" and "_mode" keywords.

Matters: Not used in processings to create matters

*sample/matter_processing*_date	date	P/U [m]	Proces L5	F	YYYY-MM-DD	Date of the processing step

Sample/Matter processings: processes and conditions

sample/matter_processing_types	***List [L6]***	[!o]				£: Types of processing steps of the material(s), matter(s) or sample(s)
*sample/matter_processing*_type	enum(text)	S [!o_m]	Proces L5	F	--	Type(s) of processing step of the initial precursor material(s), matter(s) or sample(s), of produced intermediate material(s), of a sample layer, or of the full sample before start of the experiment.

			L6			Enum: {no, mixing, layer formation, thermal, pressure, mechanical, fluid physical, chemical, irradiation} *Condition:* mandatory when *"processings*_title" ≠ 'NULL' *Definitions:* - *'mixing':* Mode of mixing of the different precursor materials or matters in the 'precursor layer' or in the 'sample layer' and its physical characteristics. - *'layer formation':* Mode of formation of a 'precursor layer' or 'sample layer' and its physical characteristics. - *'thermal'*: temperature cycling of the material(s), layer, or sample - *'pressure'*:mechanical pressure cycling of the material(s), layer or sample - *'mechanical'*: mechanical stress or alteration of the material(s), layer or sample - *'fluid physical'*: contact of a fluid (or vacuum) with the material(s), layer, or sample - *'chemical'*: reaction of a fluid with the material(s), layer, or sample - *'irradiation'*: irradiation of the material(s), layer, or sample by energetic photons (γ, X, UV-Vis-IR, microwaves, …) or particles (e^-, protons, ions, …). *Note:* multiple types may occur simultaneously, e.g. T and P increase. If processings are successive then it is better (necessary ?) to define several processing steps with they order of occurrence
*sample/matter_processing*_proces s	blob	U [!o_m]	Proces L5	F	--	Description of the type of process(es) and its conditions during the processing step of the material(s), matter(s), layer or sample. *Condition:* mandatory when *"processings*_title" ≠ 'NULL' *Note:* the numbers are given only as text but it is requested to expres all their physical units in an homogeneous way by using the one defined as "*sample*_xxx_unit" *Definitions per type:* ⇨ *'mixing':* Describe the mode of mixing (at the grain level) of precursor

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materials in the ‘precursor layer’ (matters) or in the ‘sample layer’ (e.g. homogeneous mixing, heterogeneous mixing, grains in fluid, fluid in porous solid, ...) and its physical characteristics

⇨ *‘layer formation’*: Describe the mode of formation (condensation, manual deposition, …) of the ‘precursor layer’ (matters) or the ‘sample layer’ and the physical characteristics of this layer (thickness, mass, texture, porosity, density, substrate, …)

⇨ ‘*thermal*’: Temperature of the material(s)/layer/sample during thermal processing + uncertainty and duration (time) of the thermal stage

Unit: use “*sample*_temperature_unit” and “*sample*_time_unit”

Note: it can also describe any type of temperature change (step, ramp, cycle, …). A series of freeze-thaw cycles can be described in one thermal processing step (instead of several at low and high T)

Ex: ‘125 +/- 1K during 250 min’

⇨ ‘*pressure*’: Hydrosatatic pressure of the material(s)/layer/sample during pressure processing + uncertainty and duration (time) of the pressure stage

Unit (sample): use “*sample*_pressure_unit” and “*sample*_time_unit”

Note: it can also describe any type of pressure change (step, ramp, cycle, …).

Ex: ’25 GPa during 10 min’

⇨ ‘*mechanical*’: Mechanical processing (stressing, grinding, crushing, sieving, manual selection, section, polishing, …) of the material(s)/layer/sample during mechanical processing + method/technique used + forces applied (stress, crushing, …) + duration (time) of the mechanical stage

Unit (sample): use “*sample*_xxx_unit”(s)

Definitions:

- ‘stressing’: technique, stress type and value of forces applied,

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…

- ‘crushing’: technique (press, manual, …), force applied and thickness (+ uncertainty) after crushing, …

  Ex: single grain crushing
- ‘sieving’ technique (manual, mechanical, …), size(s) of the sieving mesh(s), …

  Ex: direct deposition by sieving
- ‘grain selection’: technique (manually or micromanipulator) and mode (magnet, needle, paint brush, under binocular, …), selection criteria, …

  Ex: selective adding, moving or removing of grains in/from a layer
- ‘section’: technique (cutting, FIB, microtomed, ultra-microtomed, polishing, …), type of section (ultra-thin, ultra-thin in epoxy, ultra-thin on glass slide, …) and thickness
- ‘surface preparation‘: flattening or shaping surface, roughening, …
- ‘surface polishing’: polishing method (…, polishing in epoxy), degree of polishing (micro-roughness: …, no polishing) and roughness value (rms, …)

Ex: ’sieving the mineral matter between 50 and 100 µm meshs during gravitational deposition of the layer’

⇨ ‘*fluid physical’*: Type of fluid (gas, liquid, liquid solution) and molecule(s) or matter(s), with their mole fraction(s), in contact with the material(s)/layer/sample during fluid processing. Temperature, pressure and pH of the fluid in contact with the material(s)/layer/sample during fluid processing + uncertainties and duration (time) of the fluid stage

Unit (sample): use ”*sample*_temperature_unit”, ”*sample*_pressure_unit” and “*sample*_time_unit"

Notes:

– During deposition under vacuum, or under ambient conditions, the fluid composition is the residual gas or ambient air,

respectively

- process can be a fluid that will produce either a coating shell on the material(s) or an additional layer on the layer/sample itself (if not porous), or will penetrate/alter the layer/sample either physicaly or chemicaly (reactions to be described as "chemical"). This coating will be one new constituent (coating shell) of the material(s) or one new material in the layer, or one new layer on the sample. They need to be described in the final sample/ layer(s)/ material(s)/ constituents(s)/ specie(s) structure with comments on their origin.
- During deposition under vacuum, or under ambient conditions, the fluid pressure is the residual gas pressure or the ambient pressure, respectively

Ex: 'CO2 (15%) + N2 (85%) gas, 125 +/- 1K at 100Pa', 'fluoridric acid (30%) aqueous solution, pH=5.2 during 250 min', 'Air with 400ppm CO2 and 2% H2O', 'unknown residual gas', 'ultra-high vacuum, 2e-8 mbar', …

⇨ '*chemical*': Nature and composition of the reactant(s), chemical method, protocol and reactions of formation/alteration of the material(s)/ constituents(s)/ species(s) in the sample/ layer/ material(s) during chemical processing, temperature, pressure and pH of the reactants + uncertainties and duration (time) of the chemical stage

Note: include material synthesis by various types of chemical vapor deposition (CVD, PECVD, …)

⇨ '*irradiation*': Type of irradiation (photons of all energies) or particle bombardment (ions, electrons, …) + irradiation source (type + model), filter, irradiation energy (+ distribution) of the material(s)/layer/sample during irradiation processing. Irradiation or particle bombardment conditions (flux or power, duration (time), dose or energy dose, …) of the material(s)/layer/sample during irradiation processing

Unit (sample): use "*sample*_irradiation_particle_energy_unit" or "particule", "*sample*_time_unit" and cm^{-2} or m^{-2}

Ex: 'UV-Vis photons from Hg lamp (Zeiss HBO 100W), lines 250-

						600nm, bandpass filter 200-650nm, 25mW.cm-2 during 30s, total: 0.75 J.cm-2', 'Ar+ ions, 3e+5 particule.s-1.cm-2 during 1500 s, total 4.5e+8 particule.cm-2'. **Matters:** the physical units are not specified in "matters" (contrary to "sample") but it is requested to express all them in an homogeneous way by choosing ONE of each of the following units: • Temperature: {K, °C} • Pressure: {Pa, hPa, mbar, bar, atm, torr} • Time: {s, min, h, d} • Energy: {J, kJ, eV, keV, MeV, A, nm, micron, cm-1}
*sample/matter_processing_*changes	blob	U [m]	Proces L5	F	--	Observed/expected physical and chemical changes of the material(s), layer or sample during the processing step. *Note:* physical changes (textural/structural/phase, …), or chemical changes (chemical reaction(s), compostion, …) *Note:* the final result, in term of composition and texture of the sample, of all the successive processing step(s) (i.e. after the very last processing step just before experiment start) should be described in the Sample/ Layers/ Materials/ Constituents/ Species structure
*sample/matter_processings_*comments	blob	U [m]	Proces	F	--	Additional or synthetic information on the whole processing of the material(s), layer or sample.

11. INSTRUMENTS – INSTRUMENT PARAMETERS

11.1 Description

The instrument data model is intended to give all information relative to the spectroscopic instrument used, as well as on the specific technics implemented on it. It is split on three parts: the “laboratory” table which gives basic information on the laboratory in which the experiment is performed; the “instrument” table which gives information on all types of instruments and technics that can be used, and the “instrument parameters” table which gives the values of the spectral parameters of the instrument (wavelength range/resolution/sampling) but also some specific information related to particular instrument and techniques such as angles for goniometric and ellipsometric techniques, spatial extent/resolution/sampling for micro-spectroscopy, and/or polarization parameters (bot incident and measured).

Wavelength range: We did not put limits on the spectroscopic instrument except it should measure electromagnetic waves and its wavelength range should be comprised between the VUV (about 100nm - 100 000 cm^{-1}) and the mm ranges (about 1 mm - 10 cm^{-1}). So currently, X-ray and gamma spectroscopy on one side, and radio waves on the other sides are excluded.

- The **instrument** is defined by *“instrument and technique descriptions” and* by a set of “*Instrument references”* These descriptions are stored in a *“fundamental”* database to which the **instrument parameters** will refer.

We will feed this database with all relevant combinations of instrument and technique (named with “*instrument*_technique_name”). Specific generic instrument/techniques will be generated for high levels products which may combine several spectral ranges (and possibly several instruments).

- The **instrument parameters** are then described for each experiment, mainly with their *“data acquisition parameters”* and *“spectral parameters”* and with a link to the corresponding instrument. Depending on the instrument and technique used there are also additional or optional *"spatial modes and parameters"*, *"angular parameters"*, and/or *"polarization parameters"*.

11.2 Instrument Table

Root of the table: ***instrument***

Data type: 'Instrument'

Key-word	Type	Level	Table	Exp	Unit	Description
Instrument import mode and indexes						
*instrument*_import_mode	enum(text)	P [!!_m]	Instru	F	--	Mode of import of the "instruments" data (global for the template) Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*instrument*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Instru	(V)	--	Name of the storage copy of the xml import file of the instrument metadata ➔ determined automatically during import (from "*instrument*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*instrument*_index [**][-xml]	int(10)	B [!!_g]	Instru	F	--	Automatic random but unique number (internal ID) given to new instrument/technique set.
*instrument*_uid [**]	varchar(255)	S0/S1 [!!_m]	Instru	F	--	Unique identifier code (UID) given to the instrument+technique set or to a numerical model (to be created) *Nomenclature:* Create this code name with 'INSTRU_' in order to be unique. For an instrument+technique the UID should be of the style 'INSTRU_InstrumentName_Technique_LabAcronym' where 'InstrumentName' is the instrument name, 'Technique' is a short but unambiguous version of the technique name, and 'LabAcronym' is the acronym of the laboratory where it is situated. For Numerical model (case of spectrum simulations) the UID should be of the style 'MODEL_ModelName_ModelYear/Version' where 'ModelName' is the

name of the numerical model, and 'ModelYear/Version' is either the year of the model or its version number.

Notes:

- each couple of instrument + technique is described independently. Ex: for an instrument that has 4 sets of source/detector/beamsplitter to cover the whole visible-IR wavelength range, it is necessary to describe 4 instrument/techniques, one for each set (i.e. wavelength range).
- as similar instrument+technique can be present in different laboratories it is necessary to distinguish them with '_LabAcronym'
- for widely distributed commercial instruments used without modification, only its name may be sufficient (and may be created at the common SSHADE level, but difficult to manage …).

Ex:

- INSTRU_Nicolet800_Vis_IPAG, INSTRU_Nicolet800_NIR_IPAG, INSTRU_Nicolet800_MIR_IPAG, INSTRU_Nicolet800_FIR_IPAG
- INSTRU_Vertex+Hyperion_mono_trans_NIR_IAS, …
- MODEL_Hapke_1986, MODEL_SPECTRIMAG_v3 (numerical models)

instrument_manager_databases	***List [L0]***	[!!]				£: databases which manage this laboratory
*instrument*_manager_database_uid [*]	varchar(255)	S1 [!!o_m]	Instru DatBas L0	F	--	Link(s) to the existing UID(s) of the database which manages this instrument information *Condition:* at least one database *Note:* For instrument that did not belong to one laboratory which has a database (and not managed by a database) or for widely distributed models, it should be 'DB_SSHADE'
instrument_laboratories	***List [L1]***	[!!]				£: current and previous laboratory(ies) of the instrument *Note:* this list should be ordered from the oldest to the current (or most recent

						lab)
*instrument*_laboratory_order [-xml]	int(4)	U [!!_c]	Instru L1	F	--	Order of the laboratory Note: calculated from the order of the "*instrument_laboratories"*
*instrument*_laboratory_current	boolean(flag)	S3 [!!_m]	Instru L1	F	--	Flag telling if this laboratory is the current one BoolEnum: {yes, no} or {true, false}
*instrument*_laboratory_uid [*]	varchar(255)	S1 [!!_m]	Instru Labo L1	F	--	Link to the existing UID of the current or previous laboratory(ies) where the instrument or model is currently, or was, located. *Note xml:* Can also be found with "*laboratory*_acronym" *Note:* For widely distributed models, it may be IPAG (@SSHADE)
*instrument*_laboratory_comments	blob	U [m]	Instru L1	F	--	Additional information on the instrument in this laboratory. *Ex:* years in the laboratory, …

Instrument description

*instrument*_type	varchar(255)	S0 [!!_m]	Instru	F	--	Type of instrument or of model FreeList: {FTIR spectrometer, grating spectrometer, AOTF spectrometer, CRDS spectrometer, laser diode spectrometer, SWIFT spectrometer, µSPOC spectrometer, narrow-band filters spectrometer, grating imaging spectrometer, grating hyperspectral imaging system, ImSPOC imaging spectrometer, narrow-band filters imager, spectro-gonio radiometer, Raman spectrometer, Raman micro-spectrometer, FTIR micro-spectrometer, spectrofluorometer, ellipsometer, X-ray absorption spectrometer, gamma-ray spectrometer, Mossbauer spectrometer, vector network analyzer, radiative transfer simulation, quantum mechanical simulation, …} *Definitions:* - 'FTIR spectrometer': - 'grating spectrometer': - 'AOTF spectrometer':

- ‘CRDS spectrometer’:
- ‘laser diode spectrometer’:
- ‘SWIFT spectrometer’:
- ‘µSPOC spectrometer’:
- ‘narrow-band filters spectrometer’:
- ‘grating imaging spectrometer’ or ‘grating hyperspectral imaging system’:
- ‘ImSPOC imaging spectrometer’:
- ‘narrow-band filters imager’:
- ‘spectro-gonio radiometer’:
- ‘Raman spectrometer’:
- ‘spectrofluorometer’:
- ‘Raman micro-spectrometer’:
- ‘FTIR micro-spectrometer’:
- ‘ellipsometer’:
- ‘X-ray absorption spectrometer’:
- ‘gamma-ray spectrometer’:
- ‘Mossbauer spectrometer’:
- ‘vector network analyzer’: VNA
- ‘impedance spectrometer’
- ‘radiative transfer simulation’:
- ‘quantum mechanical simulation’:

*instrument*_name	varchar(255)	S0 [!!_m]	Instru	F	--	Specific name and model of the instrument or of the numerical model Free list: use the following style: *Spectrometers:* Nicolet 800, Brucker Vertex 70v, Brucker Vertex 80v, Jobin Yvon Horiba - Labram HR800 Vis, Jobin Yvon Horiba - Labram HR800 UV, XY Dilor, … *Radiative transfer models*: Lommel-Seeliger, Minnaert 1941, Lumme and Bowell 1981, Hapke 1986, Douté & Schmitt 1998, DISORT, Shkuratov, RTLS 2000, … *Note:* for “instrument_type” = ‘radiative transfer simulation’ or ‘quantum mechanical simulation’: name of radiative transfer model or quantum mechanical model (theories) used to simulate the spectra.

						Note: Need to maintain a (open) external list of instrument names
*instrument*_technique	openum(text)	S0/S1s [!!_m]	Instru	F	--	Instrumental technique. OpenEnum: {transmission, reflection-absorption, ATReflection, specular reflection, ellipsometry, bidirectional reflection, biconical reflection, confocal reflection, diffuse reflection, directional-hemispherical reflection, hemispherical-directional reflection, scattering, thermal emission, Raman scattering, fluorescence emission, gamma emission, Mossbauer absorption, permittivity, time-domain, dual polarisation interferometry} *Definitions:* It is combined with the instrument type: For FTIR, grating, CRDS, ... spectrometers: - 'transmission (absorption)': - 'reflection-absorption' (absorption, called RAIRS): - '(surface) bidirectional reflection': incidence and emergence angles are well defined and with only in a small conic solid angle (typically both with less than 5° half angle) - '(surface) biconical reflection': a bidirectional reflection technique but with a large conic solid angle (typically between 5° and 45° half angle) - '(surface) diffuse reflection': also called DRIFTS. The central incidence and emergence angles and ranges are not well defined (frequently asymmetric ellipsoid mirrors) - '(surface) directional-hemispherical reflection': incidence is defined within a small to medium conic solid angle (<45° half angle), but emergence is integrated over (almost) an hemisphere - '(surface) hemispherical-directional reflection': incidence comes from (almost) an hemisphere and emergence is defined within a small to medium conic solid angle (<45° half angle) - '(surface) specular reflection':identical incidence and emergence angles within very small conic solid angle (typically both with less than 1° half angle) - '(surface) thermal emission': - 'ATReflection' (also called MIR), - '(grains) scattering': - '(grains) thermal emission':

						For spectro-gonio radiometers: - '(surface) bidirectional reflection': For Raman spectrometers: - 'fluorescence emission': generally measurement integrated over a very wide angle (almost hemisphere) of diffuse fluorescence emission triggered by a source lamp, or a laser - 'Raman scattering': generally measurement integrated over a very wide angle (almost hemisphere) of diffuse Raman scattered light triggered by a laser For Gamma spectrometers - 'gamma emission': - 'Mossbauer absorption': For impedance spectrometers - 'permittivity': - 'time-domain': For ellipsometers: - 'ellipsometry': - 'dual polarisation interferometry': *Notes:* - for "*instrument*_type" = 'radiative transfer simulation': type of technique simulated by radiative transfer model: '(surface) bidirectional reflection', '(surface) thermal emission', '(grains) scattering', '(grains) thermal emission', ... - for "*instrument*_type" = 'quantum mechanical simulation': type of technique/process simulated by quantum mechanical theory: 'transmission (absorption)', 'thermal emission', 'fluorescence emission', 'Raman scattering', …
*instrument*_technique_name	varchar(255)	S0/S1 [!!_m]	Instru	F	--	Name describing the combination of instrument, technique and spectral range used. *Ex:* - *For spectrometers:* Nicolet 800 – transmission NIR, Vertex 70v – micro-transmission MIR, Labram HR800 micro-Raman Vis - 488 nm, Labram HR800 Raman UV - 244 nm, Spectro-gonio radiometer –

bidirectional reflection Vis+NIR,

- *For Radiative transfer models*: Hapke 1989 - surface reflectance RT model, Douté & Schmitt 1998 – Spectrimag surface reflectance RT model, DISORT - doubling-adding surface reflectance RT model, Machin 2012 - grains thermal emission RT model, … Truc 2013 - ab-initio QM emission model, ...

Note: for "instrument_type" = 'radiative transfer simulation' or 'quantum mechanical simulation': Specific name and technique of the radiative transfer model or quantum mechanical model used to simulate spectra

Note: need to maintain a (free) external correspondence table between:

- instrument_technique_name

and

- spectral_range_min/_max
- spatial_resolution
- angle_resolution

in order to help filling manually these keywords

Instrument techniques description

*instrument*_microscopy_imaging	enum(text)	S1/S1b [!_m]	Instru	F	--	Tell if the instrumental technique use a microscope, a micro-imager, an imager or not. Enum: {macroscopic, microscopy, linear scan, linear micro-scan, imaging, micro-imaging} *Definitions:* It is combined with the instrument technique: - '*macroscopic'*: individual macroscopic measurements (scale > 100 µm) *Ex*: for all instrument techniques - '*microscopy'*: individual microscopic measurements (scale < 100 µm) *Ex*: for 'transmission micro-spectroscopy', 'reflection micro-spectroscopy', 'ATR micro-spectroscopy', 'fluorescence micro-spectroscopy', 'Raman micro-spectroscopy' - '*linear scan'*: 1D measurements at macroscopic scale (scale > 100 µm) for linear (or curved) scans *Ex*: scan of a surface by a plane/drone with a monodetector

- '*linear micro-scan'*: 1D measurements at microscopic scale (scale < 100 µm) for linear (or curved) scans
- '*imaging'*: 2D measurements (polychromatic images or spectro-images) at macroscopic scale (scale > 100 µm)
  Ex: for 'reflection imaging spectroscopy' (Spectro-imager)
- '*micro-imaging'*: 2D measurements (polychromatic images or spectro-images) at microscopic scale (scale < 100 µm)
  Ex: for 'transmission imaging micro-spectroscopy', 'reflection imaging micro-spectroscopy' (IR microscope)

*instrument*_optical_accessory	varchar(255)	S2 [m]	Instru	F	--	Type of additional optical accessory installed in the instrument FreeList: {Ge ATR crystal, KRS-5 crystal, ZnSe ATR crystal, Si ATR crystal, biconical diffuse reflectance, diffuse reflectance (DRIFTS), multipass cell, integrating sphere, absolute specular reflectance, blue filter, red filter, linear polarizer, Vis confocal microscope in reflection, IR microscope in transmission, IR microscope in reflection, IR microscope in ATR, …}
*instrument*_source	varchar(255)	S2 [!_m]	Instru	F	--	Light source type of the instrument FreeList: {Tungsten/Halogen lamp, Globar-IR, Hydrogen arc lamp, Deuterium arc lamp, Hg lamp, Xe arc lamp, He-Ne laser, laser diode, Ar+/Kr+ laser, Ar+ laser, frequency-doubled Ar+ laser, Nd:YAG laser, frequency-doubled Nd:YAG laser, pulsed laser, synchrotron - bending magnet, synchrotron - undulator, synchrotron - wiggler, Sun, no, , …} *Note:* 'no' (or 'NULL') for simulation ("instrument_type" = 'radiative transfer simulation' or 'quantum mechanical simulation')
*instrument*_source_wavelength	varchar(255)	S2 [!_m]	Instru	F	--	General spectral range, precise wavelength (laser), or wavelength range (laser diode) of the source FreeList: {gamma, hard X, soft X, EUV, VUV-UV, Vis-NIR, UV-NIR, MIR, FIR, MIR-FIR, submm, mm, 90GHz, 6050-6900 cm-1, 244 nm, 457.9 nm, 488 nm, 514.5 nm, 532 nm, 632.8 nm, 647.1 nm, …} *Note:* cf. *"parameters_instrument*_spectral_range_type" for the typical spectral ranges. If spectral range is more limited, then specify in

						"*instrument*_comments" *Note:* for simulation: can be the range of simulation possible with the model ("*instrument*_type" = 'radiative transfer simulation' or 'quantum mechanical simulation')
*instrument*_source_power	varchar(255)	S3 [!o_m]	Instru	F	var.	Power of the source *Condition:* Mandatory only when "*instrument*_technique" = {Raman scattering, fluorescence emission} *Unit*: give the unit after the value. It can be W, W/cm2, …. *Notes:* - 'no' (or 'NULL') for simulation ("instrument_type" = 'radiative transfer simulation' or 'quantum mechanical simulation') - power of the laser pulse in the case of Raman and fluorescence spectroscopy (the power received by the sample, mandatory, should be given in "*sample_irradiation_radiant_flux*")
instrument_spectral_analyzers	***List [L2]***	[!]				£: Spectral analyzers of the instrument.
*instrument*_spectral_analyzer	varchar(255)	S2 [!_m]	Instru L2	F	--	Type of spectral analyzer of the instrument FreeList: {Quartz beamsplitter, CaF2 beamsplitter, KBr/Ge beamsplitter, Si beamsplitter, Mylar 20µm beamsplitter, diffraction grating 1200 l/mm - 250nm, diffraction grating 600 l/mm - 400nm, diffraction grating 300 l/mm - 1000nm, diffraction grating 150 l/mm - 4000nm, diffraction grating 3600 l/mm, diffraction grating 1800 l/mm, diffraction grating 1200 l/mm - 1200nm, diffraction grating 600 l/mm - 550nm, diffraction grating 150 l/mm, Ge AOTF 1.5-3 µm, 2-crystal monochromator Si[111], 2-crystal monochromator Si[220], 2-crystal monochromator Si[311], crystal analyzer Ge [110], crystal analyzer Ge [111], crystal analyzer Ge [331], crystal analyzer Si [111], X-ray polychromator, narrow-band filters, no, …} *Note:* 'no' (or 'NULL') for simulation ("instrument_type" = 'radiative transfer simulation' or 'quantum mechanical simulation')

instrument_detectors	***List [L3]***	[!]				£: Detectors of the instrument
*instrument*_detector	varchar(255)	S2 [!_m]	Instru L3	F	--	Detector type of the instrument FreeList: {Si, Si drift, Ge array, InSb (liq. N2 cooled), InSb (cryocooler), InGaAs, PbS, PbSe, MCT (liq. N2 cooled), DTGS-KBr, DTGS-PE, Ge bolometer (He cooled), Si bolometer (He cooled), MCT array (liq. N2 cooled), CCD, CCD (liq. N2 cooled), LSO:Tb scintillator, other, no, …} *Note:* 'no' (or 'NULL') for simulation ("instrument_type" = 'radiative transfer simulation' or 'quantum mechanical simulation')
*instrument*_comments	blob	U [m]	Instru	F	--	Additional information on the instrument and technique (special configuration, use of cryogenic/thermal/vacuum cells ...), or simulation model.

Instrument references

instrument_documentations	***List [L4]***	[O]				£: documentations describing the instrument and its associated techniques
*instrument*_documentation_name	varchar(255)	U [m]	Instru L4	F	--	Name of the documentation describing the instrument, its associated techniques and performances *Ex:* 'Spectro-gonio radiometer at IPAG', 'SPECTRIMAG user manual', …
*instrument*_documentation_filename	varchar(255)	U [O!_m]	Instru L4	F	--	Link to documentation describing the instrument, its associated techniques and performances, i.e. all parameters described in this "instrument" part. *Condition:* mandatory when "*instrument*_documentation_name" ≠ Ø *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, …
instrument_links	***List [L5]***	[O]				£: web sites describing the instrument and techniques, or the model.
*instrument*_link_name [*xxx*_link_name]	varchar(255)	U [m]	Instru L5	F	--	Name of the web page(s) describing the instrument, technique or the associated cells used, or the simulation model. *Ex:* 'Spectrometer Brucker Vertex 70v', 'Microscope Hyperion 3000',

						‘SPECTRIMAG radiative transfer model’, …
*instrument*_link_url [*xxx*_link_url]	CS-varchar(255)	U [O!_m]	Instru L5	F	--	Link(s) to web sites describing the instrument, technique or the associated cells used, or the simulation model. *Condition:* mandatory when "*instrument*_link_name" ≠ Ø *Notes*: - can link to a publication by giving its url address, preferably through its DOI. *Ex*: https://doi.org/10.1002/ejic.200700067
instrument_publications	***List [L6]***	[O]				£: Publications describing the instrument and techniques, or the model.
*instrument*_publication_uid [*]	varchar(255)	U [m]	Instru Publi L6	F	--	Link to the existing UID of the publication(s) describing the instrument, technique or the associated cells used, or the simulation model. *Note:* these papers should be in the bibliography database, with “*publication*_content” = 'instrument-technique'

11.3 Instrument parametersTable

Root of the table: ***parameters_instrument***

Data type: in 'Experiment and spectra'

Note: These parameters will be first defined for the whole experiment in *"experiment_parameters_instruments"* (see *"Experiment"* table) and then possibly modified for each spectrum in *"sample_parameters"* (see *"Spectrum"* table) ,except for *"spectrum_parameters_instruments*_instrument_sample_holder".

Key-word	Type	Level	Table	Exp	Unit	Description
Instrument parameters indexes						
*parameters_instrument*s	***List [L0]***	[!!]				£: measurement parameters of the instrument(s) used ***Variable: spectrum*** *Note xml:* when a 'multiple items' bloc is changed, all the items of the bloc should be (re-)defined
*parameters_instrument*_index [**][-xml]	int(10) [Virtual index]	B [!!_v]	ParIns L0	F	--	Automatic random but unique number (internal ID) given to a new instrumental parameter set.
Instrument and sample holder						
*parameters_instrument*_instrument_uid [*]	varchar(255)	B [!!_m] [V:££om]	ParIns Instr L0	F	--	Link to the existing UID of the instrument used to do the measurements (or to measure the original spectra used to produce high level spectra) *Note:* In *"sample_parameters_instruments"* it is necessary to use one of the UID defined in *"experiment_parameters_instruments"* ***Variable: spectrum*** *Condition:* absolute compulsory when a parameter is changed or when there are several instruments *Notes*:

						* when there is only one instrument - absolute compulsory to give "instrument_uid" when one or more parameter(s) is changed * when there are several instruments - if no "instrument_uid" is given: all instruments are taken by default - if only one instrument is used then it is compulsory to give its "instrument_uid" even if no parameter is changed - absolute compulsory to give all "instrument_uid" when one or more parameter(s) is changed in one instrument - if no
*parameters_instrument*_instrument_carrier	blob	S1b [!o_m]	ParIns L0	F	--	Type and name of the carrier of the instrument *Condition:* mandatory when *"experiment*_type" = {low altitude field measurement, satellite remote sensing} *Notes:* - mostly used for remote sensing experiments - for '*low altitude field measurement*': provide the type of low altitude flying device (plane, helicopter, UAV, drone, … and eventually some flying info (altitude range, …) *Ex*: 'Hexacopter, flying altitude between 10 and 120 m' - for '*satellite remote sensing*' provide the name of the satellite carrying the instrument, and eventually some orbit info (altitude, orbit type) *Ex*: 'Mars Express spacecraft, quasi-polar elliptic orbit (perihelion: 298 km, aphelion: 10,107 km, period: 7.5hours)' - for '*field measurement*' you can tell if the instrument is fixed on a tripod, or carried by a people during measurement, … ***Variable: spectrum*** *Note xml:* This KW did not appear in the xml in the bloc "*spectrum*_parameters_instrument" as the carrier of the instrument is fixed for the experiment ("*experiment*_parameters_instrument_carrier")

*parameters_instrument*_instrument_sample_holder	blob	U [$_m]	ParIns L0	F	--	Sample holder and/or type of confinement cell used with the instrument *Free List:* {Glass plate in room air, KBr window cooled by He cryostat in UHV chamber, CSi window cooled by He cryostat in UHV chamber, Saphire window inside cell filled with Ar, Polished aluminum cube, Cooper closed cell 8mm thick with MgF2 windows cooled by He cryostat in UHV chamber, SERAC environmental cell: Aluminum sample holder 12 cm diameter and 2 cm depth (?) inside P-T controled chamber closed by saphire window and cooled by Peltier elements, CarboN-IR environmental cell: P-T controled cooper cylinder 8 cm diameter and 6 cm depth closed by a saphire window and cooled by a He cryostat in UHV chamber, …} *Notes:* – It is strongly recommended to provide this information! (but not mandatory only for programming reasons) – It is good to prepare a list of all available sample holders and cells for each instrument of each lab to help fill homogeneously this information ***Variable: spectrum*** *Note xml:* This KW did not appear in the xml in the bloc "*spectrum*_parameters_instrument" as the sample holder of the instrument is fixed for the experiment ("*experiment*_parameters_instrument_sample_holder")
Instrument data acquisition parameters						
*parameters_instrument*_spectrum_scan_number	int(11)	U [m] [V: m]	ParIns L0	V	--	Total number of individual spectra of the sample co-added to get the spectrum *Note:* for "*parameters_instrument*_spatial_observation_mode" = 'rastered' and 'rastered image' it is the total number of scans for all the spatial spots averaged, defined in "spatial_spots_number" *Note:* filling less useful for spectra levels 3 and 4
Instrument spectral parameters						
parameters_instrument_spectral		[!!o]				£: instrument spectral parameters

		[V: £O]				***Variable: spectrum*** *Condition:* compulsory to give the effective value for the spectrum if it changed compared to the global value given in experiment
*parameters_instrument*_spectral_ unit	enum(text)	U [!!_m] [V: m]	ParIns L0	V/Vv [Ver]	--	Unit in which all the spectral parameters are entered Enum: {m-1, cm-1, angstrom, nm, micron, mm, m, km, Hz, kHz, MHz, GHz, eV, keV} *Note:* it is necessary here to set the spectral unit because the "*parameters_instrument*_spectral_sampling" and "*parameters_instrument*_spectral_resolution" parameters are constant in one specific unit depending on the type of instrument and cannot be expressed simply in one unique standard unit (like cm^{-1}) *Note DB:* all wave data (spectra, bandlist, …) will be stored in the database in wavenumber "cm^{-1} " unit whatever is the unit in which they are entered. ***Variable: spectrum*** *Note:* generally unchanged as it only depends on the instrument
*parameters_instrument*_spectral_s tandard	enum(text)	U [!!_m] [V: m]	ParIns L0	V/Vv [Ver]	--	Medium in which the wavenumber/wavelength/frequency scale is given Enum: {vacuum, air, unknown} *Definitions:* - '*vacuum'*: reference wavelength is in vacuum (no correction) - '*air'*: reference wavelength is in air (correction: $\nu_0 = \nu_{air}/1.000272$) - '*unknown'*: unknown reference wavelength (no correction) ➔ conversion to vacuum reference to be done at the import of the file and after conversion to wavenumber 'ν' in cm^{-1} - $\nu_0 = \nu_{air}/1.000272$ *Notes:* - *'air'* corresponds to "standard air" @633nm corrected to 20°C (1013 hPa with 0.033 % CO_2) - n(air) = 1.000278 (400nm) - 1.000268 (20µm)

- see Birch and Down Metrologia, 30, 155 / 31, 315 (1993/94)

Notes:

- Case of Infrared measurements
- correction useful for resolution power $R = \lambda/\Delta\lambda = \nu/\Delta\nu > 350$ (i.e. correction > $\Delta\lambda/10$)
- **correction necessary for resolution power R > 1000 (i.e. correction > $\Delta\lambda/3$).**
- Average shift is 0.0275% (i.e. 1cm^{-1} at 3600cm^{-1}).
- applying a constant correction with n=1.000272 (@633nm, standard air at 20°C, 1 atm) gives an accuracy of correction better than 0.1 cm^{-1} from < 500 to 23000 cm^{-1} (0.43 to >20µm) and better than 0.3 cm^{-1} from < 500 to 30000 cm^{-1} (0.33 to >20µm).
- a change of 10°C induces a change of ~0.9 10^{-5}.
- a change of P of 40mb induces a change of ~1.1 10^{-5} (i.e. 0.1cm^{-1} at 10000 cm^{-1}).
- the effects of CO_2 and H_2O abundances in air are both negligible at our resolutions.
- Case of Raman measurements
    - with 514nm (19455 cm^{-1}) laser excitation the reference shift is ~5.4 cm^{-1}
    - $\nu_{laser0} - \nu_0 = (\nu_{laser} - \nu_{air})/1.000278$ (@400nm)
    - So same correction and rule on R apply when using Raman shift
    - Average shift is 0.0278% (i.e. 1cm^{-1} at 3600cm^{-1}).

Notes:

- all FTIR measurements are given with wavenumber vacuum standard (given by vacuum He-Ne laser wavelength).
- a number of grating spectrometer measurements are given with wavelength air standard, but correction will depend on the calibration conditions and references and any possible changes of T and P (altitude, wheather conditions) between calibration and measurement.
- Raman spectra seemsto be given with wavenumber air standard

Variable: spectrum

						Note: generally unchanged as it only depends on the instrument
*parameters_instrument*_spectral_observation_mode	enum(text)	S2 [!!_m] [V: m]	ParIns L0	V	--	Mode of spectral observation Enum: {spectrum, multi wavelengths, single wavelength, multi spectral averages, single spectral average} *Definitions:* - '*spectrum'*: measurement of a continuous set of a large number of wavelengths, typically evenly sampled, and with (almost) the same resolution (in some unit) or resolution power over its range (or over a part of the range). - '*multi wavelengths'*: measurement at a limited number of wavelengths (~3-15), with generally varying spectral spacing and/or bandwidths. These data have generally angular or spatial variations, such as BRDF, or image. - '*single wavelength'*: measurement at a single wavelength, generally with a wide spectral bandwidth. These data need to have angular or spatial variation, such as BRDF, or image. - '*multi spectral averages'*: several values averaged over a set of spectral ranges. It can be the integration over specific spectral ranges of a spectral measurement (e.g. RGB channels, standard set of filters). These data have generally angular or spatial variations, such as BRDF, or image - '*single spectral average'*: single value averaged over a spectral range. It can be the integration over a narrow or wide spectral range of a spectral measurement (e.g. bond albedo). These data need to have angular or spatial variation, such as BRDF, or image. ***Variable: spectrum*** *Note:* effective spectral observation mode for this spectrum
parameters_instrument_spectral_range_types	***List [L1]***	[!!] [V: O]		V/Vv [Ver]		£: Typical spectral ranges

*parameters_instrument*_spectral_range_type	varchar(255)	S0 [!!_m] [V: m]	ParIns L0 L1	V/Vv [Ver]	--	Typical spectral range Enum: {gamma, hard X, soft X, EUV, VUV, UV, Vis, NIR, MIR, FIR, sub-mm, mm, cm, UHF, VHF, HF, MF, LF, VLF, ULF, SLF, ELF} *Definitions:* • '*gamma*': Gamma rays 0.1-10pm (12-0.12 MeV) • '*hard X*': hard X-rays 0.01-0.2nm (100-5 keV) • '*soft X*': soft X-rays (0.1-)0.2-10nm ((12-)6-0.12 keV) • '*EUV*': Extreme Ultraviolet 10-120 nm (120-10 eV) • '*VUV*': Vacuum Ultraviolet (10-)120-200 nm (10-6 eV) Also called 'FUV': Far Ultra-Violet • '*UV*': Ultraviolet 200-400 nm (6-3 eV) Also called 'NUV': Near Ultra-Violet • '*Vis*': Visible 400-800(-1000) nm • '*NIR*': Near-InfraRed 1-2.5(-5)µm • '*MIR*': Mid-InfraRed 2.5-15(-50) µm • '*FIR*': Far-InfraRed 15-300(-500)(-1000) µm • '*sub-mm'*: Sub-millimeter 300-1000 µm • '*mm*': millimeter wave 1-10 mm (300GHz-30GHz) also called 'EHF': Extremely High Frequency or microwaves • '*cm*': centimeter waves 1-10 cm (30GHz-3GHz) also called 'SHF': Super High Frequency or microwaves • '*UHF*': Ultra high frequency 0.1-1m (3GHz-300MHz) also called decimeter radio waves • '*VHF*': Very high frequency 1-10m (300-30MHz) also called meter radio waves • '*HF*': High frequency 10-100m (30-3MHz) also called decameter radio waves • '*MF*': Medium frequency 100-1km (3MHz-300kHz) also called hectometer wave • '*LF*': Low frequency 1-10km (300-30kHz) also called kilometer wave

						• '*VLF*': Very Low frequency 10-100km (30-3kHz) also called myriameter wave • '*ULF*': Ultra Low frequency 100-1000km (3kHz-300Hz) • '*SLF*': Super Low frequency 1000-10 000km (300-30Hz) • '*ELF*': Extremely Low frequency 10 000-100 000km (30-3Hz) frequently extended to all waves down to 0Hz *Note:* this spectral range is indexed to an equivalence table in term of typical minimum and maximum wavenumbers/wavelength/frequency ***Variable: spectrum*** *Note*: effective spectral range type for this spectrum
*parameters_instrument*_spectral_range_number [-xml]	int(10)	U [!_c] [V: m]	ParIns L0	V/Vv [Ver]	--	Number of spectral ranges of valid measurements ➔ calculated from the list of "*parameters_instrument*_spectral_range_min" and "*parameters_instrument*_spectral_range_max"
parameters_instrument_spectral_ranges	***List [L2]***	[!!]		V/Vv [Ver]		£: Spectral ranges of valid data measurements (or analysis) *Note:* they can be non-continuous valid parts of a spectrum, or a series of overlapping ranges with different samplings/resolutions (as for grating spectrometers), or a series of broad/narrow-band filters (it is then the number of filters if not overlapping).
*parameters_instrument*_spectral_range_min	float	S2 [!!_m] [V: !o_m]	ParIns L0 L2	V/Vv [Ver]	var.	Start(s) of each spectral range of valid measurement (or analysis) *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted in 'cm^{-1}' unit in the database but provided to user in the unit specified in SSHADE *Note:* - for a series of broad/narrow-band filters this correspond to about the lowest wavenumber filter - for spectral products the spectral range correspond to the valid range of data after analysis

						Variable: spectrum *Condition*: Mandatory if at least one value of the bloc "*parameters_instrument_spectral_ranges"* is changed *Note*: effective start of valid spectral range for this spectrum
*parameters_instrument_*spectral_range_max	float	S2 [!!_m] [V: !o_m]	ParIns L0 L2	V/Vv [Ver]	var.	End(s) of each spectral range of valid data measurement (or analysis) *Other notes:* same as for *"parameters_instrument_*spectral_range_min" *Note:* - for a series of broad/narrow-band filters this correspond to about the highest wavenumber filter - for a single broad/narrow-band filter (in case of single wavelength BRDF) this value should be the same as "*parameters_instrument_*spectral_range_min" ***Variable: spectrum*** *Condition*: Mandatory if at least one value of the bloc "*parameters_instrument_spectral_ranges"* is changed *Note*: effective end of valid spectral range for this spectrum
*parameters_instrument_*spectral_range_absorption_edge_element_uid [*]	varchar(255)	S2 [£!o_m] [V: !o_m]	ParIns Atom L0 L2	V/Vv [Ver]	-	Link to the existing UID of the chemical element corresponding to the measured absorption edge in X Absorption Spectroscopy. *Condition*: Compulsory only for X-ray absorption spectrometer *Condition*: Mandatory when "*parameters_instrument_*spectral_range_absorption_edge_type" ≠ Ø *Note:* link to the natural atom as all isotopes have same electronic structure. ***Variable: spectrum*** *Condition*: Mandatory when "*parameters_instrument_*spectral_range_absorption_edge_type" ≠ Ø *Note*: effective chemical element corresponding to the measured absorption edge for this spectrum

*parameters_instrument*_spectral_range_absorption_edge_type	enum(text)	S2 [£!o_m] [V: !o_m]	ParIns L0 L2	V/Vv [Ver]	-	Type of absorption edge measured in X Absorption Spectroscopy. Enum: {K, L, L1, L2, L3, L2-3, M, M1, M2, M3, M4, M5, M4-5, N, N1, N2, N3, N4, N5, N6, N7, O, O1, O2, O3, O4, O5, O6, O7} *Condition*: Compulsory only for X-ray absorption spectrometer *Condition*: Mandatory when "*parameters_instrument*_spectral_range_absorption_edge_element_uid" ≠ Ø *Notes*: - L2-3 and M4-5 are used for spectra spanning these 2 edge ranges - The use of the generic edges L, M, N, and O is not recommended, but may be used for spectra spanning other multiple edges. See: - https://github.com/XraySpectroscopy/XAS-Data-Interchange/blob/master/specification/dictionary.md - http://old.iupac.org/publications/analytical_compendium/Cha10sec348.pdf ***Variable: spectrum*** *Condition*: Mandatory when "*parameters_instrument*_spectral_range_absorption_edge_element_uid" ≠ Ø *Note*: effective type of absorption edge for this spectrum
*parameters_instrument*_spectral_sampling	float	U [m] [V: m]	ParIns L0 L2	V/Vv [Ver]	var.	Spectral sampling(s) of each spectral range given *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • stored in the database and provided to user in "*parameters_instrument*_spectral_unit" (later in 'user unit' => calculation => file) *Defintion:* it is the regular spacing (in the spectral unit) between recorded spectral points. *Note:* - no value for broad/narrow-band filters, except if their spacing is regular in the spectral unit. Their individual position is given in "*parameters_instrument*_spectral_filter_center"

						- for instruments that have a no constant spectral sampling neither in wavenumber/frquency nor in wavelength unit, it is necessary to to give an average value here and provide more detailed information in "*parameters_instrument*_spectral_comments" --- ***Variable: spectrum*** *Note*: effective end spectral sampling for this spectrum
*parameters_instrument*_spectral_resolution	float	U [!_m] [V: !o_m]	ParIns L0 L2	V/Vv [Ver]	var.	Optical spectral resolution(s) (FWHM of intensity collected at a particular wavelength/wavenumber) of each spectral range *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • stored in the database and provided to user in "*parameters_instrument*_spectral_unit" (later in 'user unit' => on-the-flight calculation => interface) *Defintion:* it is the width at half maximum (in the spectral unit) of an infinitely narrow line (Dirac) as measured by the instrument. *Notes:* - it should be constant within each spectral range. - for instruments that have no constant spectral resolution neither in wavenumber/frquency nor in wavelength unit, it is necessary to give an average value here and provide more detailed information in "*parameters_instrument*_spectral_comments" - for broad/narrow-band filters their individual FWHM is given in "*parameters_instrument*_spectral_filter_width", so no value is needed here (put 'NULL') ***Variable: spectrum*** *Condition*: Mandatory if at least one value of the bloc "*parameters_instrument_spectral_ranges"* is changed *Note*: effective spectral resolution for this spectrum
*parameters_instrument*_spectral_position_error	float	U [m] [V:	ParIns L0	V/Vv [Ver]	var.	Error (+/-) on the wavenumber/wavelength/frequency value of the position of the points in the spectral file

		m]	L2			*Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • stored in the database and provided to user in "*parameters_instrument*_spectral_unit" (later in 'user unit' => on-the-flight calculation => interface) *Notes:* - it should be constant within each spectral range. - If not constant in the spectral unit then give average value here and more info in "*parameters_instrument*_spectral_comments". ***Variable: spectrum*** *Note*: effective spectral position error for this spectrum
parameters_instrument_spectral_filters	***List [L3]***	[!o] [V: O]		V/Vv [Ver]		£: filters or diaphragm used to bandpass or attenuate the flux. *Notes*: For multispectral measurements: - it is highly recommended to enter the filters in increasing order of central wavelength. - the filters should not change between spectra (parameters type="spectrum")
*parameters_instrument*_spectral_filter_type	varchar(255)	U [!o_m] [V: !o_m]	ParIns L0 L3	V/Vv	--	Type of filter (and its transmission information) or diaphragm (size), if any *Condition #1:* Mandatory when "*instrument*_technique" = {Raman scattering, fluorescence emission} OR *Condition #2:* Mandatory for multispectal measurements, i.e. when "*parameters_instrument*_spectral_observation_mode" = {multi wavelengths, single wavelength, multi spectral averages, single spectral average} *Ex:*'neutral density 10%', 'bandpass 650nm, FWHM 200nm, 60%', 'diaphragm 3 mm', 'no', … ***Variable: spectrum*** *Condition*: Mandatory if at least one value of the bloc

						"*parameters_instrument_spectral_filters"* is changed *Note*: effective type of spectral filter used for this spectrum
*parameters_instrument*_spectral_filter_place	varchar(255)	U [m] [V: m]	ParIns L0 L3	V/Vv	--	Placement of the filter used to bandpass or attenuate the flux reaching the detector. *Ex:*'in front of the detector', 'in front of the source','at the focus of the illumination beam', …
*parameters_instrument*_spectral_filter_center	float	U [!o_m] [V: !o_m]	ParIns L0 L3	V/Vv	var.	Central (or edge) wavelength/wavenumber/frequency(s) of the filter *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted and stored in 'cm-1' unit in the database but provided to user in the unit specified by the data provider in "*parameters_instrument*_spectral_unit" *Condition:* Mandatory only when "*parameters_instrument*_spectral_filter_type" ≠ Ø (if a filter/diaphragm is used) *Notes:* - used in particular to specify the position of a series of narrow bandpass filters - can also be used to specify the edge of a low/high pass filter ***Variable: spectrum*** *Condition*: Mandatory if at least one value of the bloc "*parameters_instrument_spectral_filters"* is changed *Note*: effective central/edge wavelength of spectral filter used for this spectrum
*parameters_instrument*_spectral_filter_width	float	U [!o_m] [V: !o_m]	ParIns L0 L3	V/Vv	var.	Full width at half maximum of the filter *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • stored in the database and provided to user in "*parameters_instrument*_spectral_unit" *Note*: - Conversion from wavenumber ν (cm^{-1}) to wavelength λ (µm):

=> width(λ) = 10000/(center(ν)+width(ν)/2) -10000/(center(ν)-width(ν)/2)

- Conversion from wavelength λ (µm) to wavenumber ν (cm^{-1}):
  => width(ν) = 10000/(center(λ)+width(λ)/2) -10000/(center(λ)-width(λ)/2)

Condition: Mandatory only when "*parameters_instrument*_spectral_filter_type" ≠ Ø (if a filter/diaphragm is used)

Notes:

- used in particular to specify the width of a series of narrow bandpass filters
- generally not used for low/high pass filters

Variable: spectrum

Condition: Mandatory if at least one value of the bloc "*parameters_instrument_spectral_filters"* is changed

Note: effective width of spectral filter used for this spectrum

*parameters_instrument*_spectral_comments	U [m] [V: m]	ParIns L0	V/Vv [Ver] Aj	--	Additional information on spectral parameters: special range type, narrow-band filter peak transmission and transmission shape, info on variable spectral resolution, uncertainties, ...

Instrument angular parameters (goniometer, ellipsometer)

Definition: The angles follow the « positive & same origin and direction » notation as defined for physics, i.e all angles are positive with the following ranges: i (0-90°), e (0-90°), az (0-360°) with origin (0°) at nadir for incidence 'i' and emergence 'e' and 0° for azimuth 'az' (increasing clockwise) when the direction of i and e are both in the same quadrant of the principal plane. The specular geometry is thus for i = e, az = 180° and the opposition geometry is for i = e, az = 0°.

Definition (short): incidence and emergence angles are positive with origin at nadir and azimuth origin (increasing clockwise) is for i = e (opposition geometry).

Note: the « positive & opposite » notation defined for remote sensing, i.e all angles are positive with the following ranges, is the following: i (0-90°), e (0-90°), az (0-360°) with 0° at nadir for i and e and 0° for azimuth (increasing clockwise) when the direction of i and e are opposite in the principal plane. The specular geometry is thus for i=e, az = 0° and the opposition geometryis for i=e, az=180°.

Note: The "*parameters_instrument*_angle_incidence/_emergence/_azimuth" need only to be given for spectra with a single geometry ("*parameters_instrument*_angle_observation_mode" = 'fixed angles'). For multi-angles data the set of 'i,e,az' values are either given manually with each spectral file (using "*spectrum*_file_angle_incidence/_emergence/_azimuth/_phase"), or are provided directly inside the file "*spectrum*_file_filename"

parameters_instrument_angle		[!o] [V: £O]				£: instrument angular parameters *Condition:* Mandatory only for "*instrument*_technique" = {specular reflection, ellipsometry, bidirectional reflection, biconical reflection, directional-hemispherical reflection, hemispherical-directional reflection, scattering, thermal emission} ***Variable: spectrum*** *Condition:* compulsory to give the effective value for the spectrum if it changed compared to the global value given in experiment
*parameters_instrument*_angle_observation_geometry	enum(text)	S1 [!!o_m] [V: m]	ParIns L0	V	--	Type of angular geometry of the illumination and observation Enum: {direct, specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical, hemispherical-directional, hemispherical-conical, bihemispherical, directional, conical, hemispherical, other geometry, various, unknown, N/A} *Condition:* absolute mandatory only when "*parameters_instrument*_instrument_uid" / "*instrument*_technique" = {specular reflection, ellipsometry, bidirectional reflection, biconical reflection, confocal reflection, diffuse reflection, directional-hemispherical reflection, hemispherical-directional reflection, scattering, thermal emission} *Default* = • 'direct' when "*instrument*_technique" = {transmission, Mossbauer absorption, permittivity} • 'specular' when "*instrument*_technique" = {reflection-absorption, ATReflection} • 'other geometry' when "*instrument*_technique" = {Raman scattering, fluorescence emission, gamma emission, time-domain, dual polarisation interferometry} *Definitions:*

- ‘*direct’*: measurement exactly in the same axis as the illumination (mostly for transmission)
- ‘*specular’*: bidirectional observation at the opposite angle to illumination incidence angle relative to the normal of the surface
  Ex: ellipsometry
- ‘*bidirectional’*: illumination at a well defined incidence angle and observation at well defined emergence and azimuth angles. Both the angular ranges (angular width of cones) of illumination and observation are small (< 10°?)
- ‘*directional-conical’*: illumination at a well defined incidence angle (angular range < 10°?) and observation integrated over a large regular angular range (cone) (> 10°?)
- ‘*conical- directional’*: illumination over a large regular angular range (cone) (> 10°?) and observation at a well defined emergence and azimuth angles (angular range < 10°?)
- ‘*biconical’*: illumination and observation at well defined central angle of incidence and observation but with large regular angular ranges (cones) (> 10°?)
- ‘*directional-hemispherical’*: illumination at a well defined incidence angle and observation integrated over (almost) the whole hemisphere. The angular range of illumination is small (< 10°?)
- ‘*conical-hemispherical’*: illumination over a large regular angular range (cone) (> 10°?) and observation integrated over (almost) the whole hemisphere. The angular range of illumination is small (< 10°?)
- ‘*hemispherical-directional’*: diffuse illumination over (almost) the hemisphere and observation at well defined emergence and azimuth angles. The angular range of observation is small (< 10°?)
- ‘*hemispherical-conical’*: diffuse illumination over (almost) the hemisphere and observation integrated over a large regular angular range (cone) (> 10°?)
- ‘*bihemispherical’*: diffuse illumination over the hemisphere and observation integrated over (almost) the whole hemisphere.
- ‘*directional’*: measurement at well defined emergence and azimuth angles, but with no illumination (thermal)
- ‘*conical’*: measurement at well defined central angle of observation but

with large regular angular ranges (angular width of cone) (> 10°?), and with no illumination (thermal).

- '*hemispherical'*: observation integrated over (almost) the whole hemisphere but with no illumination (thermal).
- '*other geometry'*: measurement with a illumination-observation geometry not described above. Describe the geometry in "*parameters_instrument*_angle_comments"
  Ex: ATR transmission geometry
  Ex: reflectance measurements in special attachments in FTIR spectrometers: the 'bi-conical' geometry of the illumination and observation (central angles, and solid angles shape) is not simple.
- '*various'*: measurements over various geometries within the experiment. Provide the different geometries in "*parameters_instrument*_angle_comments".
  Note: 'various' used only for "experiment", not for "spectrum"
- '*unknown'*: measurement over an unknown or incompletely known geometry. Provide what you know on the geometry in "*parameters_instrument*_angle_comments".
- '*N/A*': measurement for which angles have no signification, e.g., optical constants, …

Variable: spectrum

Notes:

- effective angular geometry of observation for this spectrum

*parameters_instrument*_angle_observation_mode	enum(text)	S3 [!!o_m] [V: m]	ParIns L0	V	--	Mode of angular variation of the illumination and observation geometries Enum: {fixed angles, one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set, unknown, N/A} *Condition:* absolute mandatory only when "*parameters_instrument*_instrument_uid" / "*instrument*_technique" = {specular reflection, ellipsometry, bidirectional reflection, biconical reflection, confocal reflection, diffuse reflection, directional-hemispherical reflection,

hemispherical-directional reflection, scattering, thermal emission}

Default = 'fixed angles' when "*instrument*_technique" = {transmission, reflection-absorption, ATReflection, Raman scattering, fluorescence emission, gamma emission, Mossbauer absorption, permittivity, time-domain, dual polarisation interferometry}

Definitions:

- '*fixed angles'*: measurement at a single combination of illumination and observation angles (or single observation angle)
- '*one variable angle'*: measurement with one of either the illumination (incidence) or the observation angles (emergence, azimuth) varying in a few discrete values in the dataset.
  Ex: Bidirectional spectra at i=0° and e=15, 30, 45, 60°
- '*two variable angles'*: measurement with two of either the illumination (incidence) or the observation angles (emergence, azimuth) varying in a few discrete values in the dataset.
  Ex: bidirectional spectra at all combinations of i=0, 15, 30, 45, 60° and e=15, 30, 45, 60°
- '*three variable angles'*: measurement with all three illumination (incidence) and observation angles (emergence, azimuth) varying in a few discrete values in the dataset.
- '*fixed phase angle':* measurement at a fixed phase angle but for a few couples of illumination and observation (and possibly azimuth) angles.
  Ex: bidirectional spectra at fixed phase angle for a set of 5 (i,e) couples: (0,15°), (15, 30°), (30,45°), (45,60°), (60,75°)
- '*mono-angular function'*: measurement with one of either the illumination (incidence) or the observation angles (emergence, azimuth) varying continuously over a large number of angles, typically evenly sampled over a wide range. The other angles may have a few values.
  Ex: BRDF in the principal plane for a large set of observation angles but at a single illumination angle.
- '*bi-angular function'*: measurement with two of either the illumination (incidence) or the observation angles (emergence, azimuth) varying continuously over a large number of angles, typically evenly sampled

over wide ranges. The other angle may have a few values.

Ex: BRDF in the principal plane for a large set of illumination and observation angles (azimuth = 0, 180°)

Ex: BRDF in the whole observation hemisphere for a single illumination angle.

- '*tri-angular function'*: set of measurements with all three illumination (incidence) and observation angles (emergence, azimuth) varying continuously over a large number of angles, typically evenly sampled.

  Ex: whole BRDF in the whole observation hemisphere for a large set of illumination angles.
- '*fixed phase angle function':* measurement at a fixed phase angle but for different couples of illumination and observation (and possibly azimuth) angles varying continuously over a large number of angles, typically evenly sampled.

  Ex: bidirectional spectra in the principal plane at fixed phase angle g=5° for i=[0-75°], every 1°
- '*other geometry set'*: measurement with a combination of angles and sampling not described above. Describe the set of geometries in "*parameters_instrument*_angle_comments".

  Ex:
- '*unknown'*: measurement over an unknown or incompletely known geometry set. Provide what you know on the geometry set in "*parameters_instrument*_angle_comments".
- '*N/A*': measurement for which angles have no signification, e.g., optical constants, …

Notes:

- 'variable angles' are typically for 2 to 4 different values for each angles, or for unevenly spaced measurements

  Ex: '*two variable angles'* (i,e) = (0,10), (0,30), (0,60), (30,0), (30,40), (30,60), (60,0), (60,30), (60,70), az=0°
- 'angular functions' are typically for ≥ 5 different values (~evenly spaced) for each angle.

  Ex:
  - '*mono-angular function'*: i= 0, 30°, e = 0, 15, 30, 45, 60, 75°, az=0, 180°

							○ '*bi-angular function'*: i = 0, 15, 30, 45, 60, 75°; e = 0, 15, 30, 45, 60, 75°; az= 0, 90, 180° ○ '*tri-angular function'*: i = 0, 15, 30, 45, 60, 75°; e = 0, 15, 30, 45, 60, 75°; az= 0, 30, 60, 90, 120, 150, 180° ***Variable: spectrum*** *Note*: - effective angular mode of observation for this spectrum - for "*spectrum*_files_parameter_type" ='simple spectrum' it will be always '*fixed angles'*
parameters_instrument_angle_incidences [-xml]	***List [L4]***	[!o_c] [V: c]					£: instrument incidence angles (multiple for BRDF only)
*parameters_instrument*_angle_incidence	float	S3 [!o_m] [V: m]	ParIns L0 L4	**V+**	deg	Incidence angle 'i' of illumination relative to the normal to the sample surface • stored in the database and provided to user in 'deg' unit *Condition:* Mandatory only when "*parameters_instrument*_angle_observation_mode" = 'fixed angles' AND when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical} *Constraints:* ➔ filled automatically for the other observation modes using the values of each spectrum of the experiment either from "*spectrum*_file_multiangle_angle_incidence" or from the values in the file "*spectrum*_file_filename" ("*parameters_instrument*_angle_observation_mode" = {one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set}) *Definition:* - the incidence angle is measured from the normal to the sample surface

and is always positive from 0° to 90°

Note xml:

- for multi-angles experiments (BRDF, M/SBRDF, …) the full list of values of incidence angles has not to be filled manually: it will be calculated either from "*spectrum*_file_multiangle_angle_incidence" or from the file "*spectrum*_file_filename"

Variable: spectrum

Constraints:

➔ filled automatically for the other observation modes using the values of "*spectrum*_file_multiangle_angle_incidence" or from the values in the file "*spectrum*_file_filename"

Notes:

- effective incidence angle for this spectrum
- or the whole series of incidence angles for (spectro-)photometric data

parameters_instrument_angle_emergences [-xml]	***List [L5]***	[!o_c] [V: c]				£: instrument emergence angles (multiple for (S)BRDF and (S)DEDF only)
*parameters_instrument*_angle_emergence	float	S3 [!o_m] [V: m]	ParIns L0 L5	**V+**	deg	Emergence angle 'e' of observation relative to the normal to the sample surface • stored in the database and provided to user in 'deg' unit *Condition:* Mandatory only when "*parameters_instrument*_angle_observation_mode" = 'fixed angles' AND when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, hemispherical-directional, hemispherical-conical, directional, conical} *Constraints:* Same as for "*parameters_instrument*_angle_incidence" but with "*spectrum*_file_multiangle_angle_emergence" *Definitions:*

- the emergence angle is measured from the normal to the sample surface and is always positive from 0° to 180°
- For particle scattering the emergence is defined relative to the plane perpendicular to illumination.

Notes:

- for reflection measurements the angle should have values between 0° and 90°
- for 'specular reflection' and 'ellipsometry' it should be equal or close to the incidence angle
- for transmission measurements the angle should have values between 90° and 180° (i.e. '180° - incidence': e.g. emergence = 180° for incidence = 0°)
- for scattering measurements the angle can have values from 0 to 360° (0-90°+270-360°: backward, 90-270°: forward) but if the scatterer is symmetrical relative to the incidence direction then azimuth is unimportant and values simply varies from 0 to 180°

Note xml:

- for multi-angles experiments (BRDF, M/SBRDF, DEDF, M/SDEDF, scattering …) the full list of values of emergence angles has not to be filled manually: it will be calculated either from "*spectrum*_file_multiangle_angle_emergence " or from the file "*spectrum*_file_filename"

Variable: spectrum

Constraints:

Same as for "*parameters_instrument*_angle_incidence" but with "*spectrum*_file_multiangle_angle_emergence"

Notes:

- effective emergence angle for this spectrum,
- or the whole series of emergence angles for (spectro-)photometric data

parameters_instrument_angle_azimuths [-xml]	***List [L6]***	[!o_c] [V: c]

£: instrument azimuth angles (multiple for (S)BRDF and (S)DEDF only)

*parameters_instrument*_angle_azimuth	float	S3 [!o_mc] [V: mc]	ParIns L0 L6	**V+**	deg	Azimuth angle ‘az’ of observation relative to the plane perpendicular to the surface and containing the illumination beam – stored in the database and provided to user in ‘deg’ unit *Condition:* Mandatory only when “*parameters_instrument*_angle_observation_mode“ = ’fixed angles’ AND when “*parameters_instrument*_angle_observation_geometry” = {bidirectional, directional-conical, conical-directional, biconical} AND when “parameters_instrument_angle_phase" = {Ø, NULL} *Constraints:* Same as for “*parameters_instrument*_angle_incidence” but with “*spectrum*_file_multiangle_angle_azimuth" ➔ calculated when “*parameters_instrument*_angle_azimuth" = Ø and when “*parameters_instrument*_angle_phase" ≠ {Ø, NULL} using the incidence, emergence and phase angles. ⇨ “angle_azimuth” = arcos[(cos(angle_phase) - cos(angle_incidence) * cos(angle_emergence))/(sin(angle_incidence) * sin(angle_emergence))] *Definitions:* – For a surface the azimuth angle is measured in the plane of the surface and its origin is in the principal plane (plane perpendicular to the surface and containing the illumination beam), but on the opposite side of the illumination. It is always positive from 0° to 360° and is counted in the counter-clock (trigonometric) direction. – A value of 0° corresponds to an observation in the principal plane and in the forward direction, while a value of 180° is in the backward direction (i.e. same side as incidence angle). – For particle scattering or for emission the azimuth is defined in the plane perpendicular to the illumination and from an arbitrary origin azimuth. *Notes:*

- should be set to '0' for normal illumination (incidence angle = 0, where azimuth is indefinite)
- for ‘specular reflectance’ and ‘complex reflectance ratio’ this angle is generally = 0, but some specular reflection studies can explore small azimuth angles.
- In the case of aerosols scattering azimuth is generally set to 0, except if the medium is anisotropic or scatter anisotropically. A reference azimuth must then be defined.
- for emission and scattering measurements a reference azimuth should be defined
- not defined for 'directional-hemispherical reflection' and 'hemispherical-directional reflection'

Note xml:

- for multi-angles experiments (BRDF, M/SBRDF, …) the full list of values of azimuth angles has not to be filled manually: it will be calculated either from “*spectrum*_file_multiangle_angle_azimuth" or from the file "*spectrum*_file_filename"

Variable: spectrum

Condition: Mandatory only when
“*parameters_instrument*_angle_observation_mode“ = ’fixed angles’
AND
when “*parameters_instrument*_angle_observation_geometry” = {bidirectional, directional-conical, conical-directional, biconical}
AND
when “*parameters_instrument*_angle_phase" = {Ø}

Constraints:

Same as for “*parameters_instrument*_angle_incidence” but with “*spectrum*_file_multiangle_angle_azimuth"

Notes:

- effective azimuth angle for this spectrum
- or series of azimuth angles for (spectro-)photometric data

parameters_instrument_angle_phases [-xml]	***List [L6b]***	[!o_c] [V: c]				£: instrument phase angles (multiple for (S)BRDF only)
*parameters_instrument*_angle_phase	float	S3 [!o_cm] [V: !o_cm]	ParIns L0 L6b	**V+**	deg	Phase angle ‘ph’ between the incident illumination and the observation directions - stored in the database and provided to user in ‘deg’ unit *Condition:* Mandatory only when “*parameters_instrument*_angle_observation_mode“ = ’fixed angles’ AND when “*parameters_instrument*_angle_observation_geometry” = {bidirectional, directional-conical, conical-directional, biconical} AND when “*parameters_instrument*_angle_azimuth” = {Ø, NULL} *Constraints:* Same as for “*parameters_instrument*_angle_incidence” but with “*spectrum*_file_multiangle_angle_phase" ➔ set to ‘0’ when both “*parameters_instrument*_angle_azimuth" and "_phase” = Ø ➔ calculated when “*parameters_instrument*_angle_phase" = Ø and when “*parameters_instrument*_angle_azimuth" ≠ {Ø, NULL} using the incidence, emergence and phase angles. ⇨ “angle_phase” = arcos[cos(angle_incidence) * cos(angle_emergence) + sin(angle_incidence) * sin(angle_emergence) * cos(angle_azimuth)] *Definition:* - the phase angle is the absolute value of the angle between the incident illumination and the observation directions in the plane containing both the illumination and observation directions. It is always positive from 0° to 180° *Notes*: - for ‘specular reflection’ it should be generally equal to 2 times the incidence angle

Note xml:

- The phase angle can also be set manually in the xml
- for multi-angles experiments (BRDF, M/SBRDF, …) the full list of values of phases angles has not to be filled manually: it will be taken or calculated either from "*spectrum*_file_multiangle_angle_incidence/_emergence/_azimuth/_phase" or from the file "*spectrum*_file_filename"

Variable: spectrum

Condition: Mandatory only when
"*parameters_instrument*_angle_observation_mode" = 'fixed angles'
AND
when "*parameters_instrument*_angle_observation_geometry" = {bidirectional, directional-conical, conical-directional, biconical}
AND
when "*parameters_instrument*_angle_azimuth" = {Ø}

Constraints:

Same as for "*parameters_instrument*_angle_incidence" but with "*spectrum*_file_multiangle_angle_phase"

Note:

- effective phase angle for this spectrum
- or series of phase angles for (spectro-)photometric data

*parameters_instrument*_angle_resolution_illumination	float	U [!o_m] [V: m]	ParIns L0	V	deg	Angular optical resolution of the illumination (incident) beam (defined as the FWHM of the intensity of the beam) • stored in the database and provided to user in 'deg' unit *Condition:* Mandatory only when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical} *Notes:* - = '180°' for 'hemispherical-directional reflection' - *Note:* for 'biconical reflection' it is the angular width of the observation

						cone. - also useful for fixed angle spectrometers (non-parallel or focused illumination, …) ***Variable: spectrum*** *Note*: effective angular optical resolution of the illumination (incident) beam for this spectrum.
*parameters_instrument*_angle_resolution_observation	float	U [!o_m] [V: m]	ParIns L0	V	deg	Angular optical resolution of the detection system (defined as the FWHM of the intensity collected) • stored in the database and provided to user in 'deg' unit *Condition:* Mandatory only when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, hemispherical-directional, hemispherical-conical, directional, conical} *Notes:* - = '180°' for 'directional-hemispherical reflection' - for 'biconical reflection' it is the angular width of the observation cone. - also useful for fixed angle spectrometers (collection angle, …) ***Variable: spectrum*** *Note*: effective angular optical resolution of the detection system for this spectrum.
Anisotropic sample orientation		[O]				Used to define the relative orientation of an anisotropic sample (monocrystals, anisoptropic roughness, …) relative to the illumination or observation beams
*parameters_instrument*_angle_anisotropic_reference_axis	varchar(255)	U [!o_m] [V: m]	ParIns L0	V	--	Illumination or observation reference axis used to define the anisotropic sample orientation Enum: {illumination, observation, other, unknown} *Condition:* mandatory when *"parameters_instrument*_angle_anisotropic_sample_angle" ≠ Ø *Notes:*

- for a reference axis other than the illumination or observation axis, provide the information in "*parameters_instrument*_angle_comments"

Variable: spectrum

Note:

- effective illumination or observation reference axis used to define the anisotropic sample orientation for this spectrum.
- better to keep the definition of this reference axis constant over the experiment.

*parameters_instrument*_angle_anisotropic_sample_axis	varchar(255)	U [!o_m] [V: m]	ParIns L0	V	--	Definition of an axis of the anisotropic sample used to measure its angle relative to the reference axis *Condition:* mandatory when *"parameters_instrument*_angle_anisotropic_sample_angle" ≠ Ø *Definition:* define a physical or an arbitrary axis of the sample taking into account its anisotropy (principal axis, crystal axis, …) *Ex:* - for a sample with an anisotrope surface o simple textual description of a main axis of the sample: *Ex*: 'axis perpendicular to the ripples' o definition of the axis relative to geographic orientation (for field measurement) *Ex*: 'geographic N, WGS84' - for a monocrystals: o simple textual description of a main axis: *Ex*: 'c axis of hexagonal H2O ice' o Direction indices of the crystallographic axe (perpendicular to the plane defined with same Miller indices). *Ex*: '[010] direction' *Note*: to write a negative coordinate use LaTeX: '[1\overline11]' for $[1\bar{1}1]$ o Miller's hkl indices, or description, of the crystalline plane of the monocrystal used to measure its angle relative to the reference axis

							Definition: a family of lattice planes is determined by three integers h, k, and ℓ, the Miller indices. They are written '(hkℓ)', and denote the family of planes orthogonal to $hb_1 + kb_2 + \ell b_3$. where b_i are the basis of the reciprocal lattice vectors *Ex*: 'normal to (010) plane' *Ref*: https://en.wikipedia.org/wiki/Miller_index *Notes:* - 'random orientation' can be used for isotropically oriented powders, and 'unknown' if this angle may be of importance but is unknown ***Variable: spectrum*** *Note*: - effective axis of the anisotropic sample, of the crystalline plane of the monocrystals…, used to measure its angle relative to the reference axis for this spectrum. - better to keep the definition of this axis constant over the experiment.
*parameters_instrument*_angle_anisotropic_sample_angle	varchar(255)	U [m] [V: m]	ParIns L0	V	deg	Angle (+ error) of the sample axis relative to the reference axis • Unit: provide angle and error in deg *Note:* the sample axis is defined in *"parameters_instrument*_angle_anisotropic_sample_axis" and the reference axis in *"parameters_instrument*_anisotropic_reference_axis" Ex: '15 +/- 0.5 deg' or '15° +/- 0.5°' or '$15\deg \pm 5 \deg$ ***Variable: spectrum*** *Note*: Angle (+ error) of the sample axis relative to the reference axis for this spectrum.
*parameters_instrument*_angle_comments	blob	U [m] [V: m]	ParIns L0	V Aj	--	Additional information on angular parameters: angular resolution functions, *Note*: uncertainties, ... ***Variable: spectrum***

						Note: additional comments for this spectrum.
Instrument polarization parameters (goniometer, ellipsometer, …)						
parameters_instrument_polarization		[O] [V: £O]				£: instrument polarization parameters ***Variable: spectrum*** *Condition:* compulsory to give the effective value for the spectrum if it changed compared to the global value given in experiment
*parameters_instrument*_polarization_type_illumination	enum(text)	S1 [!o_m] [V: m]	ParIns L0	V	--	Type of polarization of the incident illumination beam (linear, circular, …) Enum: {linear, circular, elliptic, no} *Condition:* Mandatory only when "polarization_polarizer_illumination" ≠ Ø *Note:* to be filled when an illumination polarizer is used
*parameters_instrument*_polarization_type_observation	enum(text)	S1 [!o_m] [V: m]	ParIns L0	V	--	Type of polarization of the observation system (linear, circular, …) Enum: {linear, circular, elliptic, no} *Condition:* Mandatory only when "polarization_polarizer_observation" ≠ Ø *Note:* to be filled when an observation polarizer is used
*parameters_instrument*_polarization_polarizer_illumination	varchar(255)	U [m] [V: m]	ParIns L0	V	--	Type of polarizer of the incident illumination beam
*parameters_instrument*_polarization_polarizer_observation	varchar(255)	U [m] [V: m]	ParIns L0	V	--	Type of polarizer of the observation system
*parameters_instrument*_polarization_rejection_illumination	varchar(255)	U [!o_m]	ParIns L0	Vc	--	Rejection rate of the polarization of the incident illumination beam *Condition:* only when "polarization_type_illumination" = {linear, circular, elliptic}

		[V: m]				*Definition:* it is the ratio between the wanted and unwanted polarizations. *Notes:* – it can be given for a few wavelengths/wavenumbers – It can be expressed as a ratio, a percentage, or in dB
*parameters_instrument*_polarization_rejection_observation	varchar(255)	U [!o_m] [V: m]	ParIns L0	Vc	--	Rejection rate of the polarization of the observation system *Condition:* only when "polarization_type_observation" = {linear, circular, elliptic} *Definition:* see above *Note:* – it can be given for a few wavelengths/wavenumbers – It can be expressed as a ratio, a percentage, or in dB
*parameters_instrument*_polarization_angle_illumination	float	S3 [!o_m] [V: m]	ParIns L0	**V+**	deg	Polarization angle of the linearly polarized incident illumination beam relative to the illumination plane normal to the surface • stored in the database and provided to user in 'deg' unit *Condition:* only when "polarization_type_illumination" = {linear} *Note:* p-polarization corresponds to angle = 0° s-polarization corresponds to angle = 90°
*parameters_instrument*_polarization_angle_observation	float	S3 [!o_m] [V: m]	ParIns L0	**V+**	deg	Polarization angle of the observation system relative to the observation plane normal to the surface • stored in the database and provided to user in 'deg' unit *Condition:* only when "polarization_type_observation" = {linear} *Note:* p-polarization corresponds to angle = 0° s-polarization corresponds to angle = 90°
*parameters_instrument*_polarization_comments	blob	U [m]	ParIns L0	V Aj	--	Additional information on polarization parameters: polarization rejection spectral function, modulation of polarization, orientation of polarization relative to some axis (crystal, ...), ...

[V: m]

Instrument spatial modes and parameters (microscope, …)

Note: several of these parameters are only for IR or Raman microscopies

parameters_instrument_spatial		[!o] [V: £O]		V/Vv [Ver]		£: Instrument spatial parameters *Condition:* all keywords, except "*parameters_instrument*_spatial_observation_mode" are Mandatory only when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {linear scan, linear micro-scan, micro-imaging, imaging} (for linear scan and imager) ***Variable: spectrum*** *Condition:* compulsory to give the effective value for the spectrum if it changed compared to the global value given in experiment
*parameters_instrument*_spatial_observation_mode	enum(text)	S1b/Uu [!!_m] [V: m]	ParIns L0	V/Vv [Ver]	--	Mode of macro/microscopic observation Enum: {single spot, averaged, line, image, roi averaged, rastered, rastered image} *Definitions:* - '*single spot*': single punctual measurement • spatial_sampling_x/_y" or "spatial_extent_x/_y" gives the size of the measurement spot - '*averaged*': single average of several individual and non connex spatial measurements. • "spatial_extent_x/_y" gives the approximate total extent of the area covered by all the measurements. • "spatial_sampling_x/_y" gives the physical size of the individual measurements. • the number of measurements averaged is given in "spatial_spots_number" - '*line*': spectral linear scan of total physical size "spatial_extent_x/_y" • "spatial_measures_x" give the line size in number of pixels ("spatial_measures_y"='1')

    - “spatial_sampling_x/_y” give the individual pixel size.
- ‘*image’*: spectral image of total physical size “spatial_extent_x/_y”
    - “spatial_measures_x/_y” give the image size in number of pixels
    - “spatial_sampling_x/_y” give the individual pixel size.
- ‘*roi averaged’*: single average over a ROI (Region Of Interest = one or several groups of connex pixels) in an image (but not rectangular area).
    - “spatial_extent_x/_y” gives the approximate total extent of the area of the ROI.
    - “spatial_sampling_x/_y” gives the physical size of the individual pixels
    - the number of pixels averaged in the ROI can is in “spatial_spots_number”
- ‘*rastered’*: single average over a rectangular area of connex pixels in an image
    - “spatial_extent_x/_y” gives the total extent of the rectangular area
    - “spatial_sampling_x/_y” gives the physical size of the individual pixels
    - the number of pixels averaged in the rectangle is given in “spatial_spots_number”
- ‘*rastered image’*: part or all the pixels of an image are averaged over a grid of rectangular boxes (super-pixels)
    - “spatial_extent_x/_y” gives the total extent of the rastered area of the image
    - “spatial_measures_x/_y” give the boxes number
    - “spatial_sampling_x/_y” gives the physical size of the individual pixels
    - the number of pixels averaged in each box is given in “spatial_spots_number”

Variable: for Spectrum

Condition: same as above

*parameters_instrument*_spatial_unit	enum(text)	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	--	Unit in which all the spatial parameters are entered Enum: {nm, micron, mm, cm} *Condition:* mandatory when "*parameters_instrument*_spatial_sampling_x/_y" or "*parameters_instrument*_spatial_extent_x/_y" ≠ {Ø, NULL} OR *Condition:* compulsory when "*parameters_instrument*_spatial_resolution_width" has a value **Variable: for Spectrum** *Note:* better to keep the same for the whole experiment
*parameters_instrument*_spatial_objective	varchar(255)	U [!o_m] [V: !o_m]	ParIns L0	V	--	Type of objective (x10, x15, x40...) and focal length for microscope and spectro-imagers *Ex:* 'objective X15, focal length 40mm' *Condition:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {microscopy, linear micro-scan, micro-imaging} (for microscope) **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_spots_number	int(11)	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	--	Number of different measurement spots over the sample or number of pixels in the image averaged to get the 'averaged spectrum' *Condition:* Mandatory only for "*parameters_instrument*_spatial_observation_mode" = {averaged, roi averaged, rastered, rastered image} *Notes:* - for "*parameters_instrument*_spatial_observation_mode" = 'roi averaged', 'rastered' and 'rastered image' the "spatial_spots_number" is the number of pixels averaged - for "*parameters_instrument*_spatial_observation_mode" = 'averaged': it can be the number of individual grains of a sample (meteorite section, ...) measured to get their averaged spectrum (e.g. for Raman).

						It can be also the number of positions of the measurement spot on a sample, or the positions of a sample for bi-directional measurements (e.g. sample rotation to avoid particular specular effects). *Note:* optional for spectra levels 3 and 4 **Variable: for Spectrum** *Note:* better to keep the same for the whole experiment
*parameters_instrument*_spatial_sampling_x	float	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	var.	Spatial separation between image pixels (or pixel size) on the sample (over x axis), or separation between 'rastered' boxes when averaging is done over the x axis *Condition #1:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {linear scan, linear micro-scan, micro-imaging, imaging} (for linear scan and imager) AND *Condition #2:* Mandatory only for "*parameters_instrument*_spatial_observation_mode" = {averaged, line, image, rastered image} *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Note:* depends on "*parameters_instrument*_microscope_objective" & "observation_mode" (see these KW) **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_sampling_y	float	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	var.	Spatial separation between image pixels (or pixel size) on the sample (over y axis) or separation between 'rastered' boxes when averaging is done over the y axis *Condition #1:* Mandatory when "*instrument*_microscopy_imaging" = {micro-imaging, imaging} (for imager) AND

						Condition #2: Mandatory only for "*parameters_instrument*_spatial_observation_mode" = {averaged, image, rastered image} *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Note:* depends on "*parameters_instrument*_microscope_objective" & "observation_mode" (see these KW) **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_measures_x	int(10)	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	--	Total number of measurements over the x axis *Condition #1:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {linear scan, linear micro-scan, micro-imaging, imaging} (for linear scan and imager) AND *Condition #2:* Mandatory only for "*parameters_instrument*_spatial_observation_mode" = {line, image, rastered image} *Note:* = '1' for a 'single spot' and 'rastered' measurements, no value for 'averaged' **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_measures_y	int(10)	U [!o_m] [V: !o_m]	ParIns L0	V/Vv [Ver]	--	Total number of measurements over the y axis *Condition #1:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {micro-imaging, imaging} (for imager) AND *Condition #2:* Mandatory only for "*parameters_instrument*_spatial_observation_mode" = {image, rastered

						image} *Note:* = '1' for a ' single spot', 'line' and 'rastered' measurements, no value for 'averaged' **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_extent_x	float	U [!o_mc] [V: !o_m]	ParIns L0	V/Vv [Ver]	var.	Total spatial extent of the measurement over the x axis *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Condition:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {linear scan, linear micro-scan, micro-imaging, imaging} (for linear scan and imager) ➔ calculated (if void & condition #1) by: ⇨ spatial_extent_x = spatial_measures_x * spatial_sampling_x **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_extent_y	float	U [!o_mc] [V: !o_m]	ParIns L0	V/Vv [Ver]	var.	Total spatial extent of the measurement over the y axis *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Condition:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {micro-imaging, imaging} (for imager) ➔ calculated (if void & condition #1) by: ⇨ spatial_extent_y = spatial_measures_y * spatial_sampling_y **Variable: for Spectrum** *Note:*

*parameters_instrument*_spatial_distance_z	float	U [m] [V: m]	ParIns L0	V	m	Distance between the instrument and the measured surface (z axis) *Unit:* in 'meters' *Constraint:* recommended when "*experiment*_type" = {field measurement, low altitude remote sensing, satellite remote sensing} *Note*: can be a vertical elevation over the surface, but can be also any distance, even horizontal, from the instrument to the target. **Variable: for Spectrum** *Note:*
parameters_instrument_spatial_resolutions	***List [L7]***	[!o]		V/Vv [Ver]		£: Spatial resolutions on the sample at different wavenumbers/wavelengths *Condition:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {microscopy, linear scan, linear micro-scan, micro-imaging, imaging} (for microscope, linear scan and imager)
*parameters_instrument*_spatial_resolution_width	float	S3 [!o_m] [V: !o_m]	ParIns L0 L7	V/Vv	var.	Optical spatial resolution(s) on the sample (FWHM of the Point Spread Function) *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Condition:* Mandatory when "*parameters_instrument*_uid/*instrument*_microscopy_imaging" = {microscopy, linear scan, linear micro-scan, micro-imaging, imaging} (for microscope, linear scan and imager) *Notes:* - it is the spot size on the sample for ponctual macroscopic measurements - if constant with wavelength/wavenumber then give a single value. - vary strongly with wavelength for microscopic measurements - depends on "*parameters_instrument*_spatial_objective" &

						"observation_mode" **Variable: for Spectrum** *Condition*: Mandatory if at least one value of the bloc "*parameters_instrument_spatial_resolutions"* is changed *Note:*
*parameters_instrument*_spatial_resolution_width_error	float	U [m] [V: m]	ParIns L0 L7	V/Vv	var.	Absolute uncertainty(ies) on the optical spatial resolutions on the sample at different wavenumbers or wavelengths *Unit:* in unit defined in "*parameters_instrument*_spatial_unit" • converted in 'm' unit in the database but provided to user in "*parameters_instrument*_spatial_unit" *Note:* may also be used to take into account (roughly) effects such as unperfect focus on sample surface and/or sampling depth.
*parameters_instrument*_spatial_resolution_position	float	U [m] [V: m]	ParIns L0 L7	V/Vv	var.	Corresponding wavenumber/wavelength/frequency at which the optical spatial resolution(s) is given *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted and stored in 'cm-1' unit in the database but provided to user in the unit specified in "*parameters_instrument*_spectral_unit" **Variable: for Spectrum** *Note:*
*parameters_instrument*_spatial_comments	blob	U [m] [V: m]	ParIns L0	V/Vv [Ver] Aj	--	Additional information on spatial parameters: spot shape, spatial resolution function, variable spatial resolution (law of variation, …), ...

12. EXPERIMENTS

12.1 Definition

An **Experiment** is first defined as “a series (or one) *spectrum* measurements of a single *sample* with a unique *instrument* and only one of its technique”.

If there are (quasi-)simultaneous measurements of a same sample with 2 or more different instruments or techniques they can be in the same *experiment* but with different *instrument* and *instrument parameters*, and referring to the same *sample*.

Multiple types of experiment (”*experiment*_type”) are allowed in a single experiment, but then it is necessary to tell for each spectrum of which type it is.

Also, for field and remote sensing measurements, all the spectra should be on the same planetary body and within the same global area (but its size can be large on the planetary body!), and not scattered at the surface of the body, in order to be able to define a pertinent geolocalization of this area.

An experiment describes a series of measurements (spectra) with a single set of homogeneous variable parameter(s) of the sample (from the same category, such as "sample temperature", “annealing_temperature” and “annealing_time”) or/and one or more variable parameters of the instrument/technique (such as incidence/emergence/azimuth angles, ...).

An experiment is characterized by some measurement parameters that are fixed during an experiment (such as the “spectral range”, “spectral sampling” and “spectral resolution” ...), and by a small set (0 to 3) of main *variable sample parameters* (only in “*sample table*”) and/or several main *variable instrument parameters* that can be selected within a limited list (tagged Exp=‘V+’ (most frequently variable parameters) or ‘V’). A few ‘secondary’ parameters (taged ‘Vc’) may change “by consequence”.

All the parameters that vary during an experiment are described as “*spectrum parameters*” and their values are given for each spectrum.

In addition to the “*sample and instrument variables parameters”* the **experiment table** contains information on “s*ample and instrument parameters links”* and on *“date and experimentalist”*.

These main types of experiments identified are described below.

12.2 Different cases of experiments

12.2.1 Experiments with changes in physical conditions of the sample

During such an experiment a **sample** can be subjected to several types of changes in physical conditions.

In order to have a simple and tracable history of the sample we have limited these *experiments* to changes in physical conditions of the sample (thermal, pressure and fluid processings) that induce ***no major irreversible chemical or physical changes in the sample*** before each spectrum recording. i.e., no significant change should occur at the Layer/Material/Constituent or Species levels.

They are:
- a temperature cycling without phase change (variable sample temperature and possibly annealing temperature and time)
- a mechanical/hydrostatic pressure cycling without phase change (variable sample pressure and possibly maximum pressure)
- a gas/liquid pressure cycling of the sample (variable fluid composition and its temperature/pressure) for adsorption/absorption studies.

Two other types of experiments based on series of measurements have also been defined:
- a series of Raman or fluorescence measurements with laser pulses (variable total time ?)
- a series of microscopic measurements performed in differents places of a sample (see 5.4)

In the cases of ***Raman or fluorescence measurements*** the irradiation effects are directly linked with the measurement technique and the irradiation variable parameters (noted '(V)') need to be used as variables. Possible sample amteration should be noted in "sample_processing_comments"

In practical cases some ***"real experiments"*** can be more complex series of physical and/or chemical changes (and corresponding series of spectral measurements) but here such complex real experiments should be cut in several "simple (database) experiments" each time the process applied to the sample changes (e.g. temperature cycling after a pressure cycling) or when the sample is strongly and irreversibly physically (phase change, …) or chemically altered (new species, …). A new sample, but linked to the previous one (the "parent sample") needs then to be created with some changes in its description (phase, composition, proccessing, …) and thus a new simple experiment can start again.

12.2.2 Experiments with changes in measurements parameters

During an experiment several types of **instruments** (measurements) **parameters** can be changed (e.g. goniometer angles, microscope spatial extent, polarization angles, …) . Their number and combinations are not restricted as they are all "reversible" and have no effect on the sample (except some Raman or fluorescence measurements with laser pulses).

However we prefer to limit the variable instrument parameters within an experiment to an homogeneous set of parameters (e.g. the 3 goniometer angles, the polarization type and the 2 polarization angles, …) and to those who did not imply many other parameters changes.

12.2.3 Case of heterogeneous matters at the microscopic level

A special case occurs with series of microscopic measurements of samples with very heterogenous composition at the microscopic scale. Each spectral measurement at a different location can see another/others constituent(s).
Such a series of microscopic spectra on a single sample is defined as an "experiment" with the unique variable "*sample*_primary_constituent_index_list".

12.3 Limitation of "experiments"

For the following 2 special types of laboratory experiments we decided to consider that they are a series of simple experiments (one spectrum) , not a single one, because major changes occur in the sample before each spectrum recording:

- Samples with a thickness varying between each spectrum (e.g. during thin film deposition): in this case the main changes occur at the material level (material_mole, material_mass) and at the layer level (layer_thickness, layer_mass) with some possible changes "by consequence" in layer texture (texture, porosity, density).

- Samples subjected to a series of irradiations: in this case some strong chemical changes may occur at the constituent and species levels, in particular the species present in the constituent may change (constituent_matterspecies_index_list, matterspecies_matter_or_species_index_link), as well as their abundance (matterspecies_mole_fraction, matterspecies_mass_fraction) and possibly their state (matterspecies_compound_state, …).

Note: in such case it may be good to define a series of samples (and experiments) that have all the species present in the final sample (precursors and products, + eventual impurities) declared for all samples but with the product species set initially to zero abundance and then varying with irradiation dose.

The parent experiment can be tracked using "*experiment*_parent_experiment_uid", its sample with "s*ample*_parent_sample_uid" and the first experiment of the series of experiments with "*sample*_first_parent_experiment_uid".

12.4 Experiment Table

Root of the table: ***experiment***

Data type: 'Experiment and spectra'

Key-word	Type	Level	Table	Exp	Unit	Description
Experiment import mode and indexes						
*experiment*_import_mode	enum(text)	P [!!_m]	Exp	(V)	--	Mode of import of the Experiment/Instrument parameters data Enum: {first import, ignore, draft, no change, correction} *Definitions:* see "*sample*_import_mode"
*experiment*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Exp	V [Ver]	--	Name of the storage copy of the xml import file of the experiment metadata ➔ determined automatically during import (from "*experiment*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to apply correction
*experiment*_index [**][-xml]	int(10)	B [!!_g]	Exp	V [Ver]	--	Automatic random but unique number (internal ID) given to new experiment and to a new version
*experiment*_uid [**]	varchar(255)	S0 [!!_m]	Exp	F	--	Unique identifier code (UID) given to the experiment table (to be created) *Nomenclature:* Create this code name with 'EXPERIMENT_' very accurately in order to be simple and unique *Note DOI:* requested in "Identifier" (for 'experiment') *Ex:* It should be of the form 'EXPERIMENT_AB_yyyymmdd_1234' where 'AB' are the initials of the person preparing the import, 'yyyymmdd' is the full date of the day (or the day of the experiment), and '1234' is an order number for that day with a maximum of 4 digits from '0001 to '9999' (or 1 to 9, or 01 o 99, or 001 to 999).

						Ex: 'SPECTRUM_BS_20181006_059', 'SPECTRUM_OB_20000101_01'
*experiment*_sshade_doi [-xml]	varchar(255)	S1 [!!_c]	Exp	V [Ver]	--	DOI code of the experiment ➔ automatically generated using the UID of the experiment ⇨ 10.26302/SSHADE.*"experiment*_uid".V"*experiment*_version" *Definition:* http://en.wikipedia.org/wiki/Digital_object_identifier *Notes:* - The DOI is determined with "*experiment*_uid" and "*experiment*_version" - the prefix '10.26302' has been attributed by INIST to OSUG-DC, who will manage the doi creations. - the url of the doi is obtained by adding 'https://doi.org/' (note: the former standard whas 'http://dx.doi.org/') - the DOI will redirect to the SSHADE page displaying the experiment metadata (through a landing page) *Ex:* 10.26302/SSHADE.EXPERIMENT_LB_20170721_001.V2
*experiment*_sshade_url [-xml]	varchar(255) [Virtual KW]	U [!_c]	Exp	V [Ver]	--	Direct web link to the SSHADE experiment page displaying the experiment metadata ➔ automatically generated and in practice not stored in database *Notes:* - can be determined by knowing the UID (not restricted to experiment) - can be also obtained by copying the URL when viewing an experiment details page. *Ex:* https://www.sshade.eu/data/experiment/EXPERIMENT_LB_20170731_002
*experiment*_import_validation [pi] *[from provider interface]*	enum(text) [Vitual KW]	S2 [!!d_m]	Exp	V [Ver] ?	--	Validation state of an imported experiment Enum: {non-validated, validated} *Definitions:* - '*non-validated':* imported experiment metadata not yet validated in the

						database - *'validated':* experiment metadata validated in database *Default:* 'non-validated' *Notes:* - it is not a 'scientific' validation, but rather the validation of the correctness of the imported data. - The 'non-validated' state allows to import data in the database and take time to fully check them online. *Note:* implemented directly in the 'provider interface' with computer controlled data access rights, not through xml.
experiment_owner_databases	***List [L1]***	[!!]				£: databases which own and manage this experiment
*experiment*_owner_database_uid [*]	varchar(255)	S1 [!!o_m]	Exp DatBas L1	V [Ver]	--	Link(s) to the existing UID(s) of the which owns this experiment and manages its information (with associated spectra) *Condition:* at least one database *Note:* this KW will be used to define the list of databases to who the experiment belong *Note:* For experiments from external laboratories, not managed by a partner database, we will create specific database(s) (ex: 'DB_external') managed by the SSHADE managers
Experiment experimentalists						
experiment_experimentalists	***List [L2]***	[!]				£: experimentalists that conducted this experiment and/or processed its spectra
*experiment*_experimentalist_uid [*]	varchar(255)	S1/S1s [!_m]	Exp Exper L2	V [Ver]	--	Link to the existing UID of the experimentalist(s) who recorded and/or processed the spectra *Note DOI:* - mandatory as "Creator / creatorName" (2.1):

Experiment description

experiment_types	***List [L3]***	[!!]				£: Types of experiment
*experiment*_type	enum(text)	S0/S0s [!!_m]	Exp L3	V [Ver]	--	Type of experiment Enum: {laboratory measurement, numerical modeling, theoretical modeling, field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing, other, unknown} *Definitions:* - '*laboratory measurement*': experiment performed with the instrument inside a laboratory to record spectra of synthetic samples or of collected natural samples *Note*: '*laboratory measurements*' are the core of the SSHADE data - '*field measurement*': experiment performed on the field, with a portable instrument to record spectra of surfaces or of collected samples *Note*: The aim is to provide spectra of reference (well characterized) or analogue Earth surfaces or materials/grains/… under natural conditions *Ex:* o Reflectance spectra of series of volcanic rocks o Reflectance spectra of snow - '*low altitude field measurement*: experiment performed using an instrument aboard a low altitude flying device, like a plane, helicopter, UAV, drone, … to record spectra of surfaces *Note*: same as for '*field measurement*' but from flying devices - '*satellite remote sensing*': observation experiment performed using an instrument aboard an orbiting satellite or an exploration satellite to record spectra of surfaces… *Note*: The aim is to provide a selection of a few typical observation spectra of (simple) solid/liquid surfaces/grains/… of objects, or of typical area of objects.

Ex:

- Reflectance spectrum of CO_2 ice slab on Mars
- Reflectance spectra of N_2-rich:CH_4:CO ice on Pluto.

- '*telescopic remote sensing'*: observation performed using an instrument in a Earth based telescope to record spectra of the surface

  Note: same as for '*satellite remote sensing*' but from Earth based observatories

  Ex:

  - Hemispherical integrated reflectance spectrum of Pluto
  - Reflectance spectra of typical asteroids
  - Transmission spectra of typical interstellar cloud
- '*numerical modeling*': experiment performed with a numerical model (radiative transfert, …) that simulate some type of spectra.

  Note: One aim is to provide reference simulated spectra comparable to observations where laboratory and field measurements currently fail to provide data.

  Ex:

  - Reflectance spectra of CH_4 ice at 40K simulated from optical constants.
  - Series of reflectance spectra of H_2O ice with different temperatures and grain sizes.
- '*theoretical modeling*': experiment performed with a theoretical model (ab-initio, …, …) that simulate some type of spectra.

  Note: One aim is to provide theoretical simulated spectra comparable to laboratory measurements and also spectra where laboratory currently fail to provide data (unstable solids, …)

  Ex:

  - Raman spectra of minerals (ex: Wurm database)
  - spectra of Polyynes: H-[C≡C-]n-H .
- '*other*': any other experiment type not listed above. Describe it in "*experiment*_comments"
- '*unknown*': unknown experiment type! (should be only for very exceptional cases)

Notes:

- Multiple types of experiment ("*experiment*_type") are allowed in a

						single experiment, but then it is necessary to tell for each spectrum of which type it is. - When "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} are combined with "*experiment*_type" = {laboratory measurement, numerical modeling, theoretical modeling} it is necessary that these last measurements and modeling are directly linked with the field measurements to share the global geolocation of the experiment. - '*satellite remote sensing*' and '*telescopic remote sensing'* are observations rather than experiments or field measurements but are added here only to provide a few typical reference spectra of objects or of types of terrains of an object.
*experiment*_title	varchar(255)	S0/S0s [!!_m]	Exp	V [Ver]	--	Title describing the experiment (with main variable parameters) *Note:* - it should contain the main info on the sample and (or series of samples) and spectra obtained during the experiment - it will be displayed as search result *Ex:* 'NIR reflectance spectra of 2 olivine/iron mixtures with 2 grain sizes (20, 30 µm) at 50 and 60K', 'Vis-NIR absorption coefficient spectrum of CH4 phase-I crystal at 30 K' 'MIR transmission spectrum of Portlandite at -10°C under 2b CO2 gas 60min' *Note DOI:* - (absolute-)mandatory as "Title" (3), option as "Title/titleType" (3.1) for 'Experiment' - This title is used to create the DOI reference of the data.
*experiment*_description	blob	U [!o_m]	Exp	V [Ver]	--	Detailled description of the experiment. *Condition*: mandatory when there are more than one value in "*experiment*_variable_parameters_type" *Notes:* - it should contain complete info on the sample (or series of samples)

and the variable parameters (with values or range of values) of this experiment, and also on the spectra types/range.
- it should describe the organization of the series and subseries of samples (described details in "experiment_structure")
- information on possible variations of the samples may be also given
- it will be displayed as detailed info on search result.

Ex: 'Near-IR reflectance spectra of 3 mixtures of olivine and iron minerals with relative abundances of 90/10, 80/20 and 70/30 w%. These mixtures are studied for 3 grain size ranges (25-50, 100-150 and 250-300 µm) at 12 temperatures between 100 and 270 K.'

Note DOI:
- Recommended option as "Description / descriptionType=Abstract" (17)

Experiment history

*experiment*_date_begin	date	S1/S1bs [!_m]	Exp	V [Ver]	YYYY-MM-DD	Starting date of the experiment *Note DOI:* - recommended as "Date/dataType=Collected" (8) for 'Experiment' o Convention: "*experiment*_date_begin"/"*experiment*_date_end" for date ranges
*experiment*_date_end	date	U [m]	Exp	V [Ver]	YYYY-MM-DD	Ending date of the experiment *Note DOI:* - see "*experiment*_date_begin"
*experiment*_version [-xml]	int(3)	S3 [!!oc]	Exp	V [Ver]	--	Version number of the experiment data ➔ Set to '1' at first experiment ingestion and then incremented automatically by the data ingestion software at each major change of at least one of the spectrum data file (when at least one "*spectrum*_import_mode" = 'new version') OR at the addition of a new spectrum ("*spectrum*_import_mode" = 'first import') OR when at least one of the spectrum is made public

						(“*spectrum*_access_right”=’public’)
						
						Definition:
						- A new experiment version is mostly the same experiment but in which either:
						  o some, or all, its spectra are modified (improved) and a new spectrum file is imported.
						  o some new spectra are added
						  o some, or all, its spectra are pushed to ‘public’ access right status (“*spectrum*_access_right”)
						
						Notes:
						- However if the modification of a spectrum produces a radical new spectral product at higher level, it is better to enter it as new spectrum of this experiment, or in a new experiment with this one as a parent, rather than as a new version of the spectrum.
						- It is tolerated to replace a spectrum by a new one but under the condition it is of same “*spectrum*_type”, it uses the same (or very similar) sample and (almost) the same instrument parameters. These parameter values will be modified in ‘spectrum’ but not in ‘experiment’
						- no new version number is generated when “*spectrum*_import_mode” = ‘correction’

*experiment*_date_created [-xml]	date	S1b/Uu [!!_c]	Exp	V [Ver]	YYYY-MM-DD	Date of first import or upgrade of one or more spectra of the experiment, i.e. date of creation of a new version. ➔ determined automatically by the data ingestion software. Initialy set to the date of entry of the experiment in the database (first import w. upload) and modified at each change (modification/upgrade) of a spectrum data file (i.e. when “*spectrum*_import_mode” = ‘new version’) or addition of a new spectrum (“*spectrum*_import_mode” = ‘first import’) *Note:* - each “*experiment*_version” has its “*experiment*_date_created” (“*experiment*_version.date_created”) - it is the date of the “*spectrum*_date_created” of the new spectrum or

						new spectrum version that triggered the version of the experiment - in the code "*experiment*.date_created" correspond to "*experiment*_version.date_created" of the first version *Note DOI:* - recommended as "Date/dateType=Created" (8/8.1): ⇨ "*experiment*_version.date_created" for each "*experiment*_version"
*experiment*_date_updated [-xml]	date	S1b/Uu [!!_c]	Exp	V [Ver]	YYYY-MM-DD	Date of update of one or more spectra of the experiment ➔ determined automatically by the data ingestion software. Initialy set to the date of entry of the experiment in the database (first import) and modified at each change (update) of a spectrum metadata (i.e. when "*spectrum*_import_mode" = 'correction') until (not included) a new version is created "*spectrum*_import_mode" = 'first import' or 'new version') *Note:* - each "*experiment*_version" has its "*experiment*_date_updated" - it is the date of the "*spectrum*_date_updated" of the new spectrum or new spectrum version that triggered the version of the experiment - in the code "*experiment*.date_updated" correspond to "*experiment*_version.date_updated" of the last version *Note DOI:* - recommend as "Date/dateType=Updated" (8/8.1): ⇨ "*experiment*_version.date_updated" for each "*experiment*_version"
*experiment*_date_released [-xml]	date	S1b/Uu [!!_c]	Exp	F [Ver]	YYYY-MM-DD	Date of the first opening to public of the experiment ➔ determined automatically by the interface when at least one "*spectrum*_access_right" is set to 'public'. Initialy set to the date of release of the first spectrum of the experiment and created for each new version of the experiment *Note:* it is the older date of all the "*spectrum*_date_released" of the experiment *Note DOI:* - mandatory as "PublicationYear" (5) for 'Experiment': ⇨ year of "*experiment*_version.date_released" for each

"*experiment*_version"

- recommended as "Date/dateType=Issued" (8/8.1):
  ⇨ "*experiment*_version.date_released" for each "*experiment*_version"

Experiment links

*experiment*_parent_experiment_uid [*]	varchar(255)	S2/S2s [£o_m]	Exp Exp	V [Ver]	-- Link to the existing UID of a possible parent experiment performed just before this one and that created the initial conditions of the current experiment. *Recommendation:* Strongly recommended when already exist in the database
*experiment*_first_parent_experiment_uid [*] [-xml]	varchar(255)	S2 [!o_c]	Exp Exp	V [Ver]	-- Link to the existing UID of a possible first parent experiment, i.e., the first experiment in a series. *Condition:* when "*experiment*_parent_experiment_uid" ≠ Φ ➔ calculated recursively using "*experiment*_parent_experiment_uid" *Note xml*: not in xml

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Experiment geolocation or laboratory

Notes:

- For all 'field experiments' and 'remote sensing' (on Earth or other bodies) it is mandatory to use a "matter_planetary" to describe the matter at its original place, and provide its geolocalisation (the body and where it is measured).
  - The sample then uses the matter and adds the environment (+ sample/layer info).
  - The geolocalisation of the « spectrum » is simply inherited from the "matter" measured 'in-situ'.
- A global 'field experiment' geolocalisation can be defined at the experiment level when there are several field spectra recorded at ('slightly') different locations: along a line, within a square box or a more complex polygonal area.
- For a 'laboratory spectrum' of a matter collected in the field there is no experiment geolocalisation (only a laboratory with

						"*experiment*_laboratory_uid"), but the original matter(s) has one.
*experiment*_laboratory_uid [*]	varchar(255)	S1/S1s [!o_m]	Exp Labo	F	--	Link to the existing UID of the laboratory where the experiment was performed, and where the instrument is located at the time of the experiment *Condition:* mandatory only when "*experiment*_type" = {laboratory measurement, numerical modeling, theoretical modeling, telescopic remote sensing} *Note*: - constraint: only data from a single laboratory par experiment - for field or remote sensing measurements it can be also the laboratory that conducted the measurements - for telescopic remote sensing, it can be the telescope facility *Note DOI:* - option as "GeoLocation / geoLocationPlace" (18.3): "*laboratory*_city, _region, _country_code"
*experiment*_body_uid [*] [*matter*_body_uid]	varchar(255)	S1 [!!o_m]	Exp Mapr Body	F	F -- --	Link to the existing UID of the planetary body where the experiment was performed. *Condition:* absolute mandatory only when "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} *Format*: 'BODY_planetaryFamily_PlanetaryName' *Note:* - constraint: only data from a single body par experiment - This body is already in all the 'matter' ("*matter_xxx*_geolocation_body_uid") of the sample of the spectra of the experiment, but for easy and univoque access it is also defined (repeated) here. - this body could refer to a solar system body with the experiment remotely sampling part of that body

*experiment*_body_coordinate_system [*matter*_body_coordinate_system]	openum(text)	U [!!o_m]	Exp	F	--	Coordinate system on the planetary body used for the geographic location of this experiment OpenEnum: {WGS84, Mars 2000, Moon 2000, Pluto 2015, …} *Condition #1:* absolute mandatory only when "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} AND *Condition #2:* when "*experiment*_body_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Definitions*: - '*WGS84*': World Geodetic System 1984 for Earth (EPSG 4326) - '*Mars 2000'*: planetocentric latitude with east longitude for Mars - '*Pluto 2015'*: - … *Notes*: - constraint: an unique coordinate system per body - It is best to use the same coordinate system as the one used to locate the individual matters measured in this experiment - Prefer 'Planetocentric latitude with east longitude' coordinate systems for planetary bodies (approved by the International Astronomical Union) - Use only 'WGS84' planetographic system for Earth
experiment_geolocations	***List [L4]***	[!O_m]		V [Ver]		£: List of the geolocations of the area on the planetary body where the experiment was performed (for field and remote sensing experiments)
*experiment*_geolocation_place [*matter*_geolocation_place]	varchar(255)	S1b [!o_m]	Exp L4	V [Ver]	--	Name or description of the general geologic formation and geographic location on the planetary body where the experiment was performed (for field and remote sensing experiments) *Condition:* mandatory only when "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} Note:

						- This geolocation place should cover globally all the geolocations described in each sample matter of each spectrum of the experiment - They should be all on the same planetary body, which is given in each matter ("*matter_planetary_body*_uid") and repeated in "*experiment*_body_uid" *Ex:* - 'Western Keivy Massif, Kola Peninsula' (Earth) - 'Etna volcano' (Earth) - 'South part of Sputnik Planitia' (Pluto) - 'Mare Tranquilitatis' (moon), *Note DOI:* - recommended option as "GeoLocation / geoLocationPlace" (18.3)
*experiment*_geolocation_region [*matter*_geolocation _region]	varchar(255)	S1b [!o_m]	Exp L4	V [Ver]	--	Region, state, province or county (administrative location) on Earth of the experiment *Condition:* mandatory and only when "*experiment*_body_uid" = 'BODY_planet_Earth' *Ex:* - 'Murmanskaja Oblast', 'Sicilia', 'Rhône-Alpes', 'Arizona', 'Zambezi'
*experiment*_geolocation_country_code [*matter*_geolocation_country_code]	enum(text)	S1b [!o_m]	Exp L4	V [Ver]	--	2-digit code of the country of the geographic location on Earth of the experiment Enum: {CH, DE, ES, FR, GB, HU, IT, PL, …} Label (code): see "*laboratory*_address_country_code" *Condition:* mandatory and only when "*experiment*_body_uid" = 'BODY_planet_Earth' *Definitions:* see "*laboratory*_address_country_code"
*experiment*_geolocation_type	enum(text)	U [!!o_m]	Exp L4	V [Ver]	--	Type of geographic location where the experiment was performed (for field and remote sensing experiments) Enum: {point, line, box, polygon}

				Condition: mandatory only when "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} AND *Condition #2:* when "*experiment*_body_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition:* absolute mandatory and only when "*experiment*_geolocation_coordinate_latitude" ≠ Ø *Definitions*: - '*point*': punctual location defined by a single point (when all spectra are measured within a very small area, typically < few 10s m) - '*line*': linear location defined by its two extreme points, or polyline defined by a series of points (line of flight, line of sight, …) - '*box*': rectangular geographic location defined by two points: SW & NE coordinates - '*polygon*': spatial limit of a place defined by an ordered series of points (image, footprint) *Note DOI:* - recommended option as "GeoLocation / geoLocationPoint" (18.1) or "/ geoLocationBox" (18.2) or "/ geoLocationPolygon" (18.4)
experiment_geolocation_coordinates [*matter_geolocation_coordinates*]	***List [L5]***	[!O]	V [Ver]	£: Geolocation on the planetary body of the place where the experiment was performed (for field and remote sensing experiments) *Condition #1:* mandatory only when "*experiment*_type" = {field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing} AND *Condition #2:* when "*experiment*_body_uid" / "*body*_family" = {planet, dwarf planet, satellite} *Condition #3:* absolute mandatory when "*experiment*_geolocation_type" ≠ Ø *Conditions:* on the number of long/lat couple: - = '1' when "*experiment*_geolocation_type" = {point}

						- = '2': when "*experiment*_geolocation_type" = {box} - = '2-n': when "*experiment*_geolocation_type" = {line} - = '3-n': when "*experiment*_geolocation_type" = {polygon} Note: - For box it is recommended to give first the NW corner and then the SE corner. - These geolocation coordinates should contain all the geolocation coordinates described in the sample matter of each spectrum of the experiment *Note DB*: will be stored in shapefile format ? *Note DOI:* - recommended option as: o "GeoLocation / geoLocationPoint" (18.1) when "*experiment*_geolocation_type" = {point} o "GeoLocation / geoLocationBox" (18.2) when "*experiment*_geolocation_type" = {box} o "GeoLocation / geoLocationPolygon" (18.4) when "*experiment*_geolocation_type" = {polygon}
*experiment*_geolocation_coordinate_latitude [*matter*_geolocation_coordinate_latitude]	float	S3 [!o_m]	Exp L4 L5	V [Ver]	deg	Latitude of one of the point defining the place where the experiment was performed *Format*: in N 'decimal degrees' in "*experiment*_body_coordinate_system" *Note DOI:* - for point: as "GeoLocation / geoLocationPoint / pointLatitude" (18.1.2) - for box: as "GeoLocation / geoLocationBox / southBoundLatitude" (18.2.3) & "/ northBoundLatitude" (18.2.4) - for polygon: as "GeoLocation / geoLocationPolygon / polygonPoint / pointLatitude" (18.4.1.2)
*experiment*_geolocation_coordinate_longitude [*matter*_geolocation_coordinate_l	float	S3 [!o_m]	Exp L4 L5	V [Ver]	deg	Longitude of one of the point defining the place where the experiment was performed *Format*: in E 'decimal degrees' (in the E direction only) in

ongitude]						"*experiment*_body_coordinate_system" *Note DOI:* - for point: as "GeoLocation / geoLocationPoint / pointLongitude" (18.1.1) - for box: as "GeoLocation / geoLocationBox / westBoundLongitude" (18.2.1) & "/ eastBoundLongitude" (18.2.2) - for polygon: as "GeoLocation / geoLocationPolygon / polygonPoint / pointLongitude" (18.4.1.1)
*experiment*_geolocation_coordinate_altitude [*matter*_geolocation_coordinate_altitude]	float	S3 [m]	Exp L4 L5	V [Ver]	m	Altitude of one of the point defining the place where the experiment was performed *Format*: in 'meter' in "*experiment*_body_coordinate_system" *Notes*: - from the body reference ellipsoid (planetographic coordinates) - or from the reference sphere (planetocentric coordinates) (altitude 0)
*experiment*_geolocation_comments [*matter*_geolocation_comments]	blob	U [m]	Exp L4	V [Ver]	--	Any additional information or comments about the geolocation of this experiment *Ex:* 'measurements points of this experiment were located inside this polygon', 'very approximate coordinates (+/- 0.2°)'…

Experiment variables

Note: only a maximum of 3 sample, environment and/or instrument/spectrum variables should change during an experiment. The definition of an experiment is wider than just the case of a single initial sample with or whitout textural, phase or composition evolution. It also encompasses homogeneous series of samples with progressive values in texture (grains size, …), phase or composition. Its organization according to these paramters is described with the "*structure*" table.

experiment_variable_parameters_types	***List [L6]***	[!_m]				£: Types of sample, environment or instrument/spectrum variable parameters of the experiment.
*experiment*_variable_parameters_type	openum(text)	S1b/S1bs/Uu	Exp L6	V [Ver]	--	Type of sample, environment, instrument or spectrum variable parameters of the experiment.

[!_m]

OpenEnum: {no, sample composition, sample abundance, sample size, sample thickness, sample texture, sample grain size, sample phase, constituent, chemical variability, formation condition, temperature, pressure, mechanical stress, reactant, time, irradiation type, irradiation energy, irradiation dose, spectrum type, spectral range, illumination-observation geometry, incidence angle, emergence angle, phase angle, azimuth angle, polarization, observation mode, other}

Definitions:

- '*no*': for the case when there is only one spectrum in the experiment (i.e. without any varying sample, environment, instrument or spectrum parameter)

Sample series

- *'sample composition'*: any variation in composition at sample, layer, material, constituent or species scale
- '*sample abundance*':
- *'sample size'*: volume,
- '*sample thickness'*: thickness, …
- *'sample texture'*: prosity, surface texture, …
- *'sample grain size'*: size, shape … of material grains
- *'sample phase'*: phase of the constituting material or constituents
- *'constituent'*: (type of) constituent in microscopic measurements
- '*chemical variability'*: variability of composition intra-sample, such as various spots on a meteorite sample.
- *'formation condition':* any formation condition sucha as temperature, formation rate, …

Environment parameters

- *'temperature'*: temperature of the sample
- *'pressure'*: machanical pressure on the sample
- *'mechanical stress'*: type or values of stress applied to the sample
- *'reactant'*: type, composition of a chemical reacting with the sample
- *'time'*: time in kinetics chemical or physical processes (at constant other parameters)
- *'irradiation type'*: type/energy of irradiation or particle bombardment
- '*irradiation energy'*:
- *'irradiation dose'*: dose of irradiation

Instrument and Spectrum parameters

- *'spectrum type'*: type of spectrum or spectral product
- *'spectral range'*: spectral range (also spectral resolution ?)
- *'illumination-observation geometry'*: at least two of incidence, emergence, azimuth (or phase) angles
- '*incidence angle'*: only incidence illumination angle
- '*emergence angle*': only emergence observation angle
- '*phase angle*': incidence, emergence, and/or azimuth angles but expressed as phase angle
- '*azimuth angle*': only azimuth angle
- *'polarization'*: type or values of polarization
- *'observation mode'*: mostly mode of microscopic observation
- '*other*': for other types of variables not listed in the Enum. The type of variable should then be given in "*experiment*_variables_comments"

Notes:

- coherent 'series' of samples with a maximum of 3 varying parameters could be combined in a single experiment.
- the number of variable environment and/or instrument/spectrum parameters for a single initial sample should also be limited to 3.
- the total number of spectra should not be too extensive (as a rule of thumb: < 50 ?).
- in such cases the "*experiment_structure*" bloc should be used to describe the sections and possibly subsections of the experiment corresponding to these series.

Exemples:

- Series of samples: mixtures of olivine powder with coal => 'sample composition'
- Series of tholins samples formed with varying initial CH4/N2 ratios => 'sample composition'
- Series of olivine powder samples with varying grain sizes of = 'sample texture'
- Series of crystalline phases of nitrogen ice => 'sample phase'
- NIR and MIR spectra of CH4 ice at various temperatures => 'spectral range' & 'temperature'

						- Transmission and absorption coefficient spectra of CH4 ice at various temperatures => ‘spectral product’ & ‘temperature’ - Full BRDF: ‘illumination-observation geometry’ - BRDF in principal plane: ‘incidence angle’ & ‘emergence angle’
*experiment*_variable_parameters_comments	blob	U [m]	Exp	V [Ver]	--	Additional or synthetic information on the sample, environment or instrument parameters varying in the experiment. *Ex:* temperature/pressure cyclings, gas/liquid exposure, angular variations in the principal plane, …
Experiment_parameters						
experiment_parameters_instruments	***List [L7]***	[!!]				1: instrument parameters used for the measurements (also to produce high level spectra) *Note*: these instrument parameters are ‘multiple’ because it is possible to run a single experiment with several types of spectral measurements in parallel, either with different instruments, or different techniques on a same instrument. This allows to have all these spectra in the same experiment. *Ex*: - Infrared and raman spectra - NIR and MIR spectral ranges - several microscopic spectra and a global macroscopic spectrum of a sample
*experiment*_parameters_instrument_index [*§][-xml]	int(11) [Virtual Link]	B [!!_v]	Exp ParIns L7	V [Ver]	--	ID of the set of instrumental parameters used *Note DB:* in practice in the database the “parameters_instrument” table is linked directly to the experiment
*experiment*_comments	blob	U [m]	Exp	V [Ver]	--	Comments about this experiment and the variables parameters set *Ex:* problems, about the set of variables parameters used (sample + instrument: combination of variables, other secondary (induced) variable parameters), ...

Experiment spectra						
*experiment*_spectra_number [-xml]	int(10)	S3 [!_c]	Exp	V [Ver]	*no*	Number of spectra of the experiment ➔ calculated from the list of "*spectrum*_uid"
Experiment spectra preview		[O]		V [Ver]		£: parameters of the automatically generated preview plot of selected spectra of the experiment *Notes*: - these parameters are optional and are used to optimize the generation of the plot - if not specified the generation tool will do its best to optimize the plot: o use "*parameters_instrument*_spectral_min/max" for X limits o detect Ymin/max from the data and add some margin. - However for plots that require Y log scales (such as optical constants) the optimization is random and controlled by noise level !
*experiment*_preview_x_axis	enum(text)	P [m]	Exp	V [Ver]	--	Type of X axis in the preview plot of selected spectra of the experiment Enum: {lin, log} *Definitions*: - '*lin*': linear axis - '*log*': logarithmic axis *Note xml:* the following 4 KW ("*experiment*_preview_x_axis/_unit/_min/_max") are grouped as tags of "*experiment*_preview_x": <x axis="" unit="" min="" max="" />
*experiment*_preview_x_unit	enum(text)	P [m]	Exp	V [Ver]	--	Unit of the X axis, if different from the original import unit, in which the preview is plotted Enum: {m-1, cm-1, angstrom, nm, micron, mm, m, km, Hz, kHz, MHz, GHz, eV, keV} *Note xml:* see *"experiment*_preview_x_axis"

*experiment*_preview_x_min	float	P [m]	Exp	V [Ver]	*var*	Minimum value of X axis in the preview plot of selected spectra • Unit: given by default by "*parameters_instrument*_spectral_unit" or by "*experiment*_preview_x_unit" when provided *Note*: plotted by default in the original import unit unit if no "*experiment*_preview_x_unit" *Note xml:* see *"experiment*_preview_x_axis"
*experiment*_preview_x_max	float	P [m]	Exp	V [Ver]	*var*	Maximum value of X axis in the preview plot of selected spectra • Unit: given by default by "*parameters_instrument*_spectral_unit" or by "*experiment*_preview_x_unit" when provided *Note*: plotted by default in the original import unit unit if no "*experiment*_preview_x_unit" *Note xml:* see *"experiment*_preview_x_axis"
*experiment*_preview_y_axis	enum(text)	P [m]	Exp	V [Ver]	--	Type of Y axis in the preview plot of selected spectra of the experiment Enum: {lin, log} *Definitions*: see "*experiment*_preview_x_axis" *Note xml:* the following 5 KW ("*experiment*_preview_y_axis/_unit/_min/_max/_offset") are grouped as tags of "*experiment*_preview_y": <y axis="" unit="”” min="" max="" offset="" />
*experiment*_preview_y_unit	enum(text)	P [m]	Exp	V [Ver]	--	Unit of the Y axis (intensity), if different from the original import unit, in which the preview is plotted OpenEnum: {cm-1, m-1, cm2.g-1, m2.kg-1, mL.g−1·cm−1, cm2·mol−1, m2·mol−1, L·mol−1·cm−1, percent, permille, deg, count.s-1, count.nm-1, S, ohm, dB, sr-1, m-1.sr-1, m2.sr-1, W.m-2, kW.m-2, W.m-2.sr-1, kW.m-2.sr-1, W.m-2.sr-1.cm-1, W.m-2.sr-1.micron-1, AU, no unit, unknown, …} *Notes*: - The unit of the intensity of the spectrum depends on the spectrum type and thus only a few pairs of conversions are allowed

						○ all spectra without intensity unit: {no unit, percent, permille} [1 percent = 10 permille] ○ reflectance/radiance factor: {no unit, sr-1} [1 sr-1 = π] ○ absorption coefficient:{cm-1, m-1} [1 cm-1 = 100 m-1] ○ mass absorption coefficient: {cm2.g-1, m2.kg-1} [1 m2.kg-1 = 10 cm2.g-1] ○ molar absorption coefficient: {cm2·mol−1, m2·mol−1} [1 m2.mol-1 = 10000 cm2.mol-1] ○ thermal radiance: { W.m-2.sr-1, kW.m-2.sr-1} [1 kW.m-2.sr-1 = 1000 W.m-2.sr-1] ○ thermal emittance: { W.m-2, kW.m-2} [1 kW.m-2 = 1000 W.m-2] *Note xml:* see *"experiment*_preview_x_axis"
*experiment*_preview_y_min	float	P [m]	Exp	V [Ver]	*var*	Minimum value of Y axis in the preview plot of selected spectra • Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit if no "*experiment*_preview_y_unit" *Note xml: see "experiment*_preview_y_axis"
*experiment*_preview_y_max	float	P [m]	Exp	V [Ver]	*var*	Maximum value of Y axis in the preview plot of selected spectra • Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit unit if no "*experiment*_preview_y_unit" *Note xml: see "experiment*_preview_y_axis"
*experiment*_preview_y_offset	float	P [m]	Exp	V [Ver]	*var*	Value of the cumulative Y offset applied to each spectrum in the preview

- Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided

Note: offset by default in the original import unit unit if no "*experiment*_preview_y_unit"

*Note xml: see "experiment*_preview_y_axis"

Ex: '0.1' will give offsets of {0; 0.1; 0.2; 0.3; ...}

*experiment*_preview_y2_axis	enum(text)	P [m]	Exp	V [Ver]	--	Type of the second Y axis (only for the real part of complex spectra) in the preview plot of selected spectra of the experiment Enum: {lin, log} *Limitation* (but cannot be constrained easily): only for "*spectrum*_files_parameter_type" = {complex spectrum, polarimetric spectrum, scattering spectrum} *Note*: - i.e., for "*spectrum*_type" = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex permeability, complex reflectance ratio, polarization parameters} *Definitions*: see "*experiment*_preview_x_axis" *Notes*: - only for complex spectra to set different parameters to the Y axis for 'imaginary part' (y axis) and 'real part' (y2 axis) - for "*spectrum*_type": o optical constants: 'n index' o complex admittance: 'conductance' o complex impedance: 'resistance' o relative complex permittivity: 'dielectric constant' o relative complex permeability: 'magnetic constant' o complex reflectance ratio: 'amplitude component' o polarization parameters: 'polarization position angle' *Note xml:* the following 4 KW are grouped as tags of "*experiment*_preview_y2":

						"*experiment*_preview_y2_axis/_min/_max/_offset".
*experiment*_preview_y2_min	float	P [m]	Exp	V [Ver]	*var*	Minimum value of the second Y axis in the preview plot of selected spectra • Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided *Notes*: - The unit of y2 axis is always the same as for the y axis - plotted by default in the original import unit unit if no "*experiment*_preview_y_unit" *Note xml: see "experiment*_preview_y2_axis"
*experiment*_preview_y2_max	float	P [m]	Exp	V [Ver]	*var*	Maximum value of the second Y axis in the preview plot of selected spectra • Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided *Notes*: see notes of "*experiment*_preview_y2_min" *Note xml: see "experiment*_preview_y2_axis"
*experiment*_preview_y2_offset	float	P [m]	Exp	V [Ver]	*var*	Value of the cumulative Y offset of the second Y axis applied to each spectrum in the preview • Unit: given by "*spectrum*_intensity_unit" of the first spectrum or by "*experiment*_preview_y_unit" when provided *Notes*: see notes of "*experiment*_preview_y2_min" *Note xml: see "experiment*_preview_y2_axis" *Ex:* '0.1' will give offsets of {0; 0.1; 0.2; 0.3; ...}
*experiment*_preview_filename	CS-varchar(255)	S3 [mc]	Exp	V [Ver]	--	Name of the file containing the preview plot of selected spectra to be displayed ➔ plot generated automatically during import if there is no file *Image formats:* .png, .jpg, (.gif)

Note:

- this plot will replace the automatically generated plot
- it should include the full "experiment_title" on top of the figure
- image size should be preferably around HxV = 650x460 pixels (note: will be resized later)
- it will be displayed in the result page for quick look at the experiment results

Note DB: this file should be zipped with the 'experiment-spectra' import xml file for import.

Experiment images and results

experiment_images	***List [L8]***	[O]				£: Pictures of the experiment and of overviews of its results
*experiment*_image_filename	varchar(255)	U [m]	Exp L8	V [Ver]	--	File name(s) (with extension) of the picture(s) of the experiment or of its results *Image formats:* .png, .jpg, (.gif) *Note:* – These files can include pictures of the whole experiment but also plots of spectra (or zooms) or produced results of the whole (or part of the) experiment. – Note that there is already a preview plot (for search results display purpose) with a limited selection of spectra (5-8) of the experiment that is generated automatically during import using the flag "*spectrum*_experiment_preview_flag". It can be also prepared and uloaded using "*experiment*_preview_filename" *Note DB:* this file should be zipped with the 'experiment-spectra' import xml file for import. *Ex*: – Picture of a special configuration of an experiment – Reflectance as a function of phase angle at a given wavelength for a BRDF experiment

						– Zoom of 3 different absorption bands, …
*experiment*_image_caption	varchar(255)	U [m]	Exp L8	V [Ver]	--	Caption(s) or comment(s) on the picture(s) of the experiment or of its results *Note:* if the image is part of a published paper, then give the reference
Experiment documentation						
experiment_documentations	***List [L9]***	[O]				£: Documentations about the experiment *Note:* can contain experimental protocol, log file of the experiment, … *Note*: these documentations can be downloaded or viewed inside another window of the web browser but cannot be viewed directly into SSHADE.
*experiment*_documentation_name	varchar(255)	U [m]	Exp L9	V [Ver]	--	Name of a documentation describing the experiment *Note:* this name will appear as the documentation title in the database *Ex:* 'Experimental protocol of Mid-IR monitoring of CH4 ice sample under VUV irradiation'
*experiment*_documentation_filename	varchar(255)	U [m]	Exp L9	V [Ver]	--	File name (with extension) of the documentation describing the experiment *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database. *Note xml*: this file should be zipped with the xml file
Experiment references						
experiment_publications	***List [L10]***	[£o]				£: Publications in which the experiment and the whole spectral data set are published *Note:* The experiment should be at least described in some details in the paper or ALL the spectra should be ploted (or at least part of each spectrum, *Ex*: for a BRDF curve versus phase angle at one given wavelength

*experiment*_publication_uid [*]	varchar(255)	S2/S2s [£o_m]	Exp Publi L10	V [Ver]	--	Link to the existing UID of the publication(s) in which the experiment or the whole spectral data set are published *Condition:* at least one compulsory when the experiment or all spectra are already published in a publication *Note:* these papers should be in the publications database, and should have "*publication*_content" = 'spectral data' or 'BRDF data' (or 'instrument-technique') *Note DOI:* - recommended option as "RelatedIdentifier / relationType=IsReferencedBy" (12.2): "*publication*_doi"
*experiment*_publication_comments	blob	U [m]	Exp	V [Ver]	--	Comments about the experiment or spectral dataset in the publication *Note*: for exemple which part of the dataset of the experiment is published, ...

Experiment sponsors

experiment_sponsors	***List [L11]***	[O]				£: List of organizations that provided ponctual financial support to the experiment *Note DOI:* - recommended option as "ContributorType=Sponsor" (7.1)
*experiment*_sponsor_acronym	varchar(255)	U [m]	Exp L11	V [Ver]	--	Acronym of the organization that provided ponctual financial support to the experiment *Notes:* - Includes organizations that issued a contract or under the auspices of which the experiment developed, etc. - Includes organizations that provide in-kind support, through donation, provision of people or a facility or instrumentation necessary for the development of the database content, etc. *Note DOI:* requested in recommended option as "Contributor / contributorType=Sponsor / contributorName" (7.2) for "Experiment".

						It will be combined with "*database*_sponsor_name": 'Institution full name (acronym)' *Ex*: 'ANR', 'Labex OSUG 2000', …
*experiment*_sponsor_name	varchar(255)	U [m]	Exp L11	V [Ver]	--	Name of the organization that provided ponctual financial support to the experiment *Notes:* see "*experiment*_sponsor_acronym" *Note DOI:* see "*experiment*_sponsor_acronym" *Ex*: 'Agence Nationale de la Recherche', 'Laboratoires d'excellence', …
*experiment*_sponsor_award	varchar(255)	U [m]	Exp L11	V [Ver]	--	Acronym, and/or title and/or award number of the sponsored award (grant). Format: 'ACRONYM: Title (award number)' *Ex*: 'SOLARYS: award 123.PB_2017', …

12.5 Experiment structure Table

Root of the table: ***structure***

Data type: in 'Experiment and spectra'

Notes:

- This structure is used to organize the experiment in sections and subsections when we want to put in a single experiment a homogeneous series of samples (or a single sample) with one to three varying sample, environment or instrument parameters (eg. mixtures of 2 materials in different proportions; same material with different grain sizes...). The organization is made according to these parameters.
- It is not used when a single initial sample (evolving or not during the experiment) has only one varying parameter during the experiment: the "spectra" structure id sufficient for this simple case. However it may be used to split the experiment in several sections 1) when at least 2 environment or instrument parameters vary successively during the experiment (e.g. several heating/cooling sequences, or pressure stages coupled with heating/cooling sequences, …), or 2) when spectra of a single initial sample have been recorded simultaneously with several instrument-techniques, or 3) when several levels of spectral products are proposed.
- The experiment, the sections and the subsections will be displayed in SSHADE in the order and with the structure defined here together with their title and the information on their type of variable parameters (variable sample, environment or instrument parameters). The section and subsection titles are subtitles of the general title of the experiment ("experiment_title").

Key-word	Type	Level	Table	Exp	Unit	Description
Structure: sections		[$o_O]		V [Ver]		*Definition:* the "sections" is the main subdivision along one of the varying sample, environment or instrument parameters. *Condition:* strongly recommended when there are more than one value in "*experiment*_variable_parameters_type" *Notes on conditions*: - strongly recommended when there is a series of initial samples with a varying parameter - recommended for single initial sample when there are two varying environment, instrument or spectrum parameters *Notes*: – a section can contain either measurements on a series of samples, or measurements of one single initial sample (but it may evolve upon

						some processing) with a second varying parameter. – when there are two varying parameters, the subdivision along the second parameter is done in "*structure*_section_spectra" – when there are three varying parameters, the subdivision along the second parameter is done in "*structure*_section_subsections" and that of the third parameter in "subsection_spectra"
*structure*_sections_variable_parameter	openum(text)	U [!_m]	Struct	V [Ver]	--	Type of sample, environment, instrument or spectrum parameter varying between the sections of the experiment. OpenEnum: {no, sample composition, sample abundance, sample size, sample thickness, sample texture, sample grain size, sample phase, constituent, chemical variability, formation condition, temperature, pressure, mechanical stress, reactant, time, irradiation type, irradiation energy, irradiation dose, spectrum type, spectral range, illumination-observation geometry, incidence angle, emergence angle, phase angle, azimuth angle, polarization, observation mode, other} *Definitions*: see "*experiment*_variable_parameters_type" *Exemples*: - Series of mixtures of olivine powder with coal => 'sample composition' - Series of tholins samples formed with varying initial CH4/N2 ratios => 'sample composition' - Series of olivine powder samples with varying grain sizes of = 'sample texture' - Series of crystalline phases of nitrogen ice => 'sample phase' - NIR and MIR spectra of CH4 ice at various temperatures => 'spectral range' - Transmission and absorption coefficient spectra of CH4 ice at various temperatures => 'spectral product'
structure_sections	***List [L1]***	[!o]				£: Main sections of the experiment

*structure*_section_order [-xml]	int(4)	P [!_c]	Spectr L1	V [Ver]	--	Order of the sections - determined automatically during import from the order of the "*structure*_section" blocs *Note*: - it should be used to sort the samples, series of samples, or environment, instrument or spectrum parameters values in order of increasing values of the first varying parameter (grain size, concentration of one material, temperature, …).
*structure*_section_title	varchar(255)	U [!_m]	Struct L1	V [Ver]	--	Title describing the sample and the fixed and variable sample, environment, instrument or spectrum parameters of this section of the experiment *Note:* - it should contain global info on the sample (or subseries of samples), on the type/range of spectra, on the varying sample, environment, instrument or spectrum parameters and on the value taken by the varying parameter in this experiment section - it will be displayed as search result. *Ex:* - 'Olivine/iron mixture (90/10w%) with two grain sizes (20, 30µm) at 50 and 60 K' - 'Olivine/iron mixture (70/30w%) with two grain sizes (20, 30µm) at 50 and 60 K' - 'Near-IR transmission spectra of solid and liquid CH4 between 10 and 120K' - 'Mid-IR transmission spectra of solid and liquid CH4 between 10 and 120K'
*structure*_section_description	blob	U [m]	Struct L1	V [Ver]	--	Detailled description of the sample and the fixed and variable sample, environment, instrument or spectrum parameters of this section of the experiment *Notes:* - it should contain complete info on the sample (or subseries of samples), or on the spectra types/range, and in particular the value

taken by the varying parameter in this experiment section, as well as possible other variable parameters (with values or range of values).
- it will be displayed as detailed info on search result.

Ex:
- ‘This experiment section contains the olivine and iron minerals mixture with relative abundance of 90/10w%. The mixture is studied for two grain size ranges (20 +/- 5 and 30 +/- 6 µm), each at two temperatures: 50 and 60 K’
- ‘This experiment section contains the olivine and iron minerals mixture with relative abundance of 70/30w%. The mixture is studied for two grain size ranges (20 +/- 5 and 30 +/- 6 µm), each at two temperatures: 50 and 60 K’
- ‘Near-IR transmission spectra of solid and liquid CH4 at temperatures between 10 and 120K with a step of 10K. Phase I at 10 and 20K, phase II between 30 and 90K, liquid above 90K’
- Mid-IR transmission spectra of solid and liquid CH4 at temperatures between 10 and 120K with a step of 10K. Phase I at 10 and 20K, phase II between 30 and 90K, liquid above 90K’

Structure: subsections [!O]

Definition: The “subsections” are the secondary subdivision of the series of samples, along the second varying parameter, when there are three varying parameters.

Condition: “subsections” is mandatory when there are three “*experiment*_variable_parameters_type“

Note: i.e. mandatory when there is a triple series of varying sample, environment, instrument or spectrum parameters

Notes:
- a subsection can contain either measurements on a series of samples, or measurements of one single initial sample (but it may evolve upon some processing) with a third varying parameter.
- when there are three varying parameters, the subdivision along the second parameter is done in “*structure*_section_subsections” and that

						of the third parameter in "*structure*_section_subsection_spectra"
*structure*_section_subsections_variable_parameter	openum(text)	U [!_m]	Struct L1	V [Ver]	--	Type of sample, environment, instrument or spectrum parameter varying between the subsections of this section of the experiment. OpenEnum: {no, sample composition, sample abundance, sample size, sample thickness, sample texture, sample grain size, sample phase, constituent, chemical variability, formation condition, temperature, pressure, mechanical stress, reactant, time, irradiation type, irradiation energy, irradiation dose, spectrum type, spectral range, illumination-observation geometry, incidence angle, emergence angle, phase angle, azimuth angle, polarization, observation mode, other} *Definitions*: see "*experiment*_variable_parameters_type" *Exemples*: see "*structure*_sections_variable_parameter"
structure_section_subsections	***List [L2]***	[!o]				£: Subsections of the experiment
*structure*_section_subsection_order [-xml]	int(4)	P [!_c]	Struct L1 L2	V [Ver]	--	Order of the subsections - determined automatically during import from the order of the "*structure*_subsection" blocs *Note*: it should be used to sort the sample (for sample series), environment, instrument or spectrum parameters values (for single initial sample) in order of increasing values of the second varying parameter (grain size, concentration of one material, temperature, …).
*structure*_section_subsection_title	varchar(255)	U [!_m]	Struct L1 L2	V [Ver]	--	Title describing the sample and the fixed and variable sample, environment, instrument or spectrum parameters of this subsection of the experiment *Note:* - it should contain global info on the sample, on the type/range of spectra, on the varying sample, environment, instrument or spectrum parameters and on the value taken by the varying parameter in this experiment subsection - it will be displayed as search result.

						Ex: - 'Olivine/iron mixture (90/10w%) with grain sizes 20µm at 50 and 60K' - 'Olivine/iron mixture (90/10w%) with grain sizes 30µm at 50 and 60K'
*structure*_section_subsection_description	blob	U [m]	Struct L1 L2	V [Ver]	--	Detailled description of the sample and the fixed and variable sample, environment, instrument or spectrum parameters of this subsection of the experiment *Notes:* - it should contain complete info on the sample, or on the spectra types/range, and in particular the value taken by the varying parameter in this experiment section, as well as possible other variable parameters (with values or range of values). - it will be displayed as detailed info on search result. *Ex:* - 'This experiment subsection contains the olivine and iron minerals mixture with relative abundance of 90/10w% and grain size ranges 20 +/- 5 µm at two temperatures: 50 and 60 K' - 'This experiment subsection contains the olivine and iron minerals mixture with relative abundance of 90/10w% and grain size ranges 30 +/- 6 µm at two temperatures: 50 and 60 K'
Structure: spectra		[!o]				*Note*: this bloc is either in the subsection or in the section bloc depending if there are, or not, subsections. *Condition*: "*structure*_section_spectra" mandatory when "*structure*_section_subsections" = Ø *Condition*: "*structure*_section_subsection_spectra" mandatory when "*structure*_section_subsections" ≠ Ø
*structure*_section_(subsections)_spectra_variable_parameter	openum(text)	U [!_m]	Struct L1	V	--	Type of sample, environment, instrument or spectrum parameter varying between the spectra of this (sub)section of the experiment.

			L2	[Ver]		OpenEnum: {no, sample composition, sample abundance, sample size, sample thickness, sample texture, sample grain size, sample phase, constituent, chemical variability, formation condition, temperature, pressure, mechanical stress, reactant, time, irradiation type, irradiation energy, irradiation dose, spectrum type, spectral range, illumination-observation geometry, incidence angle, emergence angle, phase angle, azimuth angle, polarization, observation mode, other} *Definitions:* - see "*experiment*_variable_parameters_type" - '*no*': for the case when there is only one spectrum for a series or subseries of sample (i.e. without any varying environment, instrument or spectrum parameter)
structure_section_(subsection)_spectra	***List [L3]***					£: List of the spectra
*structure*_section_(subsection)_spectrum_order [-xml]	int(4)	P [!_c]	Struct L1 L2 L3	V [Ver]	--	Order of the spectrum in this list - determined automatically during import from the order of the "*structure*_section_(subsection)_spectrum_uid" *Note*: - this order should be used to sort the samples, or environment, instrument or spectrum parameters values in order of increasing values of the second (in "section_spectra") or third (in "subsection_spectra") varying parameter (temperature, …).
*structure*_section_(subsection)_spectrum_uid [*]	varchar(255)	U [!!_m]	Struct Spectr L1 L2 L3	V [Ver]	--	Link to the existing UID of the spectrum belonging to this experiment (sub)section *Note:* - They should be in the order you want they appear in SSHADE - The spectra are described in the "*spectrum*" table… .

13. SPECTROSCOPIC DATA

13.1 SPECTRAL DATA

The **spectroscopic data** currently identified come from 5 different instrument types (plus their microscopic variants) and have different corresponding 'calibrated spectra' (level 1) and higher levels of products (levels 2 to 4):

Transmission spectroscopy	**Level**	**Operation**
'Transmission'	(level 1)	(calibrated spectrum + correction)
'Absorbance'	(level 2)	(math transformation)
'normalized absorbance'	(level 2)	(math transformation)
'Optical density'	(level 2)	(math transformation)
'Absorption coefficient' (unit: cm-1)	(level 3)	(fundamental solid parameter)
'Optical constants'	(level 4)	(fundamental solid parameter set)
Reflection spectroscopy		
'radiance factor'	(level 1)	(calibrated spectrum + correction)
'specular reflectance'	(level 2)	(calibrated spectrum + correction)
'reflectance factor' (include biconical, any integrated)	(level 2)	(calibrated spectrum + normalizedto cos(i))
'Spectral bidirectional reflectance distrib. function' (SBRDF)	(level 2)	(4D calibrated spectrum data set)
'Anisotropy factors	(level 3)	(integrated or not)
'Hemispherical-directional reflectance'	(level 2-3)	(measured or angular integration)
'Directional-hemispherical albedo'	(level 2-3)	(measured or angular integration)
'Bidirectional reflectance distribution function at λ' (BRDF)	(level 3)	(3D data extraction + inter/extrapolation)
'Scattering coefficients'	(level 4)	(radiative transfer parameter set)

And their different polarization variants

Emission spectroscopy		
'Thermal emission' (unit:)	(level 1)	(calibrated spectrum + correction)
'Thermal emittance'	(level 2)	(math transformation)
'Spectral directional emittance distribution function' (SDEDF)	(level 2)	(2D calibrated spectrum data set)
'Directional thermal emissivity'	(level 3)	(fundamental parameter)
'Directional emittance distribution function at λ' (DEDF)	(level 3)	(1D data extraction + inter/extrapolation)
'Spectral directional emissivity distribution function' (SDEyDF)	(level 3)	(fundamental parameter)
'Directional emissivity distribution function at λ' (DEyDF)	(level 4)	(fundamental parameter - 1D extraction)

‘Hemispherical thermal emissivity’	(level 4)	(integrated fundamental parameter)
ATReflection spectroscopy		
‘Transmission’	(level 1)	(calibrated spectrum + correction)
‘Absorbance'	(level 2)	(math transformation)
Raman spectroscopy		
‘Raman scattering’	(level 1)	(calibrated spectrum + correction)
‘Normalized Raman scattering’	(level 2)	(corrected and normalized spectrum)
‘Raman scattering efficiency’	(level 4)	(fundamental solid parameters)
Fluorescence spectroscopy		
‘Fluorescence emission’	(level 1)	(calibrated spectrum + correction)
‘Normalized fluorescence emission’	(level 2)	(corrected and normalized spectrum)
‘Fluorescence emission efficiency’	(level 4)	(fundamental solid parameters)

Note: "raw signal spectra" (level 0 product), i.e. before instrument response calibration, are not intended to be stored in this database, except special case where they may be needed as the unique source data of a product.

Definitions: cf. « *spectrum*_type »

13.2 Description

The **spectroscopic data** consist of a “*spectrum file”* and some *"file and spectrum information"*. The spectrum is linked with an "experiment" which connects to the "sample" and to the "instrument parameters" used. A spectrum can also have some specific values for a limited number of variables parameters in the "sample" (processing) and/or "instrument parameters" tables, listed in the “experiment”. These values are given in this *spectrum table*.

Each type of spectral measurement (linked with instrument type and technique used) can deliver a different type of "calibrated spectrum" (***level 1 product***) which can have a different intensity unit (e.g. transmission spectra, reflection spectra, emission spectra, ...).

In addition several types of "calibrated spectra" are frequently simply and individually normalized or converted (mathematically) in another unit (***level 2 product***) for convenience (linearization of absorption, normalization of Raman spectra (when not an absolute measurement), ...) and sometimes with additional individual processing (such as baseline removing, ...). These spectra keep all the parameters of the level 1 product from which they are derived.

At higher levels of analysis (***level 3 & 4 products***) it is possible to combine several spectra either from different spectral ranges (e.g., Vis + NIR + MIR) and/or from different but very similar samples (e.g. same samples but with different thicknesses for absorption coefficient or optical constants spectra).

Some high level spectral products are also the result of angular integrations of a set of illumination or observation geometries (e.g. spectra at various

emergence angles for directional-hemispherical albedo spectra).

Although these products strongly depend on the instrument type and technique used we have keep their metadata in a single table with most of their parameters common and a few specific to some techniques. The main changes for different instrument types and techniques will be in the instrument parameters table (fixed or variable).

The **spectrum table** contains the "*spectrum links",* information on *"spectrum type",* and *"spectrum origin and history",* the values of the *"spectrum variable parameters"* (sample and instrument), some information on "s*pectrum analysis and validation"* and *"references"* as well as links and information on the associated *"spectrum file".*

- "***Calibrated spectra***" (level 1 product) or spectra directly derived from them (level 2 products; simple transformation of level 1 spectra) are directly connected with one *sample* and one set of *instrument parameters* (trough the *experiment*). They can have a few *sample* and *instrument* variable parameters within an experiment.

These variable parameters give the values specific to the spectrum for some *instrument measurement parameters* (e.g., incidence/emergence/azimuth angles, Raman irradiation time, …), and *sample processing parameters* (temperature, annealing temperature and time, interaction with atmospheric gas (pressure, composition), …).

- For ***more evolved spectral products***, such as absorption coefficient (level 3 product) or optical constants (level 4 product) that can be the combination of several spectra either coming from measurements with different instrument parameters, or on similar samples (same composition, same intensive state parameters) but with different extensive physical state parameters (different thicknesses, …) there is no more direct link between the spectrum and one unique sample and/or one set of instrument parameters. It is thus necessary to define a "*generic sample*" (e.g., a sample with a variable thickness) and a simplified "*generic instrument parameter set*" (e.g., to redefine the spectral parameters: range, resolution and sampling) that have no real existence in order to use the same "sample table" and "instrument parameter table" than for a spectrum measured with a real instrument on a real sample.

13.3 Microscopic measurements on heterogeneous matters

A special case occurs with the microscopic measurements of samples with very heterogenous composition at the microscopic scale. A global description of the sample is not fully relevant for spectral measurements that are peformed at the constituent scale. It is thus necessary to know on which constituent each spectral measurement is made. An accurate description of the constituents (at least those measured) should thus be done and a "pointer" ("*sample*_primary_constituent_index") should tell in the spectrum table which constituent(s) is(are) probed by each microscopic spectrum.

Note: it is not always possible to have the knowledge of which constituents are effectively probed if several constituents are in the measurement spot. Their relative proportion is also generally extremely difficult to estimate, given the difficulty to define precisely the spatial resolution, horizontal and vertical, of microscope spots (probed volume).

13.4 Spectrum Table

Root of the table: ***spectrum***

Data type: 'Experiment and spectra'

Note: common to all instruments and all product levels

Key-word	Type	Level	Table	Exp	Unit	Description
Spectrum import, indexes and links						
*spectrum*_import_mode	enum(text)	P [!!_m]	Exp	V	--	Mode of import of the "spectrum" data and metadata Enum: {first import, inherited, ignore, draft, no change, correction, new version, invalidate} *Constraint:* 'invalidate' only when *"spectrum*_access_right" is already 'public' *Definitions:* There are 2 levels of import: • '*first import'*: for first import of the metadata and data • '*use existing':* use an existing table specified by its UID. Need only to give this UID and some values of KW *Note*: not used in spectrum, mostly in sample and matters) There are 2 levels of 'no correction': • *'ignore'*: fully ignore this metadata table. • '*no change'*: when there is no change in this table (for correction in others tables) but it exists already in the database (checked) There are 3 levels of correction: • '*correction':* used to correct/add values of metadata, links, or associated files for data already imported in the database. For spectra it only modifies values/links/files on the current (last) version of the metadata. It should not be used to change a spectrum file which has data modified inside its valid spectral range (or only very minor

changes). But it can be used when values of the spectrum data file are modified outside the valid spectral range

- *'new version'*: used when values of the spectrum data file are changed within the valid spectral range. This change may be simply a local or global improvement of the analysis of the data (but within the same 'spectrum_type'), a spectral extension of the data, … but it may be also a correction of a local or global error. All this will be described using the "*spectrum*_analysis", "*spectrum*_history" and/or "*spectrum*_comments" KWs with possible increase of the value of the "*spectrum*_quality" KW. It will automatically increment the version number of the spectrum (*spectrum*_version) and of the experiment ("*experiment*_version").
- *'invalidate':* used when a public spectrum is found to be mostly or fully invalid but there is no way to correct it and import a new version. This import mode did not wait for a new spectrum.

Notes:

- For *'new version'* a limited set of KW (noted by [Ver] in the 'Exp' column) of the previous version is archived, together with the "*spectrum*_previous_version_status" and "*spectrum*_previous_version_comments" KWs and the previous original spectrum file.
- For *'invalidate'* the "*spectrum*_previous_version_status" and "*spectrum*_previous_version_comments" KWs are stored with the current version and in some cases also with all the previous versions (see "*spectrum*_previous_version_status").
- If a new analysis changes the product type or level (e.g. "spectrum_type" = 'transmission' to 'absorbance') then it should be imported ('first import') as a new spectrum with the previous one as a parent.

*spectrum*_xml_filename [-xml]	varchar(255) [virtual KW]	P [!!_vc]	Spectr	V [Ver]	--	Name of the storage copy of the xml import file of the spectrum metadata ➔ determined automatically during import (from "*spectrum*_uid»?) *Note:* this file is stored in order to be able to retrieve it when it is necessary to

						apply correction or import a new version
*spectrum*_index [**][-xml]	int(10)	B [!!_g]	Spectr	V [Ver]	--	Automatic random but unique number (internal ID) given to new spectrum
*spectrum*_uid [**]	varchar(255)	S0 [!!_m]	Spectr	F	--	Unique identifier code (UID) given to the spectrum table (to be created) *Nomenclature:* Create this code name with 'SPECTRUM_' very accurately in order to be simple and unique *Ex:* It should be of the style 'SPECTRUM_AB_yyyymmdd_123...' where 'AB' is initial of people preparing the import, 'yyyymmdd' is the full date of the day, and '123...' should be alphanumeric (only with '_'), and with no more than 10 characters. *Ex:* 'SPECTRUM_BS_20181006_059', 'SPECTRUM_OB_20000101_01', 'SPECTRUM_KD_20170712_X40_300K' *Notes:* - The post-fix '123...' may just be an incremental order number for that day, or may give a short description of the varying parameter of the spectrum. *Ex:* 'SPECTRUM_KD_20170712_X50A_200K' - All the spectra of a single initial sample should be listed in chronological order (as recorded in the experiment) when an irreversible chemical, physical, or textural evolution of the sample occurs during the experiment. It is absolute mandatory when the sample description changes (changing "*spectrum*_sample_uid). And use "*spectrum*_chronologically_ordered"='yes'. - This will permit to track the history of the sample and use "*spectrum*_sample_changes" to describe the changes. - It is also better to list spectra in chronologic order for experiments with a single initial sample subjected to environmental changes (T and/or P cycles, …) that may induce slight irreversible or quasi-reversible effects. - Groups of spectra of different initial samples can be listed in any order. - The "*experiment*_structure" table will allow you to organize the order

						of presentation of the spectra according to 1 to 3 different sample, environment or instrument/spectra varying parameters. But, for practical reasons and when possible, it is recommended to follow here this same order
*spectrum*_sshade_url [-xml]	varchar(255) [Virtual KW]	U [!_c]	Spectr	V [Ver]	--	Direct web link to the SSHADE spectrum page displaying the spectrum data and its metadata ➔ automatically generated and in practice not stored in database *Note:* can be determined by knowing the UID (not restricted to spectra) *Note:* can be also obtained by copying the URL when viewing a spectrum or looking at its details. *Ex:* https://www.sshade.eu/data/SPECTRUM_LB_20170731_022
*spectrum*_experiment_type	enum(text)	S1 [!!o_m]	Spectr	F	--	Type of experiment for this spectrum Enum: {laboratory measurement, numerical modeling, theoretical modeling, field measurement, low altitude field measurement, satellite remote sensing, telescopic remote sensing, other, unknown} *Condition:* mandatory only when *"experiment*_type" has more than one value *Constraint:* should be one of the values of *"experiment*_type" ➔ calculated when *"experiment*_type" has only one value ⇨ *"spectrum*_experiment_type" = *"experiment*_type" *Definitions:* cf. *"experiment*_type" *Notes:* *Ex:* - Measurements done in the field and then spectra of the same sample recorded in the laboratory. It is then necessary to tell if the spectrum is of experiment type 'field measurement' or 'laboratory measurement'. - Laboratory or field measurements and their corresponding radiative transfert modeling

Spectrum order						
*spectrum*_chronologically_ordered	boolean	P [!!_m]	Spectr	F	--	Flag telling if the spectrum follow the previous one in chronological order BoolEnum: {yes, no} or {true, false} Note: - This will allow to automatically determine the UID of the spectrum which has been recorded before this one ("*spectrum*_previous_spectrum_uid") and thus to keep track of their chronological order. This is especially important for irreversible evolutions of the initial sample. - When the previous spectrum has been recorded on another initial sample than for this spectrum, then always put 'no'. The relative order of measurement of different samples is not considered here.
*spectrum*_previous_spectrum_uid [*]	varchar(255)	P/U [mc]	Spectr Spectr	F	--	Link to the existing UID of the spectrum preceding chronologically this spectrum - determined automatically during import from the order of "*spectrum*_uid" when the spectrum is listed in chronologic_order ⇨ "*spectrum*_previous_spectrum_uid" = previous "*spectrum*_uid" in the list when "*spectrum*_chronological_order" = 'yes' ⇨ Otherwise "*spectrum*_previous_spectrum_uid" = ''
*spectrum*_order [-xml]	int(4)	B [!_c]	Spectr	F	--	Order of the spectrum in this list ➔ determined automatically during import from the order of "*spectrum*_uid"
Spectrum title and type						
*spectrum*_title	varchar(255)	S1 [!!_m]	Spectr	V [Ver]	--	Title describing the spectrum *Note:* It should contain complete info on the sample and spectrum (spectral range type, spectrum type + sample name + main parameters, …) *Ex:* 'Vis-NIR absorption coefficient spectrum of CH4 phase-I crystal at 30 K'

						‘MIR transmission spectrum of Portlandite at -10°C under 2b CO2 gas 60min’ **Spectrum version** It should reflect the changes of the version if they affect one element of the title
*spectrum*_type	enum(text)	S0 [!!_m]	Spectr	Vc [Ver]	--	Type of spectrum intensity, depending on the instrument and level of product Enum: {raw, transmission, absorbance, normalized absorbance, optical depth, absorption coefficient, optical constants, ATR transmission, ATR absorbance, corrected ATR absorbance, complex admittance, complex impedance, relative complex permittivity, dielectric loss tangent, relative complex permeability, magnetic loss tangent, bidirectional reflectance, bidirectional reflectance distribution function, radiance factor, reflectance factor, normalized reflectance, albedo, anisotropy factor, complex reflectance ratio, Stokes parameters, normalized Stokes parameters, polarization parameters, thermal emission, thermal radiance, thermal emittance, thermal emissivity, scattering intensity, differential scattering cross section, normalized differential scattering cross section, scattering cross section parameters, scattering efficiency factor parameters, single scattering albedo, Raman scattering intensity, normalized Raman scattering intensity, Raman scattering coefficient, Raman scattering efficiency, fluorescence emission, normalized fluorescence emission fluorescence emission efficiency, radiative transfer model parameters} *Constraint*: for “*spectrum*_import_mode = {correction, new version} “*spectrum*_type” can be changed only to a type with the same “*spectrum*_files_parameter_type” *Ex*: - can change ‘absorbance‘ to ‘absorption coefficient’ - cannot change ‘absorbance‘ to ‘optical constants’ *Definitions:* - ‘*raw*’: for any raw measurement, i.e. raw detector signal before division by a background or reference spectrum. *Note*: This case is rarely used and not recommended. It is mostly used to provide the background or reference spectrum for first

level products. It is also used to provide the measurements used for higher levels when the first level is missing. (e.g. raw spectra to calculate the polarization degree, angle and Pq when reflectance spectra not available).

- '*transmission*': simple ratio of transmited to incident intensity of light, I/Io
- '*absorbance*': it is the common logarithm of the ratio of incident to transmitted spectral radiant power through a material (A = - log (T)).
- '*normalized absorbance'*: It is the absorbance normalized to '1' at a given wavelength/wavenumber/frequency, to be defined in "*spectrum*_reference_position". Formerly called 'optical density' (discouraged use).
- '*optical depth'*: it is the natural logarithm of the ratio of incident to transmitted spectral radiant power through a material (OD = - ln (T)).
  Note: OD = A * ln(10)
- '*absorption coefficient'*: absorption/attenuation coefficient in various units. Include 'mass absorption/attenuation coefficient' and 'molar attenuation coefficient'
  Note: unit to be defined in "*spectrum*_intensity_unit").
- '*optical constants'*: real and imaginary parts of the refractive index
  - associated with "*spectrum*_files_parameter_type"='complex spectrum'
- '*ATR transmission'*: Attenuated Total Reflectance transmission spectra trough an ATR crystal
- '*ATR absorbance'*: Attenuated Total Reflectance spectra converted to absorbance
- '*corrected ATR absorbance'*: ATR absorbance spectra corrected from the effects caused by the dependence of penetration depth on wavelength (relative band intensity distortion), by dispersion of the refractive index (shift of bands to lower wavenumber) and by non-polarization effects (deviation from Beer's Law).
  Note: they are model dependent, so it is good to tell in "*spectrum*_analysis" which model is used.
- '*complex admittance*': Y = 'conductance' G (real part) + 'susceptance' B (imaginary part)

    - associated with "*spectrum*_files_parameter_type"='complex spectrum'
- '*complex impedance*': Z = 'resistance' R (real part) + 'reactance' X (imaginary part)
    - associated with "*spectrum*_files_parameter_type"='complex spectrum'
- '*relative complex permittivity'*: ε_r relative complex permittivity (ratio relative to the permittivity of vacuum ε_0 called the 'electric constant') = 'dielectric constant' ε'_r (real part) + 'relative electric conductivity' ε''_r (imaginary part)
    - associated with "*spectrum*_files_parameter_type"='complex spectrum'
- '*dielectric loss tangent'*: dielectric loss tangent tan $\delta_e = \varepsilon'' / \varepsilon'$ (for mm-cm-m-km wavelengths)
- '*relative complex permeability'*: μ_r relative complex permeability (ratio relative to the permeability of vacuum μ_0 called the 'magnetic constant') = 'magnetic constant' μ'_r (real part) + 'relative magnetic conductivity?' μ''_r (imaginary part)
    - associated with "*spectrum*_files_parameter_type"='complex spectrum'
- '*magnetic loss tangent'*: magnetic loss tangent tan $\delta_m = \mu''/ \mu'$ (for mm-cm-m-km wavelengths)

'*bidirectional reflectance*': r(i,e,g). The bidirectional reflectance is the ratio of the radiance of a surface at a given illumination and viewing geometry, L(i,e,g), to the collimated incident irradiance, F, perpendicular to the direction of travel of the light.

Notes:

- unit: sr^{-1}

Constraint: used only with "parameters_instrument_angle_observation_geometry" = {specular, bidirectional}

'*bidirectional reflectance distribution function*': BRDF(i,e,g), r_{brdf}. The bidirectional reflectance distribution function is the ratio of the radiance of a surface at a given illumination and viewing geometry, L(i,e,g), to the incident irradiance on the surface, E(i) = F. cos(i)

Notes:

- unit: sr^{-1}
- it is the 'bidirectional reflectance' divided by the cosine of the incident illumination: BRDF(i,e,g) = r(i,e,g) / cos(i)

Constraint: same as for 'bidirectional reflectance'

- *'radiance factor'*: RADF(0,e,g), r_f . The (bidirectional) radiance factor is the ratio of the radiance of a surface at a given illumination and viewing geometry, L(i,e,g), to the radiance of a perfect Lambert surface illuminated and viewed normally (i=e=0°), $L_{Lamb}(0,0,0)$.

  Notes:

  - it has no unit
  - frequently called 'I/F', or the 'apparent albedo'
  - it is the reflectance factor for normal illumination: REFF(0,e,g)
  - RADF(0,e,g) = π . r(i,e,g) = π . cos(i) . BRDF(i,e,g)

  Constraint: can be of any type of illumination-observation geometry (i,e,g)

- *'reflectance factor'*: REFF(i,e,g), r_c . The (bidirectional) reflectance factor is the ratio of the radiance of a surface at a given illumination and viewing geometry, L(i,e,g), to that of a Lambertian surface illuminated and viewed in the same geometry $L_{Lamb}(i,e,g)$

  Notes:

  - it has no unit
  - it is the radiance factor divided by the cosine of the incident illumination: REFF(i,e,g) = RADF(0,e,g) / cos(i)
  - REFF(i,e,g) = π . BRDF(i,e,g) = π . r(i,e,g) / cos(i)
  - sometimes called the 'Radiance coefficient', the 'Lambert albedo', or the 'reflectance coefficient' r_c

  Constraint: can be of any type of illumination-observation geometry (i,e,g)

- *'normalized reflectance':* any type of the above reflectance normalized to '1' at a given wavelength/wavenumber/frequency, to be defined in "*spectrum*_reference_position".
- *'albedo'*: all types of albedos, including spectrally integrated reflectance factors.

Note: The different albedos are mostly differentiated by their type of angular integration, which will be defined by "*parameters_instrument*_angle_observation_geometry", but they all bear the same global definition.

- *Normal albedo*, $A_n(0,0,0)$ (or normal reflectance r_n): case for a surface illuminated and viewed perpendicularly; L(0,0,0)
  - $A_n(0,0,0) = REFF(0,0,0) = RADF(0,0,0)$
  - It is a particular bidirectional reflectance
- *Directional-hemispherical albedo*, $A_h(i)$ (or reflectance r_h): ratio of the total reflected power, in all directions in the upper hemisphere, to the collimated irradiance incident from a given direction on the surface:
  - also called hemispherical albedo, or plan albedo
  - case of the angular integration of the illumination over the hemisphere.
- *Hemispherical-directional albedo*, $A_{hd}(e)$ (or reflectance r_{hd}): ratio of the reflected radiance in a given direction, in all directions, to to the total incident power on the surface:
  - case of the angular integration of the reflectance over the hemisphere.
- *Bihemispherical albedo*, A_s (or reflectance r_s): ratio of the total reflected power, in all directions in the upper hemisphere, to the total incident power on the surface:
  - also called spherical albedo
  - case of the angular integration of both the illumination and reflectance over the hemisphere.

Notes:

- The type and spectral range of integration should be specified in "*parameters_instrument*_spectral_observation_mode" and "*experiment/_spectrum*_spectral_comments"
- The type and angular range of integration should be specified in "*parameters_instrument*_angle_observation_geometry" and "*experiment/_spectrum*_angle_comments"

- '*complex reflectance ratio'*: composed of an 'amplitude component'

and the ‘phase difference’ (for ellipsometry)

- ‘*Stokes parameters’*: set of the four Stokes parameters: I, Q, U, V
  - Stokes parameter I = I(0°,0°)+I(90°,0°). Total intensity.
  - Stokes parameter Q = I(0°,0°)-I(90°,0°)
  - Stokes parameter U = 2I(45°,0°)-I(0°,0°)-I(90°,0°)
  - Stokes parameter V = 2I(45°,90°)-I(0°,0°)-I(90°,0°)

  Notes:
  - used for spectro-angular files containing all or part of these 4 parameters, instead to have them in separate files
  - sometimes the parameter ‘I’ is given separately in its intensity type (e.g. transmission, reflectance, …)
  - associated with "*spectrum*_files_parameter_type"=’polarimetric spectrum’
- ‘*normalized Stokes parameters’*: set of the three normalized Stokes parameters: I, Q/I, U/I, V/I
  - used for spectro-angular files containing all these 3 parameters, instead to have them in separate files
  - associated with "*spectrum*_files_parameter_type"=’polarimetric spectrum’
- ‘*polarization parameters’*: set of the (3 or) 4 polarization parameters: contrast, linear polarization (DoLP), position angle, and circular polarization
  - *‘polarization contrast’*: It is equal to the reduced Stokes parameter Pq which is the ratio between the Stokes parameter Q and the total intensity of light (I = I0 + I90). (Pq = Q/I)

    Note: may be also called: reduced Stokes parameter Pq, contrast, fraction of linear polarization Q, degree of linear polarization Q. polarization (%), Q, Pq
  - ‘*degree of linear polarization’*: Fraction of light which is polarized. (DolP = $(Q^2+U^2)^{1/2}$/I)

    Note: may be also called: total degree of linear polarization, PL, fraction of linear polarization, DoLP, m_L
  - ‘*polarization position angle’*: is the angle between the direction of maximum polarization and the direction perpendicular to the scattering plane. (χ= ½.atan(U/Q))

Note: may be also called: Angle of polarization, AoP, or position angle

- '*degree of circular polarization':* It is equal to the reduced Stokes parameter Pv which is the ratio between the Stokes parameter V and the total intensity of light (I = I0° + I90°). (Pv= V/I)

Note: may be also called: reduced Stokes parameter Pv, fraction of circular polarization V, degree of circular polarization V, circular polarization (%), V, DoCP, m_C

Notes:

- used for spectro-angular files containing all or part of these 4 parameters, instead to have them in separate files
- associated with "*spectrum*_files_parameter_type"='polarimetric spectrum'

- '*thermal emission'*: Thermal radiation power per unit area of radiating surface per unit of solid angle and per unit frequency
- '*thermal radiance'*: Radiant flux emitted by a surface, per unit area of radiating surface per unit solid angle. It is a directional quantity.
- '*thermal emittance'*: or radiant exitance (or radiant emittance) is the radiant flux emitted by a surface per unit area
- '*thermal emissivity'*: is the effectiveness of a surface in emitting energy as thermal radiation
- '*scattering intensity'*: intensity scattered by a medium (particles, solid, liquid) and collected by a detector
- *'differential scattering cross section':* angular dependence of scattering cross section ($dC_{sca}/d\alpha$) of a particle
- *'normalized differential scattering cross section', p*: angular dependence of scattering cross section ($dC_{sca}/d\alpha$) of a particle normalized to its total cross section C_{sca}
- *'scattering cross section parameters':* set of the 3 scattering cross section parameters: scattering, absorption, extinction
  - '*scattering cross section',* C_{sca}: total scattering cross section
    Note: It is the hemispherical integral of the *differential scattering cross section'*
  - '*absorption cross section',* C_{abs}: total absorption cross section

Note: Related with the absorption coefficient α: $\sigma = \alpha/N$ (N: molecule or particles number density)

- '*extinction cross section',* C_{ext}: sum of the absorption and scattering cross sections of a particle, $C_{sca} + C_{abs}$.
- associated with "*spectrum*_files_parameter_type"='scattering spectrum'

- *'scattering efficiency factor parameters':* set of the 3 scattering efficiency factor parameters: scattering, absorption, extinction
  - '*scattering efficiency factor',* Q_{sca}: which is defined as the ratio of the scattering cross-section to the geometrical cross-section πa^2.
    Note: Also simply called *'scattering efficiency'*
  - '*absorption efficiency factor',* Q_{abs}: which is defined as the ratio of the absorption cross-section to the geometrical cross-section πa^2.
    Note: Also simply called *'absorption efficiency'*
  - '*extinction efficiency factor',* Q_{ext}: which is defined as the ratio of the extinction cross-section to the geometrical cross-section πa^2.
    Note: Also simply called *'extinction efficiency'*
  - associated with "*spectrum*_files_parameter_type"='scattering spectrum'
- '*single scattering albedo*': total fraction of light reflected by a single particle. It s the ratio of scattering efficiency factor to the extinction efficiency factor.
- '*Raman scattering intensity*': intensity inelastically scattered (Raman scattering) by a medium (particles, solid, liquid) and collected by a detector
- '*normalized Raman scattering intensity'*: Raman scattering intensity normalized to '1' at a given wavelength/wavenumber/frequency, to be defined in "*spectrum*_reference_position".
- '*Raman scattering coefficient'*: ratio of the total scattered intensity per unit distance traveled by the exciting incident beam in the scattered media to the incident intensity
- '*Raman scattering efficiency*' (or cross section): ratio of the number of

photons scattered by Raman process to the total number of scattered photons
- '*fluorescence emission (intensity)*': intensity emitted by fluorescence by a medium (particles, solid, liquid) and collected by a detector
- '*normalized fluorescence emission*': fluorescence emission normalized to '1' at a given wavelength/wavenumber/frequency, to be defined in "*spectrum*_reference_position".
- '*fluorescence emission efficiency*': ratio of the number of photons emitted to the number of photons absorbed
- '*radiative transfer model parameters*': set of parameters used in radiative transfer models

Spectrum version

Constraints:
- the spectrum type mostly should not change with version but it is tolerated to upgrade it only to an upper product level of the same category of physical measurement to avoid keeping unnecessary lower level data or products
- the new "*spectrum*_type" should have the same "*spectrum*_file_type" as the original spectrum

Exemples:
- trnasmission => absorbance => normalized absorbance => absorption coefficient
- but: absorption coefficient => optical constant (file_type = 'complex') is forbidden
- optical density <=> absorbance
- ATR absorbance => corrected ATR absorbance => absorption coefficient
- Raman scattering intensity => normalized Raman scattering intensity,
- fluorescence emission => normalized fluorescence emission
- scattering intensity => differential scattering cross section => normalized differential scattering cross section => scattering cross section => scattering efficiency factor

*spectrum*_intensity_unit	openum(text)	U [!!o_m]	Spectr	Vc [Ver]	--	Unit of the intensity of the spectrum, depending on the spectrum type OpenEnum: {cm-1, m-1, cm2.g-1, m2.kg-1, mL.g−1·cm−1, cm2·mol−1, m2·mol−1, L·mol−1·cm−1, percent, permille, deg, count.s-1, count.nm-1, S, ohm, dB, sr-1, micron2, mm2, m2, m-1.sr-1, m2.sr-1, W.m-2, kW.m-2, W.sr-1, kW.sr-1, W.m-2.sr-1, kW.m-2.sr-1, W.m-2.sr-1.cm-1, W.m-2.sr-1.micron-1, AU, no unit, unknown, …} *Condition:* absolute mandatory only when *"spectrum*_type" = {absorption coefficient, complex admittance, complex impedance, bidirectional reflectance, bidirectional reflectance distribution function, thermal emission, thermal radiance, thermal emittance, scattering intensity, differential scattering cross section, normalized differential scattering cross section, scattering cross section parameters, Raman scattering intensity, Raman scattering coefficient, Raman scattering efficiency, fluorescence emission, fluorescence emission efficiency, radiative transfer model parameters} *Definitions:* - 'cm-1', 'm-1': for 'metric absorption coefficient' (cm^{-1}, m^{-1}) - 'cm2.g-1', 'm2.kg-1', 'mL.g−1·cm−1': for mass attenuation coefficient ($cm^2.g^{-1}$, $m^2.kg^{-1}$, $mL.g^{-1}·cm^{-1}$) - 'cm2·mol−1', 'm2·mol−1', 'L·mol−1·cm−1': for molar attenuation coefficient ($cm^2·mol^{-1}$, $m^2·mol^{-1}$, $L·mol^{-1}·cm^{-1}$) - 'percent': % - 'permille': ‰ - 'deg': angular ° - 'count.s-1': count/s - 'count.nm-1': count/nm - 'S': Siemens - 'ohm': Ohm (Ω) - 'dB': decibel (dB) - 'sr-1': sr^{-1} - 'micron2', 'mm2', 'm2': $µm^2$, mm^2, m^2 - 'm-1.sr-1': m^{-1}/sr - 'm2.sr-1': m^2/sr - 'W.m-2', 'kW.m-2': W/m^2, kW/m^2 - 'W.sr-1', 'kW.sr-1': W/sr, kW/sr

- ‘W.m-2.sr-1’, ‘kW.m-2.sr-1’: $W/m^2/sr$, $kW/m^2/sr$,
- ‘W.m-2.sr-1.cm-1’: $W/m^2/sr/cm^{-1}$
- ‘W.m-2.sr-1.micron-1’: $W/m^2/sr/\mu m$
- ‘AU’: Arbitrary Unit (generally simple detector signal)
- ‘no unit’:
- ‘unknown’: there is a unit but it is unknown (quite similar to AU). Typical case for “*spectrum*_type” = ‘raw’

Notes:

- The following spectrum types have always no unit:
    - absorbance, normalized absorbance, optical depth, optical constants, ATR absorbance, corrected ATR absorbance, relative complex permittivity, relative complex permeability, normalized reflectance, thermal emissivity, scattering efficiency factor parameters, single scattering albedo, anisotropy factor, normalized Raman scattering intensity, normalized fluorescence emission
- The following spectrum types have generally no unit but may be sometimes expressed as ‘%’ (percent):
    - transmission, ATR transmission, reflectance, radiance factor, reflectance factor, albedo, anisotropy factor, complex reflectance ratio, normalized Stokes parameters, polarization contrast, degree of circular polarization, degree of linear polarization
- The following spectrum types have generally no unit but may be sometimes expressed as ‘decibel’ (db):
    - dielectric loss tangent, magnetic loss tangent
- A few ones have (or may have) specific units:
    - Absorption/attenuation coefficient:
        - metric $\{cm^{-1}, m^{-1}\}$
        - mass $\{cm^2.g^{-1}, m^2.kg^{-1}, mL.g^{-1}\cdot cm^{-1}\}$
        - molar $\{cm^2\cdot mol^{-1}, m^2\cdot mol^{-1}, L\cdot mol^{-1}\cdot cm^{-1}\}$
    - complex admittance: (Siemens: S),
    - complex impedance (ohm),

- bidirectional reflectance, bidirectional reflectance distribution function: {sr^{-1}}
- Stokes parameters: {AU}
- thermal emission: {$W/m^2/sr/cm^{-1}$, $W/m^2/sr/\mu m$, }
- thermal radiance: {$W/m^2/sr$, $kW/m^2/sr$}
- thermal emittance: {W/m^2, kW/m^2}
- scattering intensity: {count/nm, $W/m^2/sr$, $kW/m^2/sr$, W/sr, kW/sr} but absolute values are rarely used
- differential scattering cross section: {m^2/sr}
- normalized differential scattering cross section: {sr^{-1}}
- scattering cross section parameters:{μm^2, mm^2, m^2}
- Raman scattering intensity: {count/nm, ...} but absolute values are rarely used
- Raman scattering coefficient: {m^{-1}/sr}
- Raman scattering efficiency (or cross section): {m^2/sr}
- fluorescence emission: {count/nm} but absolute values are rarely used
- fluorescence emission efficiency (or cross section): {m^2/sr}

- Some of the 'radiative transfer model parameters' have their own unit, e.g.:
  - mean macroscopic roughness 'Θ': {deg}
  - Henyey-Greenstein phase function 'g' (or 'b' and 'c'): no
  - opposition peak height 'Bo': no
  - opposition peak width 'h': {deg}

Spectrum version

Notes:

- the unit may change if the spectrumtype is upgraded to an upper product level of the same category of physical measurement

*spectrum*_reference_position	float	U [!o_m]	Spectr	V [Ver]	var.	Reference position (wavenumber/wavelength/frequency) of the band to which the normalized (or relative) intensity is calculated (set to intensity = 1 at this reference position).

						Unit: in unit defined by "*parameters_instrument*_spectral_unit" • Converted and stored in 'cm-1' unit in the database but displayed to the user in the unit specified by the user in SSHADE *Condition:* Mandatory when "*spectrum*_type" = {normalized absorbance, normalized Raman scattering, normalized fluorescence emission} *Note:* should be generally the strongest band, or a standard reference band. *Note:* used in particular to derive the 'normalized Raman emission' and 'normalized fluorescence emission' spectra.
spectrum_reference_spectra	***List [L1]***	[O]				£: reference spectra used to produce a relative spectrum
*spectrum*_reference_spectrum_uid [*]	varchar(255)	U [m]	Spectr Spectr L1	V [Ver]	--	Link to the existing UID of the reference spectrum(a) (if already in the database) used to produce this relative spectrum *Note:* - only for a spectrum relative to a reference spectrum (of level 1+), i.e. when a transmission/absorbance/… spectrum is divided/substracted from/by this transmission/absorbance/…reference spectrum. - not for 'raw instrument transfer function spectra' (level 0) such as the reference spectrum taken with white 'Spectralon 99' as calibration target for reflectance spectra. But you can put a true reflectance spectrum (level 1) of 'Spectralon 99'. *Ex*: you substract the initial absorbance spectrum of an ice mixture from your absorbance spectrum taken after irradiation in order to display only the spectrum of the products
*spectrum*_model_parameters	blob	U [m]	Spectr	V [Ver]	--	Model parameters for a simulated spectrum (+ errors for model fit) *Condition:* strongly recommended when "*instrument*_type" = {radiative transfer simulation, quantum mechanical simulation…} *Note*: LaTeX can be used *Notes*: - You can provide here information and parameters values (+errors) used

in radiative transfer or quantum mechanic simulations (direct or spectrum fit). This excludes the info/parameters directly linked to the "*sample*" (composition, grain size, …) or the "*instrument*" (spectral, angular, spatial … info).

- When the spectrum is simulated (direct):
    - the radiative transfer or quantum mechanic model should be described as an "*instrument*" and linked in "experiment" with "*experiment*_parameters_instrument_uid".
    - the optical constants used to simulate the sample should be noted in "*sample*_material_comments" or "*sample*_constituent_comments" (depending on the level of mixing and type of optical constants) and its reference given in "*sample*_publication".
    - The grain size of the sample material(s) should be given in "*sample*_material_grain_size_min/max/fraction"
    - The fixed model parameters (wavelength independent) are given here. For ex: the mean macroscopic roughness 'Θ', Henyey-Greenstein phase function 'g' (or 'b' and 'c'), opposition peak height 'Bo' and width 'h'. You can also repeat the name and reference of the RT/QM model used (but already in "instrument") and the optical constants used (but also in a "sample" comment).
        - *Ex*: 'Spectrimag model, Dout$\'e$ and Schmitt (1998): optical constants by Grundy and Schmitt (1998). Mean macroscopic roughness $\theta = 10°$, simple Henyey-Greenstein phase function $g = 0.4$, no opposition peak'

- If you want to put a model fit of a laboratory spectrum in the database:
    - create new (sample) and experiment with the model as the instrument and link the model spectrum to the lab spectrum with "*spectrum*_parent_spectrum_uid".
    - or do it in the same experiment by declaring 2 instruments in "*experiment*_parameter_instrument_uid": the true one and the model, and then for each spectrum you can choose with

---

"*spectrum*_parameter_instrument_uid" between the true instrument (measured spectrum) and the model (simulated spectrum).

- o you can provide here the absolute uncertainty (± errors) on the 'non-spectral' fit parameters of your spectrum.
  - *Ex*: 'Hapke surface reflectance model (1986): optical constants by Grundy and Schmitt (1998). Single scattering albedo $\omega = 0.82 \pm 0.02$ (@ 1200nm), mean macroscopic roughness $\theta = 15.5^{\circ} \pm 2.5^{\circ}$, Henyey-Greenstein phase function $b = 0.265 \pm 0.050$, $c = 0.585 \pm 0.025$, opposition peak height $B_0 = 0.15 \pm 0.03$, opposition width $h = 0.10 \pm 0.02$'

---

*spectrum*_level [-xml]	enum(text)	S3/Uu [!!_c]	Spectr	V [Ver]	--	Level of the spectrum product Enum: {0, 1, 2, 3, 4} *Notes:* - '0' corresponds to "raw signal" - '1' corresponds to "spectrum" - '2' corresponds to "intermediate spectrum": only simple math operation (normalization, …) - '3' correspond to "advanced_spectrum": moderately complex math operations (ratio between spectra, …) - '4' correspond to "advanced_spectrum": complex math operations - ('5' to '8' are reserved to "*bandlist*_level") ➔ Determined from "spectrum_type" (correspondence table below) - '0': raw - '1': transmission, ATR transmission, complex admittance, complex impedance, bidirectional reflectance, radiance factor, thermal emission, thermal radiance, scattering intensity, Raman scattering intensity, fluorescence emission - '2': absorbance, normalized absorbance, optical depth, ATR absorbance, corrected ATR absorbance, relative complex permittivity,

relative complex permeability, bidirectional reflectance distribution function, reflectance factor, normalized reflectance complex reflectance ratio, Stokes parameters, normalized Stokes parameters, thermal emittance, differential scattering cross section, normalized Raman scattering intensity, normalized fluorescence emission

- '3': absorption coefficient, dielectric loss tangent, magnetic loss tangent, albedo, anisotropy factor, polarization parameters, normalized differential scattering cross section, scattering cross section parameters, Raman scattering coefficient
- '4': optical constants, thermal emissivity, scattering efficiency factor parameters, single scattering albedo, Raman scattering efficiency, fluorescence emission efficiency, radiative transfer model parameters

Spectrum version

Notes:

- the level may change if the spectrum type is upgraded to an upper product level of the same category of physical measurement

Exemples:

- absorbance => absorption coefficient (cm^{-1})

Experiment and spectra links						
*spectrum*_experiment_uid [*§][-xml]	varchar(255) [Virtual Link]	U [!!_v]	Spectr Exper	F	--	Link to the existing UID of the experiment that produced this spectrum (this experiment provides the links to the instrument parameters) *Note xml/DB:* in practice in the database (and import xml) the "spectra" are linked directly to the experiment (same file)
spectrum_parent_spectra	***List [L2]***	[O]				£: original spectra used to produce a high-level spectrum
*spectrum*_parent_spectrum_uid [*]	varchar(255)	S2 [$o_m]	Spectr Spectr L2	V [Ver]	--	Link to the existing UID of the original spectrum(a) (if already in the database) used to produce a high-level spectrum *Recommendation:* Strongly recommended when already exist in the database *Note:* for intermediate and advanced spectra only ("spectrum_level" ≥ 2).

						For level 2: a single spectrum; for levels 3 and 4: one or more spectra. **Spectrum version** *Notes:* - the parent spectrum may change if the spectrum type is upgraded to an upper product level of the same category of physical measurement *Exemples*: - absorbance spectrum: parent = transmission spectrum - absorption coefficient spectrum: parent = absorbance spectrum
Spectrum sample						
*spectrum*_sample_uid [*]	varchar(255)	S0 [!!_m]	Spectr Sampl	F	--	Link to the existing UID of the sample on which this spectrum is recorded. *Notes:* - when the sample evolves irreversibly between two spectra (sample composition, phase or texture noticeably changing during the experiment) it is necessary to redefine a 'new' sample (composition, state, …) and to provide its "*sample*_uid" here. - It is the case in particular when chemical processes (such as irradiation, for exemple) are applied to the sample. Also, when a reversible or irreversible phase change occurs. - When more than one sample is used to obtain a high-level product ("spectrum_level" ≥ 3), it is necessary to create a "generic sample" describing only the common (and useful) properties of the different samples used. The link to the original samples (if in the database) will be done through the list of parent spectra.
*spectrum*_sample_changes	blob	U [o_m]	Spectr	F	--	Chemical, textural or physical changes of the initial sample during the experiment *Condition:* should be void ('') when *spectrum*_chronologically_ordered = 'no' or 'false' *Note*:

						- It is the known, observed or expected chemical (composition, ...), textural and/or physical (phase, ...) changes of the sample relative to the initial sample or to its state at the previous spectrum (need to tell) and produced by any processing during an experiment. - The sample changes can occur before or during spectrum recording (need to tell). - Also used to describe sample changes (irradiation effects) induced by laser during Raman or fluorescence measurements (structural and chemical). - It should not be used to tell differences between different initial samples *Ex:* - 'destruction of CH4 and formation of C2H2 and higher hydrocarbons during sample irradiation by VUV light', - 'transformation from alpha-N2 to beta-N2 ice phase during warmup', - 'sintering and small sublimation of the sample', - 'sputtering of sample surface', …
*spectrum*_sample_comments	blob	U [m]	Spectr	F	--	Additional or general information on the sample
Spectrum variable parameters: probed materials and constituents						*Condition:* specific to microscopic and imaging spectra
spectrum_sample_primary_materials	***List [L3a]***	[!o]		F		£: primary material(s) of the sample probed by a pixel or some average of an imaging measurement *Condition:* Mandatory only when "*instrument*_microscopy_imaging" = {imaging}
*spectrum*_sample_primary_material_uid [*]	varchar(255)	S1i [m]	Spectr Mater L3a	F	--	Link to the existing UID of the "primary material(s)" of the sample probed by a pixel or some average of an imaging measurement *Format:* see *"material*_uid" *Notes:* - specific to macroscopic imaging spectra. For macroscopic

					measurements the spectrum or the whole spectro-image is generaly recorded globaly on all materials of the sample. - for pixel or pixel average (ex: ROI, Region Of Interest) of imaging measurements the spectrum is recorded on one or more specific material(s) of the sample. - the location of the pixels or pixel averages probing this/these materials can be given with a picture in "*spectrum_images"* - these "*material*_uid" should be among those in the list of "*material*_material_uid" of the sample description.
*spectrum*_sample_primary_materi al_comments	blob U [m]	Spectr L3a	F	--	Additional information on the primary material(s) of the sample probed by a a pixel or some average of an imaging measurement
spectrum_sample_primary_constit uents ***List [L3b]***	[!o]		F		£: primary constituent(s) of the sample probed by a microscopic measurement *Condition:* Mandatory only when "*instrument*_microscopy_imaging" = {microscopy, micro-imaging}
*spectrum*_sample_primary_constit uent_uid [*]	varchar(255) S1i [m]	Spectr Const Solid Miner Solut L3b	F	--	Link to the existing UID of the "primary constituent(s)" of the sample probed by a microscopic measurement *Format:* see *"constituent*_uid", *"solid*_uid", *"mineral*_uid", *"liquid*_uid" *Notes:* - Specific to microscopic and micro-imaging spectra. For macroscopic and imaging measurements the spectrum or whole spectro-image is generaly recorded globaly on all constituents/materials of the sample. - for microscopic measurements the spectrum is recorded on one or more specific constituent(s) of the material/sample. But it can also correspond to a pixel, a pixel average, or to the whole spectral image, depending on the value of "*parameters_instrument*_spatial_observation_mode". - the location of the pixels or pixel averages probing this/these constituents can be given with a picture in "*spectrum_images"* - these "*constituent*_uid" should be among those in the list of

						"*material*_constituent_uid" of the sample description.
*spectrum*_sample_primary_constituent_comments	blob	U [m]	Spectr L3b	F	--	Additional information on the primary constituent(s) of the sample probed by a microscopic measurement

Spectrum variable parameters: sample environment and instrument

Environment: Used either for multi-spectra experiments (allow to modify for each spectrum the values of the variable sample parameters first defined in *sample*_parameters_sample"), or for a high level spectral product (allow to make the synthese of a set of n samples by using the sample of one of the parent_spectrum and modifying the variable sample values). But in this case it is highly recommended to define a 'generic sample' to make the synthese.

Instrument: Used either for multi-spectra experiments (allow to modify for each spectrum the values of the global instrument parameters first defined in "*experiment*_parameters_instruments"), or for a high level spectral product (allow to redefine the instrument parameters changed by the creation of a product, when some parameters are defined at 'experiment' level (instead to define them all at 'experiment level: not recommended). Not useful if generic instrument parameters are fully defined at 'experiment level (recommended).

spectrum_sample_parameters_environment	***List [L4a]***	[-]				£: Set of sample parameters specific to this spectrum *Note*: Describe the changes in the environment of the sample before/during the spectrum compared to the ones described in "*sample*_parameters_sample" (generally corresponding to its state before the first spectrum). Only the parameters that changed need to be modified
*spectrum*_sample_parameters_environment_index [*§][-xml]	int(11) [Virtual Link]	B [!o_v]	Spectr Sampl L4a	F	--	ID of the variable sample parameters specific to this spectrum *Conditions:* it is mandatory to fill only the sample parameters that changed *Note DB:* in practice the "*sample*_parameters" are linked directly to the spectrum *Note DB:* This list refers to the variable parameters (marked V) of the "*sample*" table. For practical reasons "*sample*_parameters_sample" is split in 3 tables: " physchem_environment", "fluid_composition " and "irradiation".
spectrum_parameters_instruments	***List [L4b]***	[-]		V [~Ver]		£: Set of instrumental parameters specific to this spectrum *Note*: Describe the changes in the instrument parameters used to record this spectrum compared to the ones described in

						"*experiment*_parameters_instruments" (generally corresponding to the state before the first spectrum). Only the parameters that changed need to be modified **Spectrum version** *Note*: only the blocs "*parameters_instrument*_spectral" and "*parameters_instrument*_spatial" are versioned
*spectrum*_parameters_instrument_index [*§][-xml]	int(11) [Virtual Link]	B [!o_v]	Spectr ParIns L4b	V	--	ID of the set of instrumental parameters specific to this spectrum *Conditions:* it is mandatory to fill only the instrument parameters that changed *Note:* "*parameters_instrument*_instrument_sample_holder" did not appear in the xml in "*spectrum*_parameters_instrument" as it should be fixed in "*experiment*_parameters_instrument" for all spectra made with this instrument *Note DB:* in practice the "parameters_instrument" are linked directly to the spectrum

Spectrum origin and history

*spectrum*_date_begin	date	S1 [!_m]	Spectr	F	YYYY-MM-DD	Starting date of collection of the raw spectrum or creation date of the spectrum product *Notes*: - for raw and calibrated spectra (level 1, 2): record date - for spectrum products (levels 3 and above): date of creation of product
*spectrum*_time_begin	time	U [m]	Spectr	F	HH:MM:SS	Starting time of collection of the raw spectrum (at the above collection date) *Notes*: - only for raw and calibrated spectra ("*spectrum*_level" = {1, 2}): starting time of the record - this time allows following kinetics monitored by spectra.
*spectrum*_date_end	date	U [m]	Spectr	F	YYYY-MM-	Ending date of collection of the raw spectrum *Notes*:

					DD	- only for raw and calibrated spectra ("*spectrum*_level" = {1, 2}): ending date of the record - useful in particular for sets of SBRDF or SDEDF data that can be recorded over more than one day - you can keep it void if ending date is the same as starting date
*spectrum*_time_end	time	U [m]	Spectr	F	HH:MM:SS	Ending time of collection of the raw spectrum (at the above collection date) *Notes*: - only for raw and calibrated spectra ("*spectrum*_level" = {1, 2}): ending time of the record - this time allows following kinetics monitored by spectra.

Spectrum versions and validation

*spectrum*_access_right [-xml] [+pi] *[also from provider interface]*	enum(text)	S2/Uu [!!d_m]	Spectr	V [Ver]	--	Rights of access to the spectrum. Enum: {unreleased, restricted, public} *Constraints:* - 'unreleased' is the only and default value when *"spectrum*_import_mode" = {first import} - 'unreleased' and 'restricted' cannot be used if "*spectrum*_access_right" is already set to 'public' *Definitions:* - '*unreleased*': access only to all the 'experimentalists' of the experiment and to the DB provider that imported the data. - '*restricted*': access only to the DB managers, DB providers and DB users of the database in which these data are imported, and also to access groups that get access to these data - *'public'*: access to all users *Note xml:* this KW is not mandatory in the xml, but it allows to set 'public' *Notes:* - allow to limit the access to the data first only to the experimentalists of the experiment (and the 'provider' that imported the data), or to all the

						user/provider/manager of the partner database (set by "*user*_manager_database_uid/_right") , or to everybody. - this allows to prepare data in the database and put them online 'public' (or any other group restriction) only when wanted (publication of the paper …) *Note SSHADE:* implemented directly in the 'provider interface' with computer-controlled data access rights, not through xml.
*spectrum*_import_validation [-xml] [pi] *[from provider interface]*	enum(text) [Vitual KW]	S1b/Uu [!!d_m]	Spectr	V [Ver]	--	Validation state of an imported spectrum Enum: {non-validated, validated} *Constraints:* - 'non-validated' is the only and default value when *"spectrum*_import_mode" = {first import} *Definitions:* - '*non-validated':* imported spectrum data and metadata not yet validated in the database - *'validated':* spectrum data and metadata validated in database *Default:* 'non-validated' *Notes:* - it is not a 'scientific' validation (should be done before import!), but rather the validation of the completeness and correctness of the imported data. - The 'non-validated' state allows to import data in the database and take time to fully check them online. *Note SSHADE:* implemented directly in the 'provider interface' with computer-controlled data access rights, not through xml.
*spectrum*_date_released [-xml]	date	S1b/Uu [!!_c]	Spectr	V [Ver]	YYYY-MM-DD	Date of opening the access to the spectrum to the public (current version) ➔ determined automatically by the interface when "*spectrum*_access_right" is set to 'public'. Initialy set to the date of release of the spectrum and modified at each change of the spectrum data file (i.e. when "*spectrum*_import_mode" =

						'new version') *Note:*
*spectrum*_date_created [-xml]	date	S1b/Uu [!!_c]	Spectr	V [Ver]	YYYY-MM-DD	Date of first import or upgrade of the spectrum ➔ determined automatically by the data ingestion software. Initialy set to the date of entry of the spectrum in the database (first import w. upload) and modified at each change (modification/upgrade) of the spectrum data file (i.e. when "*spectrum*_import_mode" = 'new version') *Note:* - each "*spectrum*_version" has its "*spectrum*_date_created" ("*spectrum*_version.date_created") - in the code "*spectrum*.date_created" correspond to "*spectrum*_version.date_created" of the first version
*spectrum*_date_updated [-xml]	date	S1b [!!_c]	Spectr	V [Ver]	YYYY-MM-DD	Date of update of the metadata of a version of the spectrum in the database ➔ determined automatically by the data ingestion software. Initialy set to the date of entry of the spectrum/product in the database (i.e. when "*spectrum*_import_mode" = 'first import') and modified at each change (update) of spectrum metadata (i.e. when "*spectrum*_import_mode" = 'correction') until (not included) a new version is created "*spectrum*_import_mode" = 'first import' or 'new version') *Note:* - each "*spectrum*_version" has its "*spectrum*_date_updated" - in the code "*spectrum*.date_updated" correspond to "*spectrum*_version.date_updated" of the last version
*spectrum*_version [–xml]	int(3)	S3 [!!c]	Spectr	V [Ver]	--	Version number of the spectrum data ➔ incremented automatically by the data ingestion software when "*spectrum*_import_mode" = 'new version'. Set to '1' at first spectrum data file ingestion and then incremented at each major change of the spectrum data file. *Notes:*

- there could be several reasons to upgrade a spectrum
  - ✓ improvement of the data in term of spectral and/or photometric calibration, better baseline correction, S/N, removal of spurious features or atmospheric absorption, ...
    - affect mostly the spectrum file and a few spectrum KW: _analysis, _history...
  - ✓ change of the way to make spatial average in case of roi or rastered average on images
    - affect mostly several KW of "*parameters*_instrument_spatial" as well as possibly some KW such as _title, _analysis
  - ✓ extension of the spectral range, in particular for optical constants
    - affect mostly several KW of "*parameters*_instrument_spectral" as well as KW such as _title, _analysis, _history...
  - ✓ upgrade of the data to an upper product level of the same type of measurement, such as baseline correction, normalization, quantification, ...
    - affect KW such as spectrum_title, _type, _intensity_unit, _level, _analysis..., and can affect KWsuch as _reference_position, parent_spectrum_uid,...
- no new version number generated when "*spectrum*_import_mode" = 'correction'

*spectrum*_previous_version_status	enum(text)	S2 [!!o_m]	Spectr	V [Ver]	--	Validity status of the previous version Enum: {obsolete version, partly invalidated version, invalidated version, partly invalidated data, invalidated data} *Condition:* only and absolute mandatory when *"spectrum*_import_mode" = {new version, invalidate} *Constraints*: - For *"spectrum*_import_mode" = 'new version' , this KW is archived

						with the previous version - For *"spectrum*_import_mode" = 'invalidate' AND "*spectrum*_previous_version_status" = {obsolete version, partly invalidated version, invalidated version} this KW is stored with the current version. - For *"spectrum*_import_mode" = 'invalidate' AND "*spectrum*_previous_version_status" = {partly invalidated data, invalidated data} this KW is stored with the current version and all previous versions. *Definitions:* - '*obsolete version'*: This version is still scientifically valid but the new version improved at least part of the spectrum inside its valid spectral range, or extended its valid spectral range. - '*partly invalidated version'*: This version is still scientifically valid over most of the valid spectral range but an error was found that is corrected in the new version - '*invalidated version'*: An error was found over most or all the valid spectral range of this version that is corrected in the new version - '*partly invalidated data'*: An error was found over part of the valid spectral range of the original data, but the data cannot be corrected there. The new version of the spectrum has a reduced valid spectral range. - '*invalidated data'*: An error was found over most or all the valid spectral range of the original data, but the data cannot be corrected. There is no new version of the spectrum. It invalidates all previous versions. *Note SSHADE:* This status will be clearly displayed (bold) at the beginning of the previous version spectrum page ('new version') or on all versions for 'invalidate'
*spectrum*_previous_version_comments	blob		U [!!o_m]	Spectr [Ver]	V	--	Description of the reason for the change of version or for the data invalidation *Condition:* only and absolute mandatory when *"spectrum*_import_mode" = {new version, invalidate}

						Constraints: same as "*spectrum*_previous_version_status" *Note SSHADE:* This comment will be clearly displayed after the status at the beginning of the previous version spectrum page *Exemples*: - 'OBSOLETE VERSION:' 'improved baseline correction and removal of CO2 gas absorption in version #2' - 'PARTLY INVALIDATED VERSION:' 'invalidated above 3.5 µm due to misscorrected thermal emission. Corrected in version #2' - 'INVALIDATED VERSION:' 'invalidated spectrum due to a severe calibration error. Corrected in version #2' - 'PARTLY INVALIDATED DATA:' data partly invalidated due to a calibration error. Original raw no more available for recalibation. No fully valid version available. ' - 'INVALIDATED DATA:' original raw data fully invalidated due to a severe measurement error. No valid version available. Replaced by and linked to a newly recorded spectrum'
*spectrum*_previous_version_new_spectrum_uid [*]	varchar(255)	U [$o_m]	Spectr Spectr	V [Ver]	--	Link to the existing UID of a spectrum in another experiment (if already in the database) that replaces the old spectrum in case there is no new version *Constraint:* only when *"spectrum*_import_mode" = {invalidate} *Recommendation:* strongly recommended when *"spectrum*_import_mode" = {invalidate} when this new spectrum already exist in the database *Note:* - In the cases of invalidated raw data (or lost raw data), no new analysis can correct the spectrum, but another spectrum in another similar experiment may have been uploaded to replace this one. - Another case can be that we have uploaded a better spectrum in another newest experiment and we want to redirect to this spectrum and set the older spectrum 'obsolete' - This link allows redirecting to this new spectrum instead to a new spectrum version, not available here.

*spectrum*_history	blob	U [cm]	Spectr	V [Ver] Aj	--	History of the spectrum import, upgrade or correction ➔ calculated by default and added to the current text: ”*spectrum*_date_last_updated”: “*spectrum*_import_mode” – “*spectrum*_version” – “*spectrum*_history”, where “*spectrum*_history” is the text added in the xml file. This KW is in “replace” = ‘no’ mode by default Ex: - '2009-12-25: first import - v1' [no text in “*spectrum*_history”] (c) - '2010-08-03: correction - v1: added band information on spectrum' [“*spectrum*_history” = ‘added band information on spectrum'] (c+m) - '2010-10-15: new version - v2: corrected errors in real index n values above 9000 cm-1' [“*spectrum*_history” = ‘corrected errors in real index n values above 9000 cm-1’] (c+m)

Spectrum analysis and validation

*spectrum*_analysis	blob	U [!m]	Spectr	V [Ver]	--	Textual description of spectrum analysis *Note:* - *e.g.:* baseline correction for absorbance or Raman data (function, wavelength range, …); removal of atmospheric lines, spectra averaging, normalization (relative to …), smoothing spectral/intensity concatenations for absorption coefficient; k,n indexes extraction model for optical constants; ...
*spectrum*_quality_flag	enum(int)	S3 [!o_m]	Spectr	V [Ver]	--	General quality flag on the spectrum Enum: {0, 1, 2, 3, 4, 5} *Constraint:* set to ‘0’ when “*spectrum*_import_mode” = ‘invalidate’. Can have 6 quality levels from ‘0’ to ‘5’ - ‘0’: no valid data or bad data (only used to flag older invalidated versions!) - ‘1’: low quality (only used to flag older partly invalidated versions!) - ‘2’: medium quality

- ‘3’: good data
- ‘4’: very good data
- ‘5’: excellent data

Note: will be evaluated over the valid spectral range

Notes:

- The values ‘0’ and ‘1’ is for flagging any data that are found ‘bad’ after their import in the database and are replaced (or not) by a new version. The old ‘bad’ version is maintained in the database in order to keep track of all data which may have been used, but to clearly display a warning with “*spectrum*_previous_version_status“

Spectrum version

Constraints:

- when “*spectrum*_previous_version_status” = {invalidated version, invalidated data} then “*spectrum*_quality_flag” of previous version is set to ‘0’
- when “*spectrum*_previous_version_status” = {partly invalidated version, partly invalidated data} then “*spectrum*_quality_flag” of previous version is set to ‘1’

spectrum_validators	***List [L5a]***	[O]				£: Experimentalist(s) who processed and validated the spectrum
*spectrum*_validator_experimentalist_uid [*]	varchar(255)	S1/Uu [m]	Spectr Exper L5a	V [Ver]	--	Link to the existing UID of the experimentalist(s) who processed and validated the spectrum (for data provider tracking)
*spectrum*_comments	blob	U [m]	Spectr	V [Ver]	--	General comments on the spectrum, measurements conditions or analysis

Spectrum references

spectrum_publications	***List [L5b]***	[!o]				£: Publications in which the spectrum is published

						Condition: Mandatory only when "*experiment*_publication_uid" ≠= Ø *Note:* Put 'NULL' if there is no publication
*spectrum*_publication_uid [*]	varchar(255)	S2 [!o_m]	Spectr Publi L5b	V [Ver]	--	Link to the existing UID of the publication(s) in which the spectrum has been published *Notes:* – at least one when the spectrum is already published in a publication (and when not already listed in "*experiment*_publications") – these papers should be in the publications database, with "*publication*_content" = 'spectral data' *Note DOI:* – recommended option as "RelatedIdentifier / relationType=IsReferencedBy" (12.2): "*publication*_doi"
*spectrum*_publication_comments	blob	U [m]	Spectr	V [Ver]	--	Comments about the spectrum or multi-angle dataset in the publication *Note*: for exemple which part of the spectrum or of the multi-angle spectra dataset are published, ...

Spectrum file format description

*spectrum*_files_parameter_type	enum(text)	S2 [!!_m]	Spectr	F [Ver]	--	Type of the spectral data to be uploaded Enum: {single spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum, photometric data, spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data, spectral image, photometric images, spectral images of multiangle dataset, photometric images of multispectral dataset, spectro-photometric images} *Constraints*: - "*spectrum*_files_parameter_type" = 'complex spectrum' only for "*spectrum*_type" = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex permeability}

- "*spectrum*_files_parameter_type" = 'polarimetric spectrum' only for "*spectrum*_type" = {Stokes parameters, normalized Stokes parameters, polarization parameters}
- "*spectrum*_files_parameter_type" = 'scattering spectrum' only for "*spectrum*_type" = {scattering cross section parameters, scattering efficiency factor parameters}
- "*spectrum*_files_parameter_type" = 'model parameters spectrum' only for "*spectrum*_type" = {radiative transfer model parameters}
- all the other values of "spectrum_files_parameter_type" are only for the other values of "spectrum_type"

Constraint: when "*spectrum*_import_mode" = {correction, new version} "*spectrum*_files_parameter_type" cannot be changed

Definitions:

- '*single spectrum'*: file containing a single mono intensity spectrum (transmission, …)
- '*complex spectrum'*: file containing a spectrum expressed with a real and an imaginary part, such as 'optical constants', 'complex impedance' or 'complex reflectance ratio' ("*spectrum*_type")
- '*polarimetric spectrum'*: file containing a spectrum for a set of 3-4 polarization parameters such as "*spectrum*_type":
    - 'Stokes parameters': {Stokes parameter I, Stokes parameter Q, Stokes parameter U, Stokes parameter V}
    - 'normalized Stokes parameters': {normalized Stokes parameter Q/I, normalized Stokes parameter U/I, normalized Stokes parameter V/I}
    - 'polarization parameters': {polarization contrast, degree of linear polarization, polarization position angle, degree of circular polarization}

  Note: the unit of 'polarization position angle' is 'deg' (cannot be specified in "*spectrum*_intensity_unit" because the other parameters have no unit)
- '*scattering spectrum'*: file containing a spectrum for a set of 3 scattering parameters such as "*spectrum*_type":
    - 'scattering cross section parameters': {scattering cross section,

absorption cross section, extinction cross section}
    - ‘scattering efficiency factor parameters’: {scattering efficiency factor, absorption efficiency factor, extinction efficiency factor}

- ‘*model parameters spectrum’*: file containing a series of wavelength-dependent (spectra) model parameters
- ‘*photometric data’*: file containing multi-angular photometric data at a single wavelength
- ‘*spectra of multiangle dataset:* series of files containing each a spectrum at single geometry in a multiangle dataset.
  Ex: spectra at sereral illumination-observation geometries
- *‘photometric data of multispectral dataset’*: series of files containing each multi-angular photometric data at a single wavelength in a multispectral dataset.
  Ex: photometric curves at sereral wavelengths
- ‘*spectro-photometric data’*: file containing a set of multi-angular spectro-photometric data expressed either as:
    - a single bloc of spectro-photometric data for all values of the angular and spectral parameters
    - a series of blocs of photometric data ordered by wavelengths (for multi-wavelengths photometric data)
    - a series of blocs of spectra ordered by angular geometry (mostly for multi-angles spectra)
- ‘*spectral image’*: file containing an (hyper)spectral image at a single geometry
  Note: the emergence angle may slightly vary in the image
- ‘*photometric images’*: file containing multi-angular photometric images at a single wavelength
- ‘*spectral images of multiangle dataset*: series of files containing each a (hyper)spectral image at single geometry in a multiangle dataset.
- ‘*photometric images of multispectral dataset’*: series of files containing each multi-angular photometric image at a single wavelength in a multispectral dataset.
- ‘*spectro-photometric images’*: file containing a set of multi-angular spectro-photometric images expressed either as:
    - a single bloc of spectro-photometricimages for all values of the

angular and spectral parameters
    - a series of blocs of photometric images ordered by wavelengths (for multi-wavelengths photometric images)
    - a series of blocs of spectral images ordered by angular geometry (mostly for multi-angles spectral images)

Notes:
- ‘images’ can have one (line) or two dimensions (array)
- in addition to all types of spectra with and without angular variation or spatial dimension we added photometric data and photometric images at a single wavelength or wavelength average (‘photometric data/images’)
- but we did not include simple data and images without angular dimension at a single wavelength (or wavelength average).

- Correspondance (indicative only) with "*parameters_instrument*_spectral_observation_mode", "_angle_observation_mode" and “_spatial_observation_mode” and “*spectrum*_type”:

For ‘*single spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum’* with:
    - “_spectral_observation_mode” = {spectrum, multi wavelengths, multi spectral averages}
    - “_angle_observation_mode” = {fixed angles}
    - “_spatial_observation_mode” = {single spot, averaged, roi averaged, rastered}
      = spectrum without angular variation nor spatial dimension
- ‘*single spectrum’*:
    - “*spectrum*_type” ={raw, transmission, absorbance, normalized absorbance, optical depth, absorption coefficient, ATR transmission, ATR absorbance, corrected ATR absorbance, dielectric loss tangent, magnetic loss tangent, bidirectional reflectance, radiance factor, reflectance factor, normalized reflectance, albedo, anisotropy factor, thermal emission, thermal radiance, thermal emittance, thermal emissivity, scattering intensity, differential scattering cross section,

normalized differential scattering cross section, single scattering albedo, Raman scattering intensity, normalized Raman scattering intensity, Raman scattering coefficient, Raman scattering efficiency, fluorescence emission, normalized fluorescence emission, fluorescence emission efficiency

- ‘*complex spectrum’*:
    - “*spectrum*_type” = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex permeability, complex reflectance ratio}
- ‘*polarimetric spectrum’*:
    - “*spectrum*_type” = {Stokes parameters, normalized Stokes parameters, polarization parameters}
- ‘*scattering spectrum’*:
    - “*spectrum*_type” = {scattering cross section parameters, scattering efficiency factor parameters}
- ‘*model parameters spectrum’*:
    - “*spectrum*_type” = {radiative transfer model parameters}

For ‘*spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data’* with:

- “_angle_observation_mode” = {one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set}
- “_spatial_observation_mode” = {single spot, averaged, roi averaged, rastered}

- ‘*spectra of multiangle dataset, photometric data of multispectral dataset’ for*:
    - “_spectral_observation_mode” = {spectrum, multi wavelengths, multi spectral averages}
    - “*spectrum*_type” = {raw, transmission, absorbance, normalized absorbance, optical depth, ATR transmission, ATR absorbance, corrected ATR absorbance, bidirectional reflectance, radiance factor, reflectance factor, normalized reflectance, anisotropy factor, thermal emission, thermal radiance, thermal emittance, thermal emissivity, scattering intensity, differential scattering

cross section, normalized differential scattering cross section, Raman scattering intensity, normalized Raman scattering intensity, Raman scattering coefficient, fluorescence emission, normalized fluorescence emission}

- '*photometric data, spectro-photometric data' for*:
  - "_spectral_observation_mode" = {single wavelength, single spectral average}
  - "*spectrum*_type" = same as '*spectro-photometric data'*

For '*spectral image, spectral images of multiangle dataset, spectro-photometric images'* with:

- "_spectral_observation_mode" = {spectrum, multi wavelengths, multi spectral averages}
- "_spatial_observation_mode" = {line, image, rastered image}

- '*spectral image'* for:
  - "_angle_observation_mode" = {fixed angles}
  - "spectrum_type" = same as '*spectro-photometric data'*
- '*spectral images of multiangle dataset, spectro-photometric images'* for:
  - *"_angle_observation_mode*" ={one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set}
  - "*spectrum*_type" = same as '*spectro-photometric data'*

For '*photometric images, photometric images of multispectral dataset'* with:

- "_spectral_observation_mode" = {single wavelength, single spectral average}
- "_angle_observation_mode" ={one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set}
- "*spectrum*_type" = same as '*spectro-photometric data'*

*spectrum*_files_parameter_format	enum(text)	S3/Pu [!!_m]	Spectr	V [Ver]	--	Format of the spectrum data file to be uploaded (for data import) Enum: {ascii-intensity, ascii-columns, ascii-nicolet, bin-nicolet, bin-spa-

nicolet, bin-spc-grams, bin-opus-brucker, ascii-sbrdf-ipag, ascii-sbrdf-bern, ascii-sbrdf-isep, …}

Constraint: "*spectrum*_files_parameter_format" = {ascii-sbrdf-ipag, ascii-sbrdf-bern, ascii-sbrdf-isep} only when "*spectrum*_files_parameter_type" = {photometric data, spectro-photometric data}

Definitions:

For simple spectral files:

- '*ascii-intensity'*: simple ascii files for intensity with 2 mandatory columns and 2 optionals in the following order: [position, intensity, (intensity error [+/-], intensity quality)] with 2 lines header by default or with 'n' header lines ("*spectrum*_file_header_lines_number").
  Note: Columns can be separated by spaces or tabs, but other types need to be specified in "*spectrum*_file_column_separator". No other column should be present.
- '*ascii-columns'*: multi-columns ascii files that should be described using the "*spectrum_file_columns"* versatile structure below.
  Notes:
  - It allows to specify the format for "*spectrum*_files_parameter_type" = {simple spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, photometric data, spectra of multiangle dataset, photometric data of multispectral dataset}
  - the selected columns of the file to be read should be described with "*spectrum*_file_column_type".
  - The "*spectrum*_file_column_total_number" should be given to avoid to read all other columns
  - No header line by default.
  - "*spectrum*_file_column_separator" should be specified.
- '*ascii-nicolet'*: ascii format of Nicolet spectra (with small fixed header) produced by the IGOR export routine
- '*bin-spa-nicolet'*: binary .SPA format of the Nicolet spectrometers (Nicolet/Thermo OMNIC)
- '*bin-nicolet'*: binary format (.SPTR or any other as it was free) of the Nicolet spectrometer (Nicolet 700/800)

- ‘*bin-spc-grams’*: binary format (.SPC) of the Nicolet spectrometer (Grams / "Essential FTIR" software).
- ‘*bin-opus-brucker’*: binary (.0, .1, …) format of OPUS software for Brucker spectrometers

For multi-angular spectral or multispectral files:

- ‘*ascii-sbrdf-ipag’*: multi-columns ascii file with ***
  - It is of the type *“spectrum_fi*les_parameter_type” = ’spectro-photometric data’
- ‘*ascii-sbrdf-bern’*: multi-columns ascii files of Bern University
  - It is of the type *“spectrum*_files_parameter_type” = ’spectro-photometric data’
- ‘*ascii-sbrdf-isep’*: multi-columns ascii file with 2 header lines and containing a single bloc of data either ‘mean’, ‘median’ or ‘stdev’, with one line for each wavelength and one column for each angular geometry. The values of {i, e, g, az} are given in this order in the last 4 lines.

  Notes:
  - It is of the type *“spectrum*_files_parameter_type” = ’spectro-photometric data’
  - The 3 types of data should be read with the file option “data_type”
  - The “*spectrum*_file_header_lines_number” is set to ‘2’ by default, if not filled.

Note: the unit of the position values (wavelength/wavenumber/frequency) is given in “*instrument*_spectral_unit”

*spectrum*_files_parameter_header_lines_number	int(11)	P [!!o_m]	Spectr	V [Ver]	--	Number of lines of the header before the first data line in the spectrum data file to be uploaded (for data import) *Condition:* absolute mandatory and only when “*spectrum*_files_parameter_format” = {ascii-columns} *Notes*: - default is '2' for 'ascii-intensity' - for multi-angles spectral data, all the files in

						“*spectrum*_file_multiangles“ should have the same size of the header
*spectrum*_files_parameter_nodata	varchar(255)	P [m]	Spectr	V [Ver]	--	Value of the 'nodata' code in the spectrum data file to be uploaded (for data import) *Note*: - for multi-angles spectral data, all the files in “*spectrum*_file_multiangles“ should have the same ‘nodata’
*spectrum*_files_parameter_column_separator	enum(text)	P [!!o_m]	Spectr	V [Ver]	--	Type of separator between columns in the spectrum data file (for data import) Enum: {space, tab, comma, semi-colon} *Condition:* absolute mandatory and only for “*spectrum*_files_parameter_format” = {ascii-columns} *Notes*: - default is ‘space’ or ‘tab' for 'ascii-intensity'
*spectrum*_files_parameter_column_total_number	int(3)	P [!!o_m]	Spectr	V [Ver]	--	Total number of columns in the spectrum data file *Condition:* absolute mandatory and only for “*spectrum*_files_parameter_format” = {ascii-columns} *Notes*: - allow to determine the number of non-used columns
*spectrum*_files_parameter_*column* ***List [L6]*** *s*		[!!o]		V [Ver]		£: Description of the columns of ascii data files and their type *Constraint:* only when “*spectrum*_files_parameter_type"= {single spectrum, complex spectrum, model parameters spectrum, photometric data, spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data} *Note*: for ‘spectra of multiangle dataset’ and ’photometric data of multispectral dataset’ all the files in “*spectrum*_files“ should have exactly the same format
*spectrum*_files_parameter_column_number	int(2)	P [!!o_m]	Spectr	V [Ver]	--	Number of the column of the data file *Condition:* absolute mandatory and only for

			L6			“*spectrum*_files_parameter_format” = ‘ascii-columns’ *Constraint:* “file_column_number” ≥ ‘2’
*spectrum*_files_parameter_column_type	enum(text)	P [!!o_m]	Spectr L6	V [Ver]	--	Type of data contained in the column of the data file Enum: {position, incidence angle, emergence angle, azimuth angle, phase angle, intensity, intensity mean, intensity median, intensity stdev, intensity min, intensity max, intensity error, intensity error minus, intensity error plus, intensity quality, date, time, relative time} *Condition:* at least one of {position, incidence angle, emergence angle, azimuth angle, phase angle} AND one of {intensity, intensity mean, intensity median, variable} are absolute mandatory when “*spectrum*_files_parameter_format” = ‘ascii-columns’ *Notes*: - For simple spectra (*“spectrum*_files_parameter_type” = {single spectrum, photometric data, spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data}) the type of intensity is defined by “*spectrum*_type” - For multipart spectra (*“spectrum*_files_parameter_type” = {complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum}) the type of intensity is defined by “*spectrum*_file_column_intensity_type” below. *Definitions:* - ‘*position*’: wavelength, wavenumber or frequency position - ‘*intensity*’: nominal intensity or mean intensity (when averaged spatialy or with time) - ‘*intensity mean’*: mean intensity (when averaged spatialy or with time) - ‘*intensity median’*: median intensity (when averaged spatialy or with time) - *‘intensity stdev’*: standard deviation (± 1 σ) of the intensity. Used in particular for spatial average of spectra in a spectro-image and correspond to the variability of the spectra. - ‘*intensity min/max’*: minimum and maximum values of the nominal or mean intensity

						- ‘*intensity error’*: symmetric error (negative and positive) on the nominal or mean intensity - ‘*intensity error minus/plus’*: negative error and positive error on the nominal or mean intensity - ‘*intensity quality’*: numerical flag (0 to 5, see “*spectrum*_quality_flag”) giving the relative quality of the intensity values (include absolute and relative uncertainties, noise, biases, …) - ‘*incidence angle’*, ‘*emergence angle’*, ‘*azimuth angle’*, ‘*phase angle’*: the different angles of the illumination/observation geometry for multi-angle data - ‘*date*’, ‘*time*’: absolute date and time of the measurement - ‘*relative time’*: time relative to an origin (ex: start of the experiment) *Notes*: - for symmetric error (+/-) in the file, you need to attribute it to 2 columns: ‘xxx_error_minus’ and ‘xxx_error_plus’
*spectrum*_files_parameter_column_intensity_type	enum(text)	P [!!o_m]	Spectr L6	V [Ver]	var	Type of ‘intensity’ data contained in the column of a multipart data file Enum: {real part, imaginary part, Stokes parameter I, Stokes parameter Q, Stokes parameter U, Stokes parameter V, normalized Stokes parameter Q, normalized Stokes parameter U, normalized Stokes parameter V, polarization contrast, degree of linear polarization, polarization position angle, degree of circular polarization, scattering cross section, absorption cross section, extinction cross section, scattering efficiency factor, absorption efficiency factor, extinction efficiency factor, single scattering albedo, b (HG), c (HG), opposition peak height, opposition width, mean roughness} *Condition:* absolute mandatory and only: - when *“spectrum*_files_parameter_type” = {complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum} AND - when “*spectrum*_files_parameter_format” = ‘ascii-columns’ AND - when “*spectrum*_file_column_type” = {intensity, intensity mean, intensity median, intensity stdev, intensity min, intensity max, intensity

error, intensity error minus, intensity error plus, intensity quality}

Constraints:

- should be {real part, imaginary part} when “spectrum_type” = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex permeability}
- should be {Stokes parameter I, Stokes parameter Q, Stokes parameter U, Stokes parameter V} when “spectrum_type” = {Stokes parameters}
- should be {normalized Stokes parameter Q, normalized Stokes parameter U, normalized Stokes parameter V} when “spectrum_type” = {normalized Stokes parameters}
- should be {polarization contrast, degree of linear polarization, polarization position angle, degree of circular polarization} when “spectrum_type” = {polarization parameters}
- should be {scattering cross section, absorption cross section, extinction cross section} when “spectrum_type” = {scattering cross section parameters}
- should be {scattering efficiency factor, absorption efficiency factor, extinction efficiency factor} when “spectrum_type” = {scattering efficiency factor parameters}
- should be {single scattering albedo, b (HG), c (HG), opposition peak height, opposition width, mean roughness} when “spectrum_type” = {radiative transfer model parameters}
- not for the other values of “spectrum_type”

Definitions:

Used for multipart spectra with a global name in “*spectrum*_type” but expressed with several components, such as the real and imaginary parts for ‘optical constants’,

For *“spectrum*_files_parameter_type” = ‘complex spectrum’:

For “*spectrum*_type” = ‘optical constants:

- ‘*real part’*: refractive index n
- ‘*imaginary part’*: extinction coefficient k

For “*spectrum*_type” = ‘complex admittance’:

- ‘*real part’*: conductance G
- ‘*imaginary part’*: susceptance B

For "*spectrum*_type" = 'complex impedance':
- '*real part'*: resistance R
- '*imaginary part'*: reactance X

For "*spectrum*_type" = 'relative complex permittivity':
- '*real part'*: dielectric constant ε'_r
- '*imaginary part'*: relative electric conductivity ε''_r

For "*spectrum*_type" = 'relative complex permeability':
- '*real part'*: magnetic constant μ'_r
- '*imaginary part'*: relative magnetic conductivity μ''_r

For *"spectrum*_files_parameter_type" = 'polarimetric spectrum':

For "*spectrum*_type" = 'Stokes parameters'
- '*Stokes parameter I'*:
- '*Stokes parameter Q'*:
- '*Stokes parameter U'*:
- '*Stokes parameter V'*:

For "*spectrum*_type" = 'normalized Stokes parameters'
- '*normalized Stokes parameter Q'*: Stokes parameter ratio Q/I
- '*normalized Stokes parameter U'*: Stokes parameter ratio U/I
- '*normalized Stokes parameter V'*: Stokes parameter ratio V/I

For "*spectrum*_type" = 'polarization parameters':
- '*polarization contrast'*: polarization contrast
- '*degree of linear polarization'*: degree of linear polarization DoLP
- '*polarization position angle'*: angle of linear polarization AoLP (degree)
- '*degree of circular polarization'*: degree of circular polarization DoCP

For *"spectrum*_files_parameter_type" = 'scattering spectrum':

For "*spectrum*_type" = 'scattering cross section parameters':
- '*scattering cross section',* C_{sca}: total scattering cross section
  - It is the hemispherical integral of the *differential scattering cross section'*
- '*absorption cross section',* C_{abs}*:* total absorption cross section
  - Related with the absorption coefficient α: $\sigma = \alpha/N$ *(N: molecule or particles number density)*
- '*extinction cross section',* C_{ext}: sum of the absorption and scattering

cross sections of a particle, $C_{sca} + C_{abs}$.

For "*spectrum*_type" = 'scattering efficiency parameters':

- '*scattering efficiency factor'*, Q_{sca}: ratio of the scattering cross-section to the geometrical cross-section πa^2.
    - Also, simply called *'scattering efficiency'*
- '*absorption efficiency factor'*, Q_{abs}: ratio of the absorption cross-section to the geometrical cross-section πa^2.
    - Also, simply called *'absorption efficiency'*
- '*extinction efficiency factor'*, Q_{ext}: ratio of the extinction cross-section to the geometrical cross-section πa^2.
    - Also, simply called *'extinction efficiency'*

For *"spectrum*_files_parameter_type" = 'model parameters spectrum':

For "*spectrum*_type" = 'radiative transfer model parameters'

- '*single scattering albedo':* Single scattering albedo (ω)
- *'b (HG)':* asymmetry parameter 'b' of the Henyey-Greenstein function with 1 or 2 lobes ('b', or 'b', 'c').
- *'c (HG)':* retrodiffusion fraction parameter 'c' of the Henyey-Greenstein function with 2 lobes ('b', 'c').
- *'opposition peak height':* amplitude 'Bo' of the opposition peak
- *'opposition width':* FWHM 'h' the opposition peak (degree)
- *'mean roughness'*: Mean macroscopic roughness (Θ) of the surface (in degree)

Notes:

- Mandatory columns are underlined
- The 'radiative transfer model parameters' are those of the model of Hapke (1986) and also used in Douté and Schmitt (1999)

Models and their parameters:

- '*Hapke model parameters'* file: position, single scattering albedo, b (HG), c (HG), opposition width, opposition peak height, mean roughness
- '*Doute and Schmitt model parameters'* file: position, single scattering albedo, b (HG), mean roughness

Spectrum geometries

*spectrum*_geometries_number [-xml]	int(10)		S3 [!_c]	Spectr	V [Ver]	*no*

Number of geometries of the spectrum

➔ calculated from:

- the list of "*spectrum*_file_angle" for "*spectrum*_files_parameter_type" = {spectra of multiangle dataset}
- the list of "*spectrum*_file_position" for "*spectrum*_files_parameter_type" = {photometric data of multispectral dataset}
- the list of geometries inside the file for "*spectrum*_files_parameter_type" = {photometric data, spectro-photometric data}
- "*spectrum*_geometries_number" = '1' for "*spectrum*_files_parameter_type" = {single spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum}

Notes:

- This number will allow to determine the number of spectra of the experiment by multiplying it by the number of 'data sets' of the experiment, but only for those with "*spectrum*_parameters_instrument_spectral_observation_mode" = {spectrum, multi wavelengths, multi spectral averages}

Spectrum file(s)

spectrum_files	***List [L7]***	[O]		V [Ver]

£: single file or set of files containing the spectrum or the spectro-angular data (for data import)

Notes:

- For files of various type
  - single spectrum file
  - set of spectra at single geometry in a multiangle dataset
  - set of photometric data at single wavelength in a multispectral dataset (or single photometric data at single wavelength)
  - single multi-angles spectrum file

- all the files should have exactly the same format

*spectrum*_file_filename [*spectrum*_file_filename]	CS-varchar(255)	S2/Pu [!!o_m]	Spectr L7	V [Ver]	--	Name of the file containing the spectrum or all, or part of, the spectro-photometric dataset (for data import) *Condition:* absolute mandatory only when when "*spectrum*_import_mode" = {first import, new version} *Constraints:* • absolute mandatory to fill and to zip a file when "*spectrum*_import_mode" = {first import, new version} • optional to fill and to zip a file when "*spectrum*_import_mode" = {correction} • absolute mandatory to keep void when "*spectrum*_import_mode" = {invalidate}. *File format:* It will depend on "*spectrum*_files_parameter_format" The data will be stored: o in simple spectrum format when "*spectrum*_files_parameter_type" = {single spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum} o in spectro-angular format when "*spectrum*_files_parameter_type" = {photometric data, spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data} *Note:* - for series of spectra of multiangle dataset (ex: "spectrum_type"='bidirectional reflectance') you have the choice between single spectrum or multi-angle storage formats - the data will be imported in the database after conversion to homogeneous wavenumber unit (cm^{-1}) - the original file itself will be stored for track back by data provider. *Note DB:* this file should be zipped with the 'experiment-spectra' import xml file at first import and for new versions

Option 1 for series of spectrum files at single geometry in a multiangle dataset

Definition:

- For series of files that have the data at different angular geometries stored each in a different file containing the spectral values of the data (a spectrum) at a single angular geometry.

Notes:

- These files must contain several columns providing the wavelength/wavenumber/frequency of the spectrum (position) and the values of the different data types (intensity, error, …).
- the number of the wavelength/wavenumber/frequency column and of the columns containing the different data types (intensity, error, …) should be described in "*spectrum_file_columns"*
- the set of angles (i, e, az, (g)) corresponding to each file is provided with "*spectrum*_file_angle_incidence/_emergence/_azimuth(/_phase)"
- if you choose this option the series of spectra of the multiangle dataset will be stored in spectro-photometric format (instead in a series of spectra).

*spectrum*_file_ angle_incidence	float		P [!o_m]	Spectr L7	V [Ver]	*deg*	Incidence angle of illumination of the spectrum (part of a multi-angles spectral dataset) contained in the file *Condition/Constraint:* mandatory and only when "*spectrum*_files_parameter_type"= 'spectra of multiangle dataset' AND when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical}
*spectrum*_file_ angle_emergence	float		P [!o_m]	Spectr L7	V [Ver]	*deg*	Emergence angle of observation of the spectrum (part of a multi-angles dataset) contained in the file *Condition/Constraint:* mandatory and only when "*spectrum*_files_parameter_type"= 'spectra of multiangle dataset' AND when "*parameters_instrument*_angle_observation_geometry" = {specular,

							bidirectional, directional-conical, conical-directional, biconical, hemispherical-directional, hemispherical-conical, directional, conical} *Note*:
*spectrum*_file_ angle_azimuth	float		P [!o_m]	Spectr L7	V [Ver]	*deg*	Azimuth angle of observation of the spectrum (part of a multi-angles dataset) contained in the file *Condition/Constraint:* mandatory and only when "*spectrum*_files_parameter_type"= 'spectra of multiangle dataset' AND when "*parameters_instrument*_angle_observation_geometry" = {bidirectional, directional-conical, conical-directional, biconical} *Notes*:
*spectrum*_file_angle_phase	float		P [m]	Spectr L7	V [Ver]	*deg*	Phase angle of observation of the spectrum (part of a multi-angles dataset) contained in the file *Constraint:* only when "*spectrum*_files_parameter_type"= 'spectra of multiangle dataset' *Notes*:

Option #2 for series of photometric data files at single wavelength in a multispectral dataset

Definition:

- For series of files that have the data at different wavelengths (single wavelength or multispectral) stored each in a different file containing the angular values of the data (a photometric curve) at a single wavelength/wavenumber/frequency.

Notes:

- These files must contain several columns providing the different angles (i, e, az, (g)), and the values of the different data types (intensity, error, …).
- the number of the different angles columns and of the columns containing the different data types should be described in

						"*spectrum_file_columns"* - the position (wavelength/wavenumber/frequency) corresponding to each file is provided with "*spectrum*_file_position"
*spectrum*_file_ position	float	P [!o_m]	Spectr L7	V [Ver]	*var*	Position (wavelength/wavenumber/frequency) of the angular data (part of a multi-wavelengths dataset) contained in the file • Unit: given by "*parameters_instrument*_spectral_unit *Condition/Constraint:* mandatory and only when "*spectrum*_files_parameter_type"= {photometric data, photometric data of multispectral dataset}
Option #3 for series of spectro-photometric data files with a single data type in each file						
						Definition: - For series of files that have the different types of photometric data (intensity, error, stdev, …) stored each in a different file containing the spectro-angular values (a spectro-photometric curve) for a single type of data. *Notes*: - ONLY for 'ascii-sbrdf-isep' file format - the type of data contained in each file is defined with "*spectrum*_file_data_type"
*spectrum*_file_photometric_type	enum(text)	P [!!o_m]	Spectr L7	V [Ver]	--	Type of photometric data contained in the file (only for IRAP format !) Enum: {intensity, intensity mean, intensity median, intensity stdev, intensity error} *Condition:* only and absolute mandatory when "*spectrum*_files_parameter_format"= {ascii-sbrdf-isep} *Note*: the type of intensity is defined by "*spectrum*_type" *Definitions:* see "*spectrum*_file_column_type"

*spectrum*_file_export_filename [*spectrum*_export_filename]	varchar(255)	S1b [!!_m]	Spectr	V [Ver]	--	Generic name of the data and metadata files and preview image for data export *File extension:* without format extension *Notes:* – this name needs to be the most explicit for the user, but in a condensed form (should include info as 'typical spectral range', 'spectrum type', 'sample name', 'value of main variable parameter' (put at the end of name to allow ordering), …). – It will be the default name for export but the user will have the possibility to rename it, at its own risk. – Do not use blank (space) in this name. Use instead '-' or '_' to link the different parts. – This filename will get different extensions: .dat, .txt, .xml, … depending on the export format chosen for the spectrum and metadata. – For "multiangle" spectra exported in a series of files (a possible option), the file name may get an extension characterizing either the wavelength (for single wavelength multiangle data) or the geometry (for individual spectra), or the type of values (for single value type of multiangles spectra) Ex: - SBRDF: "BRDF_Vis+NIR_chocolat_noir_99%" - BRDF: "BRDF_Vis+NIR_chocolat_noir_99%_1063nm" - Spectra: "BRDF_Vis+NIR_chocolat_noir_99%_i30_e20_az0" - Value: "BRDF_Vis+NIR_chocolat_noir_99%_mean" – It will get .png extension for the preview image of the spectrum (full scale over full valid range) that will be automatically generated during data export. – For spectro-images it may give a preview image with several typical spectra with different colors. Ex: - 'optcte-NIR_CH4-1%-betaN2_38K' - 'refl-NIR-SWy2+H2O_243K_i0-e30_16' - 'transm-NIR_Allende+KBr-pellet_heat-300C'

Preview of the spectrum

spectrum_preview		[O]		V [Ver]		£: parameters of the automatically generated preview plot of the spectrum *Notes*: - these parameters are optional and are used to optimize the individual generation of the spectrum plots (but the X and Y units are forced to be the same than the spectrum or the experiment preview) - if "*spectrum*_preview" is not specified, the parameters of the "*experiment_preview"* will be used, if specified. - if none are specified the generation tool will do its best to optimize the plot: o use "*parameters_instrument*_spectral_min/max" for X limits o detect Ymin/max from the data and add some margin. - However for plots that require Y log scales (such as optical constants) the optimization is random and controlled by noise level ! *Notes xml:* - the 3 KW ("*spectrum*_preview_x_axis"/ "_min"/ "_max") are grouped as tags of "*spectrum*_preview_x": <x axis="" min="" max="" /> - the 3 KW ("*spectrum*_preview_y_axis"/ "_min"/ "_max") are grouped as tags of "*spectrum*_preview_y": <y axis="" min="" max="" />
*spectrum*_preview_x_axis	enum(text)	P [m]	Spectr	V [Ver]	--	Type of X axis in the preview plot of the spectrum Enum: {lin, log} *Definitions*: - '*lin*': linear axis - '*log*': logarithmic axis
*spectrum*_preview_x_min	float	P [m]	Spectr	V [Ver]	*var*	Minimum value of X axis in the preview plot of the spectrum • Unit: given by default by "*parameters_instrument*_spectral_unit" or by "*experiment*_preview_x_unit" when provided *Note*: plotted by default in the original import unit

*spectrum*_preview_x_max	float	P [m]	Spectr	V [Ver]	*var*	Maximum value of X axis in the preview plot of the spectrum • Unit: given by default by "*parameters_instrument*_spectral_unit" or by "*experiment*_preview_x_unit" when provided *Note*: plotted by default in the original import unit
*spectrum*_preview_y_axis	enum(text)	P [m]	Spectr	V [Ver]	--	Type of Y axis in the preview plot of the spectrum Enum: {lin, log} *Definitions*: see "*spectrum*_preview_x_axis"
*spectrum*_preview_y_min	float	P [m]	Spectr	V [Ver]	*var*	Minimum value of Y axis in the preview plot of the spectrum • Unit: given by "*spectrum*_intensity_unit" or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit
*spectrum*_preview_y_max	float	P [m]	Spectr	V [Ver]	*var*	Maximum value of Y axis in the preview plot of the spectrum • Unit: given by "*spectrum*_intensity_unit" or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit
*spectrum*_preview_y2_axis	enum(text)	P [m]	Spectr	V [Ver]	--	Type of the second Y axis (only for the real part of complex spectra) in the preview plot the spectrum Enum: {lin, log} *Definitions*: see "*experiment*_preview_x_axis" *Constraint*: only for "*spectrum*_files_parameter_type" = {complex spectrum, polarimetric spectrum, scattering spectrum} *Note*: - only for complex spectra to set different parameters to the Y axis for 'imaginary part' (y axis) and 'real part' (y2 axis) - i.e., for "*spectrum*_type" = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex

						permeability, complex reflectance ratio} - see list in "*experiment*_preview_y2_axis" *Note*: useful for complex spectra such as optical constants to set different parameters to the Y axis for 'k' (y axis) and 'n' (y2 axis)
*spectrum*_preview_y2_min	float	P [m]	Spectr	V [Ver]	*var*	Minimum value of the second Y axis in the preview plot of the spectrum • Unit: given by "*spectrum*_intensity_unit" or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit
*spectrum*_preview_y2_max	float	P [m]	Spectr	V [Ver]	*var*	Maximum value of the second Y axis in the preview plot of the spectrum • Unit: given by "*spectrum*_intensity_unit" or by "*experiment*_preview_y_unit" when provided *Note*: plotted by default in the original import unit
*spectrum*_preview_filename	CS-varchar(255)	S3 [mc]	Spectr	V [Ver]	--	Name of the file containing the preview plot of the spectrum (or spectra) or photometric curve to be displayed ➔ plot generated automatically during import if there is no file filename *Image formats:* .png, .jpg, (.gif) *Note:* - this plot will replace the automatically generated plot - it will be displayed in the result page for quick look at the spectrum *Note DB:* this file should be zipped with the 'experiment-spectra' import xml file for import.
spectrum_experiment_preview		[!O]				Choices of the spectra for the experiment preview file
*spectrum*_experiment_preview_flag	boolean	S3 [!o_m]	Spectr	V [Ver]	--	Flag telling if the spectrum will be part of the experiment spectral preview and also of the initial spectrum selection for the dynamic plot BoolEnum: {yes, no} or {true, false}

						Condition: mandatory only when "*spectrum*_files_parameter_type" = {single spectrum, complex spectrum, polarimetric spectrum, scattering spectrum, model parameters spectrum} *Notes:* - need to select a series of 6-8 spectra maximum and well representing the spectral variations observed during the whole experiment - set to 'no' for large multi-angles files (too much spectra to be displayed) and choose a few spectra using the "*spectrum_preview_multiangles"* structure below. - can be set to 'yes' for small multi-angles data sets (< 6-8 spectra), then all its spectra will be displayed in the preview. - Not yet defined how to display photometric preview of mono-wavelength angular datasets (BRDF, DEDF, specular reflection, scattering, …) => make your own plot and use "*spectrum*_preview_filename"
spectrum_experiment_preview_fla g_multiangles	***List [L7b]***	[!O]		V [Ver]		Illumination/observation geometry of the spectra selected to be part of the spectral preview and dynamic plot of the multi-angles data set(s) *Condition:* absolute mandatory at least one when *"spectrum*_files_parameter_type" = {spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data} AND *Condition:* when "*experiment*_preview_filename" = *Ø* *Notes*: - this option is only used for large multi-angles data sets (> 6-8 spectra) *Note XML:* all three following KW ("*spectrum*_experiment_preview_flag_multiangle_angle_incidence"/ "_emergence"/ "_azimuth") are merged in a single tag "angle": <angle incidence="" emergence="" azimuth="" />
*spectrum*_experiment_preview_fla g_multiangle_angle_incidence	float	P [!o_m]	Spectr L7b	V [Ver]	*deg*	Incidence angle of illumination of the spectrum selected to be part of the spectral preview and dynamic plot of the multi-angles data set(s) *Condition:* mandatory and at least one when

					"*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical}
*spectrum*_experiment_preview_fla g_multiangle_angle_emergence	P [!o_m]	Spectr L7b	V [Ver]	*deg*	Emergence angle of observation of the spectrum selected to be part of the spectral preview and dynamic plot of the multi-angles data set(s) *Condition:* mandatory and at least one when "*parameters_instrument*_angle_observation_geometry" = {specular, bidirectional, directional-conical, conical-directional, biconical, hemispherical-directional, hemispherical-conical, directional, conical}
*spectrum*_experiment_preview_fla g_multiangle_angle_azimuth	P [!o_m]	Spectr L7b	V [Ver]	*deg*	Azimuth angle of observation of the spectrum selected to be part of the spectral preview and dynamic plot of the multi-angles data set(s) *Condition:* mandatory and at least one when "*parameters_instrument*_angle_observation_geometry" = {bidirectional, directional-conical, conical-directional, biconical} AND when "*spectrum*_experiment_preview_flag_multiangle_angle_phase" = {Ø, NULL}
*spectrum*_experiment_preview_fla g_multiangle_angle_phase	P [m]	Spectr L7b	V [Ver]	*deg*	Phase angle of observation of the spectrum selected to be part of the spectral preview and dynamic plots of the multi-angles data set(s) *Condition:* mandatory when "*spectrum*_experiment_preview_flag_multiangle_angle_azimuth" = {Ø, NULL}
*spectrum*_experiment_preview_fla g_multiangle_angle_spectrum	S3 [!!_m]	Spectr	V [Ver]	--	Flag telling if the spectrum with this geometry will be part of the spectrum spectral preview BoolEnum: {yes, no} or {true, false} *Notes:* - need to select a series of 6-8 spectra maximum and well representing the spectral variations of the multi-angle dataset

*spectrum*_experiment_preview_flag_multiangle_angle_experiment	boolean	S3 [!!o_m]	Spectr	V [Ver]	--	Flag telling if the spectrum with this geometry will be part of the experiment spectral preview BoolEnum: {yes, no} or {true, false} *Condition:* absolute mandatory when all other "*spectrum*_experiment_preview_flag_multiangle_angle_experiment" = {Ø, NULL} *Notes:* - need to select 0-3 spectra of this multi-angle dataset for a series of 6-8 spectra maximum over the whole experiment well representing the spectral variations observed during the whole experiment

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ROI files						*Condition:* mandatory only when *"parameters_instrument*_spatial_observation_mode" = {roi averaged} *Notes*: - for rastered image it can be only a single ROI file that will be linked only with the first ROI spectrum. - the location of the pixels or pixel averages probing this/these materials can be given with a picture in "*spectrum_images"*
*spectrum*_roi_export_suffix	varchar(255)	P [!o_m]	Spectr	V [Ver]	--	Suffix that will be added to the generic spectrum name to automatically create the name of the ROI file for data export *Condition:* cf. above *Notes:* - this suffix needs to be given in the image or image caption of the ROI location on the sample. - do not use blank (space) in this suffix. - the filename will get different extensions (.roi, .sav …) depending on the export format chosen for the ROI. Ex: - For a spectrum 'refl-NIR-SWy2+H2O_243K_i0-e30_16', with ROI suffix "*spectrum*_roi_export_filename" = 'roi-4' the full ROI filename

						will be ‘refl-NIR-SWy2+H2O_243K_i0-e30_16_roi-4’
*spectrum*_roi_filename	CS-varchar(255)	S3/P [!o_m]	Spectr	V [Ver]	--	Name of the file (with extension) containing the ROI data to be uploaded (for data import) *Condition:* cf. above *File format:* It will depend on “*spectrum*_roi_file_format” *Note:* - the file itself will be stored for track back by data provider. *Note XML:* this file should be zipped with the ‘experiment-spectra’ import xml file for import.
*spectrum*_roi_file_format	enum(text)	P [!o_m]	Spectr	V [Ver]	--	Format of the ROI data file to be uploaded (for data import) Enum: {envi-roi, envi-evf, sav, shp, xml, …} *Condition:* cf. above *Definitions:* - ‘*envi-roi’*: .roi files from ENVI classic software - ‘*envi-evf’’*: files from ENVI classic software - ‘*sav*: .sav files from ??? - ‘*shp*’: point shape file - ‘*xml*’: - - … *Notes:* - Currently the content of the file is not read and uploaded in the data base. Only the file is stored as it is.
Spectrum auxilliary data						
spectrum_images	***List [L8a]***	[O]		V [Ver]		£: images corresponding to this spectrum
*spectrum*_image_filename	varchar(255)	U [m]	Spectr L8a	V [Ver]	--	Filename(s) (with extension) of image(s) corresponding to this spectrum (for upload)

Image formats: .png, .jpg, (.gif)

Note: It can be:

- plot(s) of the spectrum, or part of it
- picture(s) of the sample corresponding to this spectrum, in particular when the sample displays visible changes relative to the sample picture given in "*sample*_image_filename"
- for "*instrument*_microscopy_imaging" = {micro-imaging, imaging} it could be pixels map(s) of the area probed by the micro-imaging or imaging measurement

  This/these pixel map(s) could be:
  - the pixel map (binary/coded) of the constituent(s) (UID, code, …) of a compact sample (meteorite, rock, …) inhomogeneous at the scale of the pixel
  - the pixel map (binary/coded) of the material(s) (UID, code, …) of a granular sample inhomogeneous at the scale of the pixel
  - the pixel map (binary) of the location of a sample smaller than the image
  - the pixel map (binary) of the location of a ROI (Region Of Interest) of the sample over which the spectra have been averaged
  - the pixel map of the elevation (DEM) of a sample with topography at the scale of the pixel
  - the pixel map of a spectral characteristic of the sample (reflectance at some wavelength, depth of a particular band, …)
  - any other type of pixel map …

Note: the pixel map image(s) should have the same x and y dimentions than the corresponding spectro-image. It/they should be either binary image(s) (0,1) or coded grey tone or RGB binary images (code given in caption)

Note DB: this file should be zipped with the 'experiment-spectra' import xml file for import.

*spectrum*_image_caption	varchar(255)	U [m]	Spectr L8	V [Ver]	--	Caption(s) of the image(s) corresponding to this spectrum

spectrum_documentations	***List [L8b]***	[O]		V [Ver]		£: Documentations about the spectrum *Notes:* - can contain original spectrum data file, log file of the spectrum, … - may be useful for BRDF measurements to provide original acquisition and log files of the whole BRDF data - these documentations can be downloaded or viewed inside another window of the web browser but cannot be viewed directly into SSHADE.
*spectrum*_documentation_name	varchar(255)	U [m]	Spectr L8b	V [Ver]	--	Name of the documentation describing the experiment *Note:* this name will appear as the documentation title in the database *Ex:* 'Experimental protocol of Mid-IR monitoring of CH4 ice sample under VUV irradiation'
*spectrum*_documentation_filename	varchar(255)	U [m]	Spectr L8b	V [Ver]	--	File name (with extension) of the documentation about the spectrum *File formats:* .pdf, .png, .jpg, .gif, .tiff, .txt, … *Note:* this file will be imported in the database. *Note xml*: this file should be zipped with the xml file

Spectrum band lists links

spectrum_bandlists	***List [L9]***	[O]				£: bandlist(s) describing the bands of the spectrum *Condition*: optional information
*spectrum*_bandlist_uid [*]	varchar(255)	S3/S1i/ Uu [$o_m]	Spectr Band Li L9	V [Ver]	--	Link to the existing UID of the bandlist(s) which describe the bands of the spectrum *Recommendation:* Strongly recommended when already exist in the database *Note:* these bandlists provide detailed information on the bands of each isotopic species of the molecules present in the constituents of the sample and contributing to the spectrum.

						Note: Part of the bandlist information, the one corresponding to the band characteristics listed below (see *Note:* Bandlist equivalent), can be used as individual band information for spectra visualization. *Note:* if no band or only part of the spectrum bands are described in the available band lists it is possible to complement the information for the others (some minor isotopes or minor molecules, sample impurities (solid/liquid or gaseous), mineral bands, or external miscorrected gas absorption (CO2…)) with the following "spectrum_bands" keywords.
*spectrum*_bandlist_comments	blob	U [m]	Spectr	V [Ver]	--	Comments on the bandlists and additional bands: missing information (missing bandlist, …), …
Spectrum band characteristics				[Ver]		*Notes:* - This option allows to draw on the interactive plot of the spectrum the position and some characteristics of the observed bands. - limited to bands not present in bandlists, otherwise it is much better and easier to use "*spectrum_bandlists*" - they are only for display and spectrum selection help. This info is not exported - It is a big work to prepare such data for each spectrum. It will be only on selected spectra or with limited information (e.g. wavenumber_peak & molecule_uid)
spectrum_bands	***List [L10]***	[O]		V [Ver]		£: bandlist(s) describing the bands of the spectrum *Condition:* Optional bloc - Mandatory active below when *"spectrum*_band_position_peak" ≠ 'NULL'
*spectrum*_band_position_min	float	U [m]	Spectr L10	V [Ver]	var.	Position (Wavenumber/wavelength/frequency) at half peak maximum on the low frequency side of the band *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted and stored in 'cm-1' unit in the database but provided to user in the unit he will specify in the export web interface (SSHADE)

						Note SSDM: "Bandlist" equivalent = "*band*_position_peak" – "*band*_width"/2
*spectrum*_band_position_peak	float		S3/Uu [(!!)do_m]	Spectr L10	V [Ver]	var.	Position (Wavenumber/wavelength/frequency) of the peak of the band Default = 'NULL' *Condition:* (option trigger) the filling of this KW is 'absolute mandatory' when this optional bloc is used. It triggers the 'mandatory' status of several others KW in the optional bloc. *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted and stored in 'cm-1' unit in the database but provided to user in the unit he will specify in the export web interface (SSHADE) *Note SSDM:* "Bandlist" equivalent = "*band*_position_peak"
*spectrum*_band_position_max	float		U [m]	Spectr L10	V [Ver]	var.	Position (Wavenumber/wavelength/frequency) at half peak maximum on the high frequency side of the band *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • converted and stored in 'cm-1' unit in the database but provided to user in the unit he will specify in the export web interface (SSHADE) *Note SSDM:* "Bandlist" equivalent = "*band*_position_peak" + "*band*_width"/2
*spectrum*_band_peak_intensity_relative	float		U [m]	Spectr L10	V [Ver]	*no*	Relative intensity at band peak compared to the intensity at "*spectrum*_wavelength_reference" *Note SSDM:* "Bandlist" equivalent = "*band*_peak_intensity_relative"
Spectrum bands attribution							
*spectrum*_band_primary_constituent_uid [*]	varchar(255)		S1i [o_m]	Spectr Const Solid Miner Liquid	V [Ver]	--	Link to the existing UID of the constituent producing the band. *Note SSDM:* "Bandlist" equivalent = "*bandlist*_constituent_uid" *Format:* see "*constituent*_uid" *Notes:* - the constituent can be a custom "constituent" or a "basic constituent"

			L10			made of a fundamental solid, mineral, or liquid phase - this 'constituent' information can be useful when there is more than one constituent in the sample. It allows to tell which constituent is at the origin of the band, possibly completed by 'species' information when relevant. - for fundamental solids it could be mostly an isotopic substituted variant. - minerals are with terrestrial natural abundance for complex solids: do not use this KW but describe functional groups using "*spectrum*_band_primary_species"
*spectrum*_band_primary_specie_uid [*]	varchar(255)	S1i [o_m]	Spectr Atom Chem F Molec L10	V [Ver]	--	Link to the existing UID of the species producing the band *Note SSDM:* "Bandlist" equivalent = "*bandlist*_constituent_primary_species_uid" *Definition*: - For molecular and ionic solids this species can be a molecular species of the constituent. It cannot be an atomic species (as in monoatomic covalent network) as it cannot vibrate. - for minerals the species can be a molecule (H2O, …), or an anionic radical, … - for complex solids it can be a functional group. *Notes:* - for molecular species (molecule, molecular ion, or radical) and atomic species (atom, ions) it should be mostly an isotopic species. - It is possible to put the uid of the natural terrestrial isotopic mix when the precise isotopic species is unknown. - functional groups are with terrestrial natural abundance - for minerals the functional group could be an 'anionic radical'
spectrum_band_transition_chemical_bonds	***List [L12]***	[O]				£: bonds or part of the species producing this band
*spectrum*_band_transition_chemic	varchar(255)	U	Spectr	V	--	Link to the existing UID of the bond(s), part(s) of the primary molecule, or

al_bond_uid [*]		[m]	Chem B Molec L10 L12	[Ver]		whole molecule subjected to the transition producing this band *Note:* the UID starts with either 'BOND_', 'MOLECPART_', or 'MOLEC_' depending on the number of bonds involved and size of the molecule, see below. *Note SSDM:* "Bandlist" equivalent = "*band*_transition_chemical_bond_uid" *Note:* - mostly for fundamental and overtone vibration bands (a single chemical bond). - also for simple combinations of vibration bands but limit the list to 2 chemical bonds. - above 2 bonds involved prefers "chemical_bonds" of the type 'molecule part' or take a "molecule" if the transition concerns all bonds of the molecule. not for electronic transitions in molecules or minerals
*spectrum*_band_transition_assignment	varchar(255)	U [m]	Spectr L10	V [Ver]	--	Designation of the band transition *Syntax:* LaTEX format: *Note SSDM:* "Bandlist" equivalent = "*band*_transition_assignment" *Ex:* aν_1+b$\nu_2^{dl_2}$+…+c$\nu_n^{ml_n}$+eJ+fK+gKa+hKc+iL+jTx+ kTy+lRx+pRy [...] for $a\nu_1+b\nu_2^{dl}{}_2+\ldots+\nu_n^{ml}{}_n$+eJ+fK+gKa+hKc+iL+ $jT_x+ kT_y+lR_x+pR_y$ where a,b,c,d,e,f, …,p are integers *Note:* - put 'unknown' if transition is fully unknown. If part is unknown, something like '+ ?' or + ?J', … can be added - Hot bands (lower state with at least one quantum number > 0) are expressed with the '-' sign for their lower state – LaTeX: cf. http://www.cheat-sheets.org/saved-copy/latexsheet.pdf - *Ex:* '$(2\nu_1- \nu_1)+3\nu_2-T_x$' for ν_1: 1→2 ; ν_2: 0→3 and T_x: 1→0
*spectrum*_band_vibration_mode	enum(text)	U	Spectr	V [Ver]	--	Mode of internal vibration of the molecule producing this band

		[m]	L10			Enum: {stretching, stretching sym., stretching antisym., bending, bending in-p, bending out-p, bending sym., bending antisym., bending sym. in-p (scissoring), bending antisym. in-p (rocking), bending sym. out-p (wagging), bending antisym. out-p (twisting), deformation, stretching overtone, bending overtone, combination, other, unknown} *Definitions*: – For fundamental modes see "*molecule*_vibration_mode" – For ocombination/overtone modes see "*band*_transition_vibration_mode" *Notes:* definitions at: http://en.wikipedia.org/wiki/Vibrational_spectroscopy *Note SSDM:* "Bandlist" equivalent = "*band*_vibration_mode"
*spectrum*_band_rotation_mode	enum(text)	U [m]	Spectr L10	V [Ver]	--	Mode of rotation of the molecule producing this band Enum: {free rotation, hindered rotation, libration …, unknown} *Note SSDM:* "Bandlist" equivalent = "*band*_rotation_mode"
*spectrum*_band_phonon_mode	enum(text)	U [m]	Spectr L10	V [Ver]	--	Mode of external vibrations of the molecular solid producing this band Enum: {LO, TO, LA, TA1, TA2, unknown} *Note SSDM:* "Bandlist equivalent" = "*band*_phonon_mode"
*spectrum*_band_label	varchar(255)	U [m]	Spectr L10	V [Ver]	--	Information on the spectrum band that need to appear on the spectrum (e.g. chemical formula with isotopes + vibration mode) *Note SSDM:* "Bandlist" equivalent =
*spectrum*_band_comments	blob	U [m]	Spectr L10	V [Ver]	--	Comments on the spectrum band *Note SSDM:* Bandlist equivalent = 'band_parameters_comments' + 'band_transition_comments'

14. SPECTRUM FILES

14.1 Spectrum files

The spectra themselves are stored in the data base. They are described by spectral points, with its wavenumber (cm^{-1}) and the corresponding intensity value(s) which depends on the type of spectrum. For each value there is also a quality flag (mostly 6 quality levels from '0' = "no valid data" to '5' = "excellent data") and a numerical error bar, eventually asymmetric for optical constants (minimum and maximum values). Each spectrum is linked with a small png image of the whole valid spectrum at full scale, used for fast display ("spectrum_image_filename").

The ***simple spectrum*** files of the following types ("spectrum_type") are defined by wavelength values and an associated single value of intensities:

- 'level 0': raw
- 'level 1': transmission, ATR transmission, bidirectional reflectance, radiance factor, thermal emission, thermal radiance, scattering intensity, Raman scattering intensity, fluorescence emission
- 'level 2': absorbance, normalized absorbance, optical depth, ATR absorbance, corrected ATR absorbance, bidirectional reflectance distribution function, reflectance factor, normalized reflectance, thermal emittance, differential scattering cross section, normalized Raman scattering intensity, normalized fluorescence emission
- 'level 3': absorption coefficient, dielectric loss tangent, magnetic loss tangent, albedo, anisotropy factor, normalized differential scattering cross section, Raman scattering coefficient
- 'level 4': thermal emissivity, scattering efficiency factor parameters, single scattering albedo, Raman scattering efficiency, fluorescence emission efficiency

The ***complex spectrum*** files (complex admittance, complex impedance (level 1), relative complex permittivity, relative complex permeability, complex reflectance ratio (level 2), and 'optical constants' (level 4)) are defined by wavelength values and two associated values of intensity: the 'real part' and 'imaginary part'. Errors are best defined by minimum and maximum values for 'k' and 'n'. They will have thus a specific file format with 3 columns.

The '***polarization parameters'*** files (level 2)) are defined by wavelength values and two alternative sets of four parameters: either with the raw 'Stokes parameters' (I, Q, U, V), or with the 'normalized Stokes parameters (polarization contrast, degree of linear polarization, polarization position angle, degree of circular polarization). They will have thus a specific file format with 5 columns.

The **'*scattering parameters'*** files (level 3) are defined by wavelength values and two alternative sets of three parameters: either with the 'scattering cross section parameters (scattering cross section, absorption cross section, extinction cross section), or with the scattering efficiency factor parameters (scattering efficiency factor, absorption efficiency factor, extinction efficiency factor) with 4 columns.

The '***radiative transfer model parameters'*** files (level 4) are defined by wavelength values and two or more associated values of intensity, depending on the model used and its number of parameters: for exemple, the '*single scattering albedo w*' and the '*single scattering phase function parameters'*: 'b, c1, c2' (Henyey-Greenstein). They will have thus a specific file format with an adaptable number of columns (or set to the maximum case). Error need to be given for each spectral parameter. They will have thus a specific file format with a variable number of columns.

A few products from spectra, such as the ***spectral directional emittance (or emissivity) distribution function*** (SDEDF) or the ***spectral bidirectional reflectance distribution function*** (SBRDF) (level 3), are complex spectral products as they are expressed as a function of wavelength, and emergence angle (SDEDF) or incidence, emergence and azimuth angles (SBRDF) and thus they need either specific file formats or to be extracted "on the fly" from a set of 'bi-directional reflectance' spectra. The current distribution function file thus mostly lists the directional and bidirectional geometry and the associated directional or bidirectional files (TBC).

The ***directional emittance (or emissivity) distribution function*** (DEDF) or the ***bidirectional reflectance distribution function*** (BRDF) (level 3) can be derived from the SDEDF and SBRDF respectively by extracting the values at a specific wavelength. They can also be stored in specific files.

14.2 Intensity Spectrum file

Root of the table: ***spectrum*** [-xml]

Data type: in ‘Experiment and spectra’

When “*spectrum*_files_parameter_type” = ‘simple spectrum’

“*spectrum*_type” =
- ‘level 0’: raw
- ‘level 1’: transmission, ATR transmission, bidirectional reflectance, radiance factor, thermal emission, thermal radiance, scattering intensity, Raman scattering intensity, fluorescence emission
- ‘level 2’: absorbance, normalized absorbance, optical depth, ATR absorbance, corrected ATR absorbance, bidirectional reflectance distribution function, reflectance factor, normalized reflectance, thermal emittance, differential scattering cross section, normalized Raman scattering intensity, normalized fluorescence emission
- ‘level 3’: absorption coefficient, dielectric loss tangent, magnetic loss tangent, albedo, anisotropy factor, normalized differential scattering cross section, Raman scattering coefficient
- ‘level 4’: thermal emissivity, scattering efficiency factor parameters, single scattering albedo, Raman scattering efficiency, fluorescence emission efficiency

AND
"*parameters_instrument*_angle_observation_mode" = ‘fixed angles’

These spectrum files (level 1 to 4) are defined by spectral position values and one (or more) associated value of intensities, plus an error (different formats)

Key-word	Type	Level	Unit	Description
*spectrum*_file_index	int(10)	B [!!_g]	--	Automatic random but unique number given to new spectrum file
*spectrum*_position	float	S [!!_m]	var.	Wavenumber/wavelength/frequency of the spectral point *Unit:* in unit defined by “*parameters_instrument*_spectral_unit” • Converted and stored in ‘cm-1’ unit in the database but provided to user in the unit specified in “*parameters_instrument*_spectral_unit”

*spectrum*_intensity	float	U [!!_m]	var.	Intensity *Units:* in unit defined by "*experiment*_intensity_unit" • stored in the database and provided to user in "*experiment*_intensity_unit"
*spectrum*_intensity_mean	float	U [!!_m]	var.	Mean value of the intensity *Units:* in unit defined by "*experiment*_intensity_unit" • stored in the database and provided to user in "*experiment*_intensity_unit"
*spectrum*_intensity_median	float	U [!!_m]	var.	Median value of the intensity *Units:* in unit defined by "*experiment*_intensity_unit" • stored in the database and provided to user in "*experiment*_intensity_unit"
*spectrum*_intensity_min	float	U [c/m]	var.	Minimum value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* generaly calculated from the 'error' ('+ & –' or '+/-') data ➔ "intensity_min" = "intensity" - "intensity_error_minus"
*spectrum*_intensity_max	float	U [c/m]	var.	Maximum value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* generaly calculated from the 'error' ('+ & –' or '+/-') data ➔ "intensity_max" = "intensity" + "intensity_error_plus"
*spectrum*_intensity_error	float	U	var.	Symetric error on the value of intensity

		[m/c]		*Units:* in unit defined by "*experiment*_intensity_unit"
*spectrum*_intensity_error_stdev	float	U [m/c]	var.	Standard deviation of the value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" *Note:* generally used together with "spectrum_intensity_mean" or "spectrum_intensity_mean"
*spectrum*_intensity_error_minus	float	U [m/c]	var.	Negative error on the value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit"
*spectrum*_intensity_error_plus	float	U [m/c]	var.	Positive error on the value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* this error is frequently given in the data file as a symmetric (+/-) error
*spectrum*_intensity_quality	int(1)	S [m]	--	Quality flag on the value of intensity *Note:* Mostly 6 quality levels from '0': "no valid data" to '5': "excellent data" *Note:* The value '0' is for flagging any data outside the validity range

14.3 Complex Spectrum file

Root of the table: ***spectrum_complex*** [-xml]

Data type: in 'Experiment and spectra'

When "*spectrum*_files_parameter_type" = 'complex spectrum'

"*spectrum*_type" = {optical constants, complex admittance, complex impedance, relative complex permittivity, relative complex permeability, complex reflectance ratio}

The 'complex spectrum' files are defined by spectral position values and two associated values of intensities: the 'real part' and 'imaginary part'

Key-word	Type	Level	Unit	Description
*spectrum_complex*_file_index [-xml]	int(10)	B [!!_g]	--	Automatic random but unique number given to new spectrum file
*spectrum_complex*_position	float	S [!!_m]	var.	Wavenumber/wavelength/frequency of the spectral point *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • Converted and stored in 'cm-1' unit in the database but provided to user in the unit specified in "***parameters_instrument***_spectral_unit"
*spectrum_complex*_intensity_real	float	U [!!_m]	*no*	Value of 'real index'
*spectrum_complex*_intensity_imaginary	float	U [!!_m]	*no*	Value of 'imaginary index'
*spectrum_complex*_intensity_real_min	float	U [c/m]	*no*	Minimum value of 'real index' *Note:* frequently calculated from the 'error' ('+ & –' or '+/-') data, or directly provided in the data file. ➔ "intensity_real_min" = "intensity_real" - "intensity_real_error_minus"

*spectrum_complex*_intensity_real_max	float	U [c/m]	*no*	Maximum value of ‘real index’ *Note:* frequently calculated from the ‘error’ (‘+ & –‘ or ‘+/-‘) data, or directly provided in the data file. ➔ “intensity_real_max” = “intensity_real” + “intensity_real_error_plus”
*spectrum_complex*_intensity_imaginary_min	float	U [c/m]	*no*	Minimum value of ‘imaginary index’ *Note:* frequently calculated from the ‘error’ (‘+ & –‘ or ‘+/-‘) data, or directly provided in the data file. ➔ “intensity_imaginary_min” = “intensity_imaginary” - “intensity_imag
*spectrum_complex*_intensity_imaginary_max	float	U [c/m]	*no*	Maximum value of ‘imaginary index’ *Note:* frequently calculated from the ‘error’ (‘+ & –‘ or ‘+/-‘) data, or directly provided in the data file. ➔ “intensity_imaginary_max” = “intensity_imaginary” + “intensity_imag
*spectrum_complex*_intensity_real_error_minus	float	U [m/c]	*no*	Negative error on the value of ‘real index’ *Note:* this error can be given in the data file as a symmetric (+/-) error. It may need to be calculated from “intensity_real_min”
*spectrum_complex*_intensity_real_error_plus	float	U [m/c]	*no*	Positive error on the value of ‘real index’ *Note:* this error can be given in the data file as a symmetric (+/-) error. It may need to be calculated from “intensity_real_max”
*spectrum_complex*_intensity_imaginary_error_minus	float	U [m/c]	*no*	Negative error on the value of ‘imaginary index’ *Note:* this error can be given in the data file as a symmetric (+/-) error It may need to be calculated from “intensity_imaginary_min”
*spectrum_complex*_intensity_imaginary_error_plus	float	U [m/c]	*no*	Positive error on the value of ‘imaginary index’ *Note:* this error can be given in the data file as a symmetric (+/-) error. It may need to be calculated from “intensity_imaginary_max”

*spectrum_complex*_intensity_real_quality	int(1)	S [m]	--	Quality flag on the value of ‘real index’ *Note:* Mostly 6 quality levels from ‘0’: “no valid data” to ‘5’: “excellent data
*spectrum_complex*_intensity_imaginary_quality	int(1)	S [m]	--	Quality flag on the value of ‘imaginary index’ *Note:* Mostly 6 quality levels from ‘0’: “no valid data” to ‘5’: “excellent data

14.4 Radiative Transfer Model Parameters Spectrum file

Root of the table: ***spectrum_model*** [-xml]

Data type: in 'Experiment and spectra'

When "*spectrum*_files_parameter_type" = 'model parameter spectra'

When "*spectrum*_type" = 'radiative transfer model'

The 'radiative transfer model parameters' files (level 4) are defined by spectral position values and two ('*single scattering albedo w*' and '*single scattering phase function parameter b*') or more associated parameter values, depending on the radiative transfer model used. Below are those for the Hapke (1986) model.

Key-word	Type	Level	Unit	Description
*spectrum_model*_file_index [-xml]	int(10)	B [!!_g]	--	Automatic random but unique number given to new spectrum file
*spectrum_model*_position	Float	S [!!_m]	var.	Wavenumber/wavelength/frequency of the spectral point *Unit:* in unit defined by "*parameters_instrument*_spectral_unit" • Converted and stored in 'cm-1' unit in the database but provided to user in the unit specified in "*parameters_instrument*_spectral_unit"
*spectrum_model*_single_scattering_albedo_w	Float	U [!!_m]	*no*	single scattering albedo parameter, w
*spectrum_model*_mean_roughness_teta	Float	U [m]	deg	Mean roughness parameter, Θ
*spectrum_model*_phase_coefficients_b	Float	U [!!_m]	*no*	Phase function coefficient, b
*spectrum_model*_phase_coefficients_c	Float	U [m]	*no*	Phase function coefficient, c

*spectrum_model*_opposition_peak_height_B0	Float	U [m]	*no*	Opposition peak height, B_0
*spectrum_model*_opposition_peak_width_h	Float	U [m]	*no*	Opposition peak width, h
*spectrum_model*_single_scattering_albedo_w_error	Float	U [m]	*no*	Absolute uncertainty (+/-) on value of the single scattering albedo parameter,
*spectrum_model*_mean_roughness_teta_error	Float	U [m]	deg	Absolute uncertainty (+/-) on value of the Mean roughness parameter, Θ
*spectrum_model*_phase_coefficients_b_error	Float	U [m]	*no*	Absolute uncertainty (+/-) on value of the phase function coefficient, b
*spectrum_model*_phase_coefficients_c_error	Float	U [m]	*no*	Absolute uncertainty (+/-) on value of the phase function coefficient, c
*spectrum_model*_opposition_peak_height_B0_error	Float	U [m]	*no*	Absolute uncertainty (+/-) on value of the opposition peak height, B_0
*spectrum_model*_opposition_peak_width_h_error	Float	U [m]	*no*	Absolute uncertainty (+/-) on value of the opposition peak width, h
*spectrum_model*_inversion_quality	int(1?)	S [m]	--	Global quality flag on the values of the inversion parameters *Note:* Mostly 6 quality levels from ‘0’: “no valid data” to ‘5’: “excellent data

14.5 Multi-Angles Spectra file

Root of the table: ***spectrum_multiangle*** [-xml]

Data type: in 'Experiment and spectra'

When "*spectrum*_files_parameter_type" = {photometric data, spectra of multiangle dataset, photometric data of multispectral dataset, spectro-photometric data}

"*spectrum*_type" =
- 'level 0': raw
- 'level 1': transmission, bidirectional reflectance, radiance factor, thermal emission, thermal radiance, scattering intensity, Raman scattering intensity, fluorescence emission
- 'level 2': absorbance, normalized absorbance, optical depth, bidirectional reflectance distribution function, reflectance factor, normalized reflectance, thermal emittance, differential scattering cross section, normalized Raman scattering intensity, normalized fluorescence emission
- 'level 3': albedo, anisotropy factor, normalized differential scattering cross section, Raman scattering coefficient

AND
"*parameters_instrument*_angle_observation_mode" = {one variable angle, two variable angles, three variable angles, fixed phase angle, mono-angular function, bi-angular function, tri-angular function, fixed phase angle function, other geometry set}

Key-word	Type	Level	Unit	Description
*spectrum_multiangle*_file_index [-xml]	int(10)	B [!!_g]	--	Automatic random but unique number given to new brdf table
*spectrum_multiangle*_angle_incidence	float	S [!!o_m]	deg	Incidence angle of illumination relative to the normal of the sample surface *Constraint:* not for "*spectrum*_type" = {DEDF, MDEDF, SDEDF, hemispherical-directional reflectance, directional thermal emissivity, scattering} • stored in the database and provided to user in 'deg' unit
*spectrum_multiangle*_angle_emergence	float	S [!!o_m]	deg	Emergence angle of observation in the principal (illumination) plane relative to the normal of the sample surface

				Constraint: not for "*spectrum*_type" = {directional-hemispherical albedo} • stored in the database and provided to user in 'deg' unit
*spectrum_multiangle*_angle_azimuth	float	S [!!o_m]	deg	Azimuth angle of observation relative to the plane perpendicular to the surface and containing the incidence beam *Constraint:* not for "*spectrum*_type" = {hemispherical-directional reflectance directional-hemispherical albedo} • stored in the database and provided to user in 'deg' unit *Note:* generally not for "*spectrum*_type" = {DEDF, MDEDF, SDEDF, specular reflectance, complex reflectance ratio, directional thermal emissivity, scattering}
*spectrum_multiangle*_angle_phase	float	S [!!o_c/m]	deg	Phase angle of observation relative to the plane containing the incidence beam and the obersvation direction *Constraint:* not for "*spectrum*_type" = {DEDF, MDEDF, SDEDF , hemispherical-directional reflectance, directional-hemispherical albedo, directional thermal emissivity} • calculated and stored in the database and provided to user in 'deg' unit ➔ "angle_phase" = arcos[cos(angle_incidence) * cos(angle_emergence) + sin(angle_incidence) * sin(angle_emergence) * cos(angle_azimuth)]
*spectrum_multiangle*_intensity	float	U [!!_m]	var.	Intensity with unit depending on the type of product *Units:* in unit defined by "*experiment*_intensity_unit" • stored in the database and provided to user in "*experiment*_intensity _unit"
*spectrum_multiangle*_intensity_min	float	U [c/m]	var.	Minimum value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in

				"*experiment*_intensity_unit" *Note:* generaly calculated from the 'error' ('+ & –' or '+/-') data ➔ "intensity_min" = "intensity" - "intensity_error_minus"
*spectrum_multiangle*_intensity_max	float	U [c/m]	var.	Maximum value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* generaly calculated from the 'error' ('+ & –' or '+/-') data ➔ "intensity_max" = "intensity" + "intensity_error_plus"
*spectrum_multiangle*_intensity_error_minus	float	U [m/c]	var.	Negative error on the value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* this error is frequently given in the data file as a symmetric (+/-) error
*spectrum_multiangle*_intensity_error_plus	float	U [m/c]	var.	Positive error on the value of intensity *Units:* in unit defined by "*experiment*_intensity_unit" • calculated and stored in the database and provided to user in "*experiment*_intensity_unit" *Note:* this error is frequently given in the data file as a symmetric (+/-) error
*spectrum_multiangle*_intensity_quality	int(1)	S [m]	--	Quality flag on the value of intensity *Note:* Mostly 6 quality levels from '0': "no valid data" to '5': "excellent data *Note:* The value '0' is for flagging any data outside the validity range

15. ENUMERATION PARAMETERS TABLE

15.1 Description

The **OpenEnum table** contains the keywords described by an open list of attributes, with all the valid values of the attributes and in a few case a code that replace complex or long attribute labels for filling the xml.

15.2 OpenEnum Parameters Table

Root of the table: ***openenum***

Data type: 'openenum'

Key-word	Type	Level	Table	Exp	Unit	Description
Openenum import and indexes						
*openenum*_import_mode	enum(text)	P [!!_m]	OpEnu	(V)	--	Mode of import of the "openenum" Enum: {first import, draft, no change, correction} *Definitions:* see "*spectrum*_import_mode"
*openenum*_index [**][-xml]	int(10)	B [!!_g]	OpEnu	-	--	Automatic random but unique number (internal) given to new openenum list
*openenum*_keyword	varchar(255)	S0 [!!_m]	OpEnu		--	Full name of the keyword, including the table name root *Ex:* 'mineral_dana_group'
*openenum*_table [-xml]	enum(text)	S0 [!!_m]	OpEnu		--	Table to which the keyword belongs Enum: {database, laboratory, experimentalist, access group, journal, publication, atom, chemical bond, chemical function, molecule, mineral solid, liquid, meteorite object meteorite, object micrometeorite, object idp, matter fluid, matter solid, matter carbonaceous, matter extraterrestrial, sample, layer, material, constituent, processing, instrument, experiment, spectrum, bandlist, band, state, band parameter, vibration mode parameter} ➔ calculated from "*openenum*_keyword" *Ex:* 'mineral' for 'mineral_dana_group' keyword
*openenum*_column [-xml]	varchar(255)	S0 [!!_m]	OpEnu		--	Keyword of the table ➔ calculated from "*openenum*_keyword"

					Ex: 'dana_group' for 'mineral_dana_group' keyword
Openenum attribute values					
openenum_values	***List [L1]***				£: List of the attribute values of the OpenEnum
*openenum*_value_fixed	boolean	S0 [££o_m]	OpEnu L1	--	Flag used to fix the attribute value (cannot be modified) BoolEnum: {yes, no} or {true, false} *Note xml*: placed as an attribute of the 'value' block. *Note:* - tell that this attribute value is directly used in SSHADE code for some 'mandatory condition' during import. - it cannot be removed or renamed otherwise the code will not work properly. - To avoid its removal or renaming, it is replaced by using "*openenum*_value_replace_code"
*openenum*_value_replace_code	varchar(255)	P [!!o_m]	OpEnu L1	--	Previous code (fixed) to be replaced by a new one *Note xml*: placed as an attribute of the 'value' block. *Note xml*: will work only when the special flag 'Ignore fixed OpenEnum values' is activated in the import page (only for SSHADE managers) *Note:* - used to change a fixed attribute used in 'Conditions' - allow to tell that the value defined by "*openenum*_value_code" replaces the one already in SSHADE without removing it, to avoid loosing its role in some "mandatory conditions"
*openenum*_value_code	varchar(255)	S0 [!!_m]	OpEnu L1	--	Code of the attribute of the keyword *Note:* it is the code that need to be filled in the xml file *Ex:* 'clathrate network ', 'compact porous coarse grained', '02.08.09', '09.EA'

*openenum*_value_label	varchar(255)	S0 [££_m]	OpEnu L1	--	Label of the attribute of the keyword *Constraint*: only some keywords have a couple of label/code, when the attribute description is too long or complex (with non basic ascii characters) the code is replaced by a short value, generally a number or string of numbers. *Note:* this label is used only for complex ‘text’ frequently associated with some code (like in various classifications). It is replaced by a simple numerical code to simplify xml filling. *Ex:* ’Single nets of tetrahedra with 4-, 5-, (6-), and 8-membered rings’ with “code” = ‘09.EA’