# ATLAS OF ZEOLITE FRAMEWORK TYPES

Ch. Baerlocher W.M. Meier D.H. Olson

Fifth Revised Edition 2001

Published on behalf of the Structure Commission of the International Zeolite Association

**ELSEVIER** 

# ATLAS OF ZEOLITE FRAMEWORK TYPES

# Fifth Revised Editon

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# PREFACE

A forerunner of the ATLAS was first published in 1970<sup>(1)</sup>. This early survey comprised 27 zeolite structures known at the time. Then the "Atlas of Zeolite Structure Types" by W.M. Meier and D.H. Olson, with 38 entries, was published by the Structure Commission of the IZA in 1978. This was followed by the much expanded 2<sup>nd</sup> edition of the ATLAS in 1988 comprising 64 entries, the updated 3<sup>rd</sup> edition in 1992 with 85 entries, and the fully revised 4<sup>th</sup> edition in 1996 with 98 entries. This 5<sup>th</sup> edition is again an updated version of the previous compilation, and the number of entries has risen significantly to 133.

The ATLAS contains an entry for each unique zeolite framework type. The term zeolite framework refers to a corner-sharing network of tetrahedrally coordinated atoms. In compliance with the changes in zeolite nomenclature recommended by IUPAC in 2001<sup>(2)</sup> the title of the Atlas had to be changed from 'Atlas of Zeolite Structure Types' to 'Atlas of Zeolite Framework Types'. This is because the term 'structure' implies both the framework and the extra-framework constituents of a zeolite and the latter are excluded in the framework description.

As a frequently quoted work of reference, the ATLAS must be updated on a regular basis to be of full use. Not only must new framework types be added, but corrections and new information on existing entries must also be disseminated. This compilation is based on information that was available to the authors by the end of 2000. We have been very grateful for preprints and unpublished data in a number of instances and this is acknowledged on the respective pages. New framework types (formerly called structure types) will be published on the world wide web (http://www.iza-structure.org/databases/) as they are approved.

To make it easier for the reader we have rearranged some of the data and prepared new stereo drawings. We have separated the information pertinent to the Framework Type from that corresponding to the Type Material only. In addition, we have included idealized cell parameters for the framework types, added the vertex symbols for each T–atom in a framework and have reintroduced the secondary building units (SBU's) which had been dropped in the 4<sup>th</sup> edition. The data sheets have all been generated from a zeolite database built by Ch. Baerlocher and L.B. McCusker using the contents of the 4<sup>th</sup> edition of the ATLAS as a basis. This zeolite database is also used to publish the data on the world wide web under http://www.iza-structure.org/databases/.

We wish to acknowledge the assistance and collaboration of many fellow scientists in our field. We are indebted to the members of the IZA Structure Commission for their extensive proof reading and for providing additional information. In particular we wish to express our appreciation to Dr. Lynne McCusker for maintaining the reference database, for her help in preparing the stereo drawings and last but not least for her highly valued advice throughout this work. It does not seem possible to assemble such a compilation absolutely free of errors, so the authors will be grateful for any additions and/or corrections for future updates.

February 2001

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Previous IZA Special Publications:

- W.J. Mortier, "Compilation of Extra Framework Sites in Zeolites" (1982)
- W.M. Meier and D.H. Olson, "Atlas of Zeolite Structure Types", 2nd edition (1987)
- W.M. Meier and D.H. Olson, "Atlas of Zeolite Structure Types", 3rd edition (1992)
- W.M. Meier , D.H. Olson and Ch. Baerlocher, "Atlas of Zeolite Structure Types", 4<sup>th</sup> edition (1996)
- R. von Ballmoos and J.B. Higgins, "Collection of Simulated XRD Powder Patterns for Zeolites", 2nd edition (1990)
- M.M.J. Treacy, J.B. Higgins and R. von Ballmoos, "Collection of Simulated XRD Powder Patterns for Zeolites", 3rd edition (1996)
- H. Robson and K.P. Lillerud, "Verified Synthesis of Zeolitic Materials" (1998)

# INTRODUCTION AND EXPLANATORY NOTES

Zeolites and zeolite-like materials do not comprise an easily definable family of crystalline solids. A simple criterion for distinguishing zeolites and zeolite-like materials from denser tectosilicates is based on the framework density (FD), the number of tetrahedrally coordinated atoms (T-atoms) per 1000 Å<sup>3</sup>. Figure 1 shows the distribution of these values for porous and dense frameworks whose structures are well established<sup>(3)</sup>. A gap is clearly recognizable between zeolite-type and dense tetrahedral framework structures. The lower boundary ranges from 19 to over 21 T-atoms per 1000 Å<sup>3</sup>, depending on the type of smallest rings present. Strictly speaking the boundaries defined in Figure 1 for the framework densities apply to fully crosslinked frameworks only. Therefore, Figure 1 does not include interrupted frameworks.

For each framework type code (see below), two pages of data are included in the ATLAS. The left hand page lists the information that characterizes the framework type. This includes crystallographic data (highest possible space group, cell constants of the idealized framework), coordination sequences, vertex symbols and loop configurations. Taken together the last three pieces of information define the framework type. On the second page, data for the type *material* (i.e. a real material) can be found. Although the channel dimensionality is a property of the framework type, the channel description also includes the observed ring dimensions, and must therefore refer to the type material. For all framework types, a list of isotypic materials and their references are also given. The different entries in the data sheets are described in more detail below in the order in which they appear on these pages.

# Framework Type Page

## Framework type codes (previously called structure type codes)

Following the rules set up by an IUPAC Commission on Zeolite Nomenclature in 1978<sup>(4)</sup>, designations consisting of three capital letters (in bold face type) have been used throughout. The codes are generally derived from the names of the type materials (see Appendix D) and do not include numbers and characters other than capital Roman letters. The assignment of Framework Type codes is subject to review and clearance by the IZA Structure Commission according to a decision of the IZA Council (taken at the time of the 7th IZC in Tokyo, 1986). Codes are only assigned to established structures that satisfy the rules of the IZA Structure Commission (see Appendix B for a listing of these rules). For interrupted frameworks, the 3-letter code is preceded by a hyphen. These mnemonic codes should not be confused or equated with actual materials. They only describe and define the network of the corner sharing tetrahedrally coordinated framework atoms. Thus, designations such as NaFAU are untenable. However, a material can be described using the IUPAC crystal chemical formula<sup>(2)</sup>, as  $|Na_{58}|$  [Al<sub>58</sub>Si<sub>134</sub> O<sub>384</sub>]-FAU or |Na-| [Al-Si-O]-FAU (Note that the chemical elements must be enclosed within the appropriate brackets, i.e. | | for guest species and [ ] for the framework host). Framework types do not depend on composition, distribution of the T-atoms (Si, Al, P, Ga, Ge, B, Be, etc.), cell dimensions or symmetry.



Fig. 1. Framework density vs. smallest ring in loop configuration. The + sign indicates that there are some T–positions associated with only larger rings (See Loop Configurations).

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The framework types have been arranged in alphabetical order according to the framework type code, because structural criteria alone do not provide an unambiguous classification scheme. This also facilitates later insertion of new codes and allows simple indexing. The framework type code is given at the top of each page. On the left hand page this is supplemented with the maximum space group symmetry for the framework, and on the right hand page with the full name of the type material.

# **Idealized cell parameters**

The idealized cell parameters are obtained from a DLS-refinement<sup>(5)</sup> in the given (highest possible) symmetry for the framework type. The refinement was carried out assuming a (sometimes hypothetical) SiO<sub>2</sub> composition and with the following prescribed interatomic distances:  $d_{Si-O} = 1.61$ Å,  $d_{O-O} = 2.629$ Å and  $d_{Si-Si} = 3.07$ Å using the weights of 2.0, 0.61 and 0.23, respectively.

#### Coordination sequences (CS) and vertex symbols

The concept of coordination sequences was originally introduced by Brunner and Laves<sup>(6)</sup> and first applied to zeolite frameworks by Meier and Moeck<sup>(7)</sup>. In a typical zeolite framework, each T-atom is connected to  $N_1 = 4$  neighboring T-atoms through oxygen bridges. These neighboring T-atoms are then linked in the same manner to  $N_2$  T-atoms in the next shell. The latter are connected with  $N_3$  T-atoms etc. Each T-atom is counted only once. In this way, a coordination sequence can be determined for each T-atom of the 4-connected net of T-atoms. It follows that

$$N_0 = 1$$
  $N_1 \pounds 4$   $N_2 \pounds 12$   $N_3 \pounds 36...$   $N_k \pounds 4 \cdot 3^{k-1}$ 

CS's are listed from  $N_1$  up to  $N_{10}$  for each topologically distinct T-atom in the framework structure along with the site multiplicity and the site symmetry (both in parenthesis).

The vertex symbol was first used in connection with zeolite-type networks by M. O'Keeffe and S.T. Hyde<sup>(8)</sup>. This symbol indicates the size of the smallest ring associated with each of the 6 angles of a tetrahedron (T–atom). The symbols for opposite pairs of angles are grouped together. For **FAU** the vertex symbol reads 4.4.4.6.6.12, indicating that one pair of opposite angles contains 4-rings, a second pair contains a 4-ring and a 6-ring, and the final pair of opposite angles contains a 6-ring and a 12-ring. It is useful for determining the smallest rings in a framework. In the case of **DOH**, for example, these are 4- and 5-rings, i.e. 4+. Sometimes more than one ring of the same size is found at a vertex.. This is indicated by a subscript like  $6_2$  or  $8_2$ .

The coordination sequence and the vertex symbol together appear to be unique for a particular framework topology, i.e. they can be used to distinguish different zeolite framework types unambiguously. In this way, isotypic frameworks can be easily recognized.

#### Secondary building units (SBU's)

Zeolite frameworks can be thought to consist of finite or infinite (i.e. chain- or layer-like) component units. The finite units which have been found to occur in tetrahedral frameworks are shown in Figure 2. These secondary building units<sup>a</sup>, which contain up to 16 T-atoms, are derived

<sup>&</sup>lt;sup>a</sup> The primary building units are single TO<sub>4</sub> tetrahedra.



Fig. 2. Secondary building units and their symbols. Number in parenthesis = frequency of occurrence.

assuming that the entire framework is made up of one type of SBU only. It should be noted that SBU's are invariably non-chiral<sup>a</sup>. A unit cell always contains an integral number of SBU's. As far as practicable, all possible SBU's have been listed. The number of observed SBU's has increased from 16 in 1992 to 20 at present. In some instances, combinations of SBU's have been encountered. These

<sup>&</sup>lt;sup>a</sup> This means that SBU's in the isolated state of highest symmetry are neither left- nor right-handed.

have not been listed *in extenso* because this can arbitrary. The symbols given below the drawings in Figure 2 are used in the data sheets to describe the SBU's. If more than one SBU is possible for a given framework type, all are listed. The number given in parenthesis in Figure 2 indicates the frequency of the occurrence of that SBU.

The SBU's are only theoretical topological building units and should not be considered to be or equated with species that may be in the solution/gel during the crystallization of a zeolitic material.

#### **Loop configuration of T-atoms**

The loop configuration is a simple graph showing how many 3- or 4-membered rings a given T-atom is involved in. Solid lines represent T-O-T linkages whereas dotted lines indicate non-connected T-O bonds found in interrupted frameworks. Sato<sup>(9)</sup> used the term "second coordination networks". Loop configurations are likely to be of interest to spectroscopists. These data can also be used for classification purposes and for deducing rules relating to these structures which might be of predictive value<sup>(10)</sup>. Figure 3 shows all observed loop configurations and their frequency of occurrence. The information given in the loop configuration is a subset of the vertex symbol.

#### **Framework description**

For all 15 framework types belonging to the so-called ABC-6-family the ABC stacking sequence is listed here. Listed are also some other structural relationships which are thought to be helpful.

#### Isotypic framework structures

Under this heading as-synthesized materials that have the same framework type but different chemical composition or have a different laboratory code are listed. Materials obtained by post synthesis treatment (e.g. ion exchange, dealumination, etc.) are generally not included. The type material (defined on the right hand page) is given first and marked with an asterisk. Isotypic species, which have sometimes been termed "homeotypic"<sup>(11)</sup>, are very frequent and are also listed in the isotypic material index.

Zeolite-type silicates and phosphates apparently constitute two distinctive categories of microporous materials. Table 1 (which is based on the isotypes listed in the ATLAS) shows, however, that there are three, rather than two distinct groups of framework types. Apart from those associated with silicates and phosphates there is a sizable group of structure types which have been found to occur both in silicates and phosphates.

#### References

The list of references cited is far from complete. As a general rule, references to the type materials are to the work first establishing that framework type and to subsequent work adding significant information regarding the framework topology. Thus papers on non-framework species have not been included. References to isotypes are limited to the work in which sufficient data are provided to establish the identity.



Fig. 3. Loop configurations. Number in parenthesis = frequency of occurrence.

For the 42 codes from **ABW** to **CZP**, complete references, cell constant data, space groups, site symmetries, symmetry relationships, structural diagrams, positional coordinates for all types and chemical compositions for all crystal structure determinations published up to April 2000 are to be found in: W.H. Baur and R.X. Fischer: Zeolite-Type Crystal Structures and their Chemistry<sup>(12)</sup>.

	Silicates <sup>a</sup>		Both Silicates and Phosphates	Pho	sphates <sup>b</sup>
AFG	IFR	OFF	ABW	ACO	SAO
ASV	ISV	OSO	AET	AEI	SAS
*BEA	ITE	-PAR	AFI	AEL	SAT
BIK	JBW	PAU	AFX	AEN	SAV
BOG	KFI	-RON	ANA	AFN	SBE
BRE	LIO	RSN	AST	AFO	SBS
CAS	LOV	RTE	BPH	AFR	SBT
CFI	LTN	RTH	CAN	AFS	VFI
-CHI	MAZ	RUT	CGS	AFT	WEI
CON	MEI	SFE	СНА	AFY	ZON
DAC	MEL	SFF	DFT	AHT	
DDR	MEP	SGT	EDI	APC	
DOH	MFI	STF	ERI	APD	
DON	MFS	STI	FAU	ATN	
EAB	MON	STT	GIS	ATO	
EMT	MOR	TER	LAU	ATS	
EPI	MSO	TON	LEV	ATT	
ESV	MTF	TSC	LOS	ATV	
EUO	MTN	VET	LTA	AWO	
FER	MTT	VNI	LTL	AWW	
FRA	MTW	VSV	MER	CGF	
GME	MWW	-WEN	PHI	-CLO	
GON	NAT	YUG	RHO	CZP	
GOO	NES		SOD	DFO	
HEU	NON		ТНО	OSI	

 Table 1:
 Microporous zeolite-type materials

<sup>a</sup> including germanates

<sup>b</sup> including arsenates

# **Type Material Page**

The type material is the species first used to establish the framework type. Detailed information about the material is given on this page.

# Crystal chemical data

The composition, expressed in terms of cell contents, has been idealized where necessary for simplicity. The chemical formula is given according to the new IUPAC rules<sup>(2)</sup>. The space group and cell parameters listed for each type material are those taken from the reference cited. In many instances, further refinement of the structure taking into account ordering etc. would yield a lower symmetry. It should also be noted that the space group and other crystallographic data related to the type material structure do not necessarily apply to isotypes.

In some cases, the space group setting of the type material differs from that of the framework type. In these cases, the relationship of the unit cell orientation with respect to the framework type is listed. This relationship is important when comparing the orientation of the channel direction and the viewing direction of ring drawings (which are both given for the axis orientation of the type material) with that of the framework drawing.

# Framework density (FD)

The framework density is defined as the number of T-atoms per 1000 Å<sup>3</sup>. The figures given refer to the type materials. For non-zeolitic framework structures, values of at least 20 to 21 T/1000 Å<sup>3</sup> are generally obtained, while for zeolites with fully crosslinked frameworks the observed values range from about 12.1 for structures with the largest pore volume to around 20.6. To date, FD's of less than 12 have only been encountered for the interrupted framework cloverite<sup>(13)</sup>, and for hypothetical networks<sup>(14)</sup>. The FD is obviously related to the pore volume but does not reflect the size of the pore openings. For some more flexible zeolite structure types, the FD values can vary appreciably. In these cases (e.g., gismondine) values are given for the type material and for the framework in its most expanded state. The flexibility of a framework structure is, to some extent, revealed by the possible variation in the FD. FD values may also depend on chemical composition.

### Channels

A shorthand notation has been adopted for the description of the channels in the various frameworks. Each system of equivalent channels has been characterized by

- the channel direction (relative to the axes of the type material structure),
- the number of T-atoms (in bold type) forming the rings controlling diffusion through the channels, and
- the crystallographic free diameters of the channels in Angstrom units.

The number of asterisks in the notation indicates whether the channel system is one-, two- or threedimensional. In most cases, the smaller openings simply form windows (rather than channels) connecting larger cavities. Interconnecting channel systems are separated by a double arrow ( $\hat{}$ ). A vertical bar (|) means that there is no direct access from one channel system to the other. The examples from Table 2 have been selected to illustrate the use of these notations. Cancrinite is characterized by a 1-dimensional system of channels parallel to [001] or *c* with circular 12-ring apertures. In offretite, the main channels are similar but they are interconnected at right angles by a 2-dimensional system of 8-ring channels, and thus form a 3-dimensional channel system. The channel system in mordenite is essentially 2-dimensional with somewhat elliptical 12-ring apertures. The 8-ring limiting diffusion in the [001] direction is an example of a highly puckered aperture. Zeolite rho is an example of a framework type containing two non-interconnecting 3-dimensional channel systems which are displaced with respect to one another (<100> means there are channels parallel to all crystallographically equivalent axes of the cubic structure, i.e., along x, y and z.). In gismondine, the channels parallel to [100] together with those parallel to [010] give rise to a 3-dimensional channel system which can be pictured as an array of partially overlapping tubes.

# Table 2: Examples illustrating the notation for the crystallographic characterization of the Channels

Cancrinite	[001] <b>12</b> 5.9 x 5.9*
Offretite	[001] <b>12</b> 6.7 x 6.8* ´ ^ [001] <b>8</b> 3.6 x 4.9**
Mordenite	[001] <b>12</b> 6.5 x 7.0* ([010] <b>8</b> 3.4 x 4.8 ([001] <b>8</b> 2.6 x 5.7}*
Zeolite Rho	<100> <b>8</b> 3.6 x 3.6***   <100> <b>8</b> 3.6 x 3.6***
Gismondine	{[100] <b>8</b> 3.1 x 4.5 (010] <b>8</b> 2.8 x 4.8}***

Please note: The channel direction is given for the axis orientation of the *type material*. This orientation may be different from the orientation given in the framework drawing (see the cell relationship given under "crystal chemical data" for these cases).

A summary of the channel systems, ordered by decreasing number of T-atoms in the largest rings, is given in Table 3. The free diameter values (effective pore width) given in the channel description and on the ring drawings are based upon the atomic coordinates of the *type material* and an oxygen radius of 1.35Å. Both minimum and maximum values are given for noncircular apertures. In some instances, the corresponding interatomic distance vectors are only approximately coplanar, in other cases the plane of the ring is not normal to the direction of the channel. Close inspection of the framework and ring drawings should provide qualitative evidence of these factors. Some ring openings are defined by a very complex arrangement of oxygen atoms, so in these cases other short interatomic distances that are not listed may also be observed. It should be noted that crystallographic free diameters may depend upon the hydration state of the zeolite, particularly for the more flexible frameworks. It should also be borne in mind that effective free diameters can be affected by non-framework cations and may also be temperature dependent.

# 20-, 18- &14-Ring Structures

-CLO	Cloverite	<100> <b>20</b> 4.0 x 13.2***   <100> <b>8</b> 3.8 x 3.8***
VFI	VPI-5	[001] <b>18</b> 12.7 x 12.7*
AET	AlPO-8	[001] <b>14</b> 7.9 x 8.7*
CFI	CIT-5	[010] <b>14</b> 7.2 x 7.5*
DON	UTD-1F	[010] <b>14</b> 8.1 x 8.2*
OSO	OSB-1	[001] <b>14</b> 5.4 x 7.3* ´ ^ [001] <b>8</b> 2.8 x 3.3**

# 12-Ring Structures

AFI	AlPO-5	[001] <b>12</b> 7.3 x 7.3*
AFR	SAPO-40	[001] <b>12</b> 6.7 x 6.9* (010] <b>8</b> 3.7 x 3.7*
AFS	MAPSO-46	[001] <b>12</b> 7.0 x 7.0* ´ ^[001] <b>8</b> 4.0 x 4.0**
AFY	CoAPO-50	[001] <b>12</b> 6.1 x 6.1* ´ ^ [001] <b>8</b> 4.0 x 4.3**
ASV	ASU-7	[001] <b>12</b> 4.1x 4.1*
ATO	AlPO-31	[001] <b>12</b> 5.4 x 5.4*
ATS	MAPO-36	[001] <b>12</b> 6.5 x 7.5*
*BEA	Beta	<100> <b>12</b> 6.6 x 6.7** (001] <b>12</b> 5.6 x 5.6*
BOG	Boggsite	[100] <b>12</b> 7.0 x 7.0* (010] <b>10</b> 5.5 x 5.8*
BPH	Beryllophosphate-H	[001] <b>12</b> 6.3 x 6.3* ´ ^ [001] <b>8</b> 2.7 x 3.5**
CAN	Cancrinite	[001] <b>12</b> 5.9 x 5.9*
CON	CIT-1	[001] <b>12</b> 6.4 x 7.0* (100] <b>12</b> 7.0 x 5.9*
		[010] <b>10</b> 5.1 x 4.5*
CZP	Chiral Zincophosphate	[001] <b>12</b> 3.8 x 7.2*
DFO	DAF-1	{[001] <b>12</b> 7.3 x 7.3 ´ ^ [001] <b>8</b> 3.4 x 5.6}***
		{[001] <b>12</b> 6.2 x 6.2 ^ [001] <b>10</b> 5.4 x 6.4}***
EMT	EMC-2	[001] <b>12</b> 7.3 x 7.3* ´ ^ [001] <b>12</b> 6.5 x 7.5**
FAU	Faujasite	<111> <b>12</b> 7.4 x 7.4***
GME	Gmelinite	[001] <b>12</b> 7.0 x 7.0* ´ ^ [001] <b>8</b> 3.6 x 3.9**
GON	GUS-1	[001] <b>12</b> 5.4 x 6.8*
IFR	ITQ-4	[001] <b>12</b> 6.2 x 7.2*
ISV	ITQ-7	<100> <b>12</b> 6.1 x 6.5** (001] <b>12</b> 5.9 x 6.6*
LTL	Linde Type L	[001] <b>12</b> 7.1 x 7.1*
MAZ	Mazzite	[001] <b>12</b> 7.4 x 7.4*   [001] <b>8</b> 3.1 x 3.1***

# 12-Ring Structures (cont.)

MEI	ZSM-18	[001] <b>12</b> 6.9 x 6.9* ´ ^ [001] <b>7</b> 3.2 x 3.5**
MOR	Mordenite	[001] <b>12</b> 6.5 x 7.0* $([010] 8 3.4 \times 4.8) ([001] 8 2.6 \times 5.7)$ *
MTW	ZSM-12	[010] <b>12</b> 5.6 x 6.0*
OFF	Offretite	[001] <b>12</b> 6.7 x 6.8* ´ ^ [001] <b>8</b> 3.6 x 4.9**
OSI	UiO-6	[001] <b>12</b> 5.2 x 6.0*
-RON	Roggianite	[001] <b>12</b> 4.3 x 4.3*
SAO	STA-1	<100> <b>12</b> 6.5 x 7.2** (001] <b>12</b> 7.0 x 7.0*
SBE	UCSB-8Co	<100> <b>12</b> 7.2 x 7.4**  (001] <b>8</b> 4.0 x 4.0*
SBS	UCSB-6GaCo	[001] <b>12</b> 6.8 x 6.8* ´ ^ [001] <b>12</b> 6.9 x 7.0**
SBT	UCSB-10GaZn	[001] <b>12</b> 6.4 x 7.4 * ´ ^ [001] <b>12</b> 7.3 x 7.8**
SFE	SSZ-48	[010] <b>12</b> 5.4 x 7.6*
VET	VPI-8	[001] <b>12</b> 5.9 x 5.9*

# **10-Ring Structures**

AEL	Alpo-11	[001] <b>10</b> 4.0 x 6.5*
AFO	AlPO-41	[001] <b>10</b> 4.3 x 7.0*
AHT	AlPO-H2	[001] <b>10</b> 3.3 x 6.8*
CGF	Co-Ga-Phosphate-5	$\{[100] \ 10 \ 2.5 \ x \ 9.2^* + 8 \ 2.1 \ x \ 6.7^*\}  [001] \ 8 \ 2.4 \ x \ 4.8^*$
CGS	Co-Ga-Phosphate-6	{[001] <b>10</b> 3.5 x 8.1 [100] <b>8</b> 2.5 x 4.6}***
DAC	Dachiardite	[010] <b>10</b> 3.4 x 5.3* [001] <b>8</b> 3.7 x 4.8*
EPI	Epistilbite	[100] <b>10</b> 3.4 x 5.6* (001] <b>8</b> 3.7 x 4.5*
EUO	EU-1	[100] <b>10</b> 4.1 x 5.4*
FER	Ferrierite	[001] <b>10</b> 4.2 x 5.4*  [010] <b>8</b> 3.5 x 4.8*
HEU	Heulandite	$\{[001] \ 10 \ 3.1 \ x \ 7.5^* + 8 \ 3.6 \ x \ 4.6^* \}$ [100] $8 \ 2.8 \ x \ 4.7^*$
LAU	Laumontite	[100] <b>10</b> 4.0 x 5.3*
MEL	ZSM-11	<100> <b>10</b> 5.3 x 5.4***
MFI	ZSM-5	{[100] <b>10</b> 5.1 x 5.5  [010] <b>10</b> 5.3 x 5.6}***
MFS	ZSM-57	[100] <b>10</b> 5.1 x 5.4* (010] <b>8</b> 3.3 x 4.8*
MTT	ZSM-23	[001] <b>10</b> 4.5 x 5.2*
MWW	MCM-22	^ [001] <b>10</b> 4.0 x 5.5**   ^ [001] <b>10</b> 4.1 x 5.1**
NES	NU-87	[100] <b>10</b> 4.8 x 5.7**
-PAR	Partheite	[001] <b>10</b> 3.5 x 6.9*
SFF	SSZ-44	[001] <b>10</b> 5.4 x 5.7*
STF	SSZ-35	[001] <b>10</b> 5.4 x 5.7*

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# **10-Ring Structures (cont.)**

STI	Stilbite	[100] <b>10</b> 4.7 x 5.0* <sup>(1001]</sup> <b>8</b> 2.7 x 5.6*
TER	Terranovaite	[100] <b>10</b> 5.0 x 5.0*  (001] <b>10</b> 4.1 x 7.0*
TON	Theta-1	[001] <b>10</b> 4.6 x 5.7*
WEI	Weinebeneite	[001] <b>10</b> 3.1 x 5.4* ´ [100] <b>8</b> 3.3 x 5.0*
-WEN	Wenkite	<100> <b>10</b> 2.5 x 4.8**  [001] <b>8</b> 2.3 x 2.7*

# 9-Ring Structures

-CHI	Chiavennite	[001] <b>9</b> 3.9 x 4.3*
LOV	Lovdarite	[010] <b>9</b> 3.2 x 4.5* (001] <b>9</b> 3.0 x 4.2* (100] <b>8</b> 3.6 x 3.7*
NAT	Natrolite	<100> <b>8</b> 2.6 x 3.9**  (001] <b>9</b> 2.5 x 4.1*
RSN	RUB-17	[100] <b>9</b> 3.3 x 4.4* (001] <b>9</b> 3.1 x 4.3* (010] <b>8</b> 3.4 x 4.1*
STT	SSZ-23	[101] <b>9</b> 3.7 x 5.3* (001] <b>7</b> 2.4 x 3.5*
VSV	VPI-7	[01-1] <b>9</b> 3.3 x 4.3* (011] <b>9</b> 2.9 x 4.2*
		[011] <b>8</b> 2.1 x 2.7*

# 8-Ring Structures

ABW	Li-A	[001] <b>8</b> 3.4 x 3.8*
ACO	ACP-1	<100> <b>8</b> 2.8 x 3.5** ´ [001] <b>8</b> 3.5 x 3.5*
AEI	AlPO-18	{[100] <b>8</b> 3.8 x 3.8 <sup>´</sup> [110] <b>8</b> 3.8 x 3.8
		[001] <b>8</b> 3.8 x 3.8}***
AEN	AIPO-EN3	[100] <b>8</b> 3.1 x 4.3* ´ [010] <b>8</b> 2.7 x 5.0*
AFN	AlPO-14	[100] <b>8</b> 1.9 x 4.6* ´ [010] <b>8</b> 2.1 x 4.9* ´ [001] <b>8</b> 3.3 x 4.0*
AFT	AlPO-52	^ [001] <b>8</b> 3.2 x 3.8***
AFX	SAPO-56	^ [001] <b>8</b> 3.4 x 3.6***
ANA	Analcime	irregular distorted 8-rings
APC	AlPO-C	[001] <b>8</b> 3.4 x 3.7* ´ [100] <b>8</b> 2.0 x 4.7*
APD	AlPO-D	[010] <b>8</b> 2.3 x 6.0* ´ [201] <b>8</b> 1.3 x 5.8*
ATN	MAPO-39	[001] <b>8</b> 4.0 x 4.0*
ATT	AlPO-12-TAMU	[100] <b>8</b> 4.2 x 4.6* ´ [010] <b>8</b> 3.8 x 3.8*
ATV	AlPO-25	[001] <b>8</b> 3.0 x 4.9*
AWO	AlPO-21	[100] <b>8</b> 2.7 x 5.5*
AWW	AlPO-22	[001] <b>8</b> 3.9 x 3.9*
BIK	Bikitaite	[010] <b>8</b> 2.8 x 3.7*
BRE	Brewsterite	[100] <b>8</b> 2.3 x 5.0* <sup>(1001]</sup> <b>8</b> 2.8 x 4.1*

8-Ring Structures (cont.)

CAS	Cesium Aluminosilicate	[001] <b>8</b> 2.4 x 4.7*
СНА	Chabazite	^ [001] <b>8</b> 3.8 x 3.8***
DDR	Deca-dodecasil 3R	^ [001] <b>8</b> 3.6 x 4.4**
DFT	DAF-2	[001] <b>8</b> 4.1 x 4.1* ´ [100] <b>8</b> 1.8 x 4.7* ´ [010] <b>8</b> 1.8 x 4.7*
EAB	TMA-E	^ [001] <b>8</b> 3.7 x 5.1**
EDI	Edingtonite	<110> <b>8</b> 2.8 x 3.8** (001] <b>8</b> 2.0 x 3.1*
ERI	Erionite	^ [001] <b>8</b> 3.6 x 5.1***
ESV	ERS-7	[010] <b>8</b> 3.5 x 4.7*
GIS	Gismondine	{[100] <b>8</b> 3.1 x 4.5  [010] <b>8</b> 2.8 x 4.8}***
GOO	Goosecreekite	[100] <b>8</b> 2.8 x 4.0* ´ [010] <b>8</b> 2.7 x 4.1* ´ [001] <b>8</b> 2.9 x 4.7*
ITE	ITQ-3	[010] <b>8</b> 3.8 x 4.3*  [001] <b>8</b> 2.7 x 5.8*
JBW	NaJ	[001] <b>8</b> 3.7 x 4.8*
KFI	ZK-5	<100> <b>8</b> 3.9 x 3.9***   <100> <b>8</b> 3.9 x 3.9***
LEV	Levyne	^ [001] <b>8</b> 3.6 x 4.8**
LTA	Linde Type A	<100> <b>8</b> 4.1 x 4.1***
MER	Merlinoite	[100] <b>8</b> 3.1 x 3.5*  [010] <b>8</b> 2.7 x 3.6*
		$\begin{bmatrix} 001 \end{bmatrix} \{ 8 \ 3.4 \ x \ 5.1^* + 8 \ 3.3 \ x \ 3.3^* \}$
MON	Montesommaite	[100] <b>8</b> 3.2 x 4.4*  [001] <b>8</b> 3.6 x 3.6*
MTF	MCM-35	[001] <b>8</b> 3.6 x 3.9*
PAU	Paulingite	<100> <b>8</b> 3.6x3.6***   <100> <b>8</b> 3.6 x 3.6***
PHI	Phillipsite	[100] <b>8</b> 3.8 x 3.8* <sup>(</sup> [010] <b>8</b> 3.0 x 4.3* <sup>(</sup> [001] <b>8</b> 3.2 x 3.3*
RHO	Rho	<100> <b>8</b> 3.6 x 3.6***   <100> <b>8</b> 3.6 x 3.6***
RTE	RUB-3	[001] <b>8</b> 3.7 x 4.4*
RTH	RUB-13	[100] <b>8</b> 3.8 x 4.1*  [001] <b>8</b> 2.5 x 5.6*
SAS	STA-6	[001] <b>8</b> 4.2 x 4.2*
SAT	STA-2	^ [001] 3.0 x 5.5***
SAV	Mg-STA-7	<100> <b>8</b> 3.8 x 3.8** ´ [001] <b>8</b> 3.9 x 3.9*
ТНО	Thomsonite	[100] <b>8</b> 2.3 x 3.9* <sup>(1)</sup> [010] <b>8</b> 2.2 x 4.0* <sup>(2)</sup> [001] <b>8</b> 2.2 x 3.0*
TSC	Tschörtnerite	<100> <b>8</b> 4.2 x 4.2*** ´ <110> <b>8</b> 3.1 x 5.6***
VNI	VPI-9	{<110> <b>8</b> 3.1 x 4.0  [001] <b>8</b> 3.5 x .3.6}***
YUG	Yugawaralite	[100] <b>8</b> 2.8 x 3.6*  [001] <b>8</b> 3.1 x 5.0*
ZON	ZAPO-M1	[100] <b>8</b> 2.5 x 5.1* ´ [010] <b>8</b> 3.7 x 4.4*

In some cases, the type material is not stable to heating and/or removal of the template. This has been indicated where the information was available.

#### Stereographic figures

Stereographic drawings of the framework and of the limiting channel windows are presented for all framework types. These drawings have been generated using the program CrystalMaker<sup>(15)</sup>. Although the depth fading helps in viewing the drawings, the use of a stereo viewer is recommended (these can be obtained from any electron microscopy supply house).

For the framework drawings, the coordinates of the idealized, highest symmetry structures were used. Only the positions of the T-atoms are shown and the T-O-T bridges are represented by straight lines. This idealization makes it easier to visualize the topology and the basic features of zeolite-like framework structures, which are often relatively complex. The unit cell has been outlined wherever possible.

In the ring drawings, all atoms are shown. Their positions are based on the crystal structure of the type material, and therefore the ring dimensions and the viewing direction are also those of the type material. As explained in the crystal chemical data section, for a few type materials, the orientation of the crystallographic axes is different from that given for the framework type. In these cases, the relationship given in the "crystal chemical data" section must be applied when comparing the viewing direction of the ring drawings with that of the framework drawing.

## **Supplementary Information**

# **Topological densities**

The coordination sequences (CS) can be used to calculate a topological density (TD). As might be expected, the CS is a periodic function. This has been established for all observed framework topologies by Grosse–Kunstleve, Brunner and Sloane<sup>(16)</sup>. They showed that the CS of any T–atom can be described exactly by a set of p quadratic equations

$$N_k = a_i k^2 + b_i k + c_i$$
 for  $k = i + np$ ,  $n = 0, 1, 2, ... and i = 1, 2, 3, ... p$ 

For example, the CS of **ABW** is exactly described by a set of three quadratic equations (p=3), namely

$N_k = 19/9 \ k2 \ + 1/9 \ k + 16/9$	for $k = 1 + 3n$ ,	n=0,1,2,
$N_k = 19/9 \ k2 \ - 1/9 \ k + 16/9$	for $k = 2 + 3n$ ,	n=0,1,2,
$N_k = 19/9 k2 - 0 k + 2$	for $k = 3 + 3n$ ,	n=0,1,2,

The number of equations p necessary to calculate all members of a particular coordination sequence varies from p=1 for **SOD** and p=42 for **FAU** to p=140,900,760 for **EUO**.

With growing index k (the shell number of the CS), the linear and constant coefficients,  $b_i$  and  $c_i$ , respectively, become less and less important. Therefore we can define the exact topological density TD as the mean of all  $a_i$  divided by the dimensionality of the topology (i.e. 3 for zeolites)

$$TD = \frac{\langle a_i \rangle}{3} = \frac{1}{3p} \sum_{i=1}^{p} i$$

This TD is the same for all T atoms in a given structure. The values are listed for all structure types together with the  $TD_{10}$ , which was listed in the previous editions of the ATLAS, in Appendix C. There is a simple relationship between TD and  $TD_{10}$ :  $TD_{10} \sim TD *1155$ . Since  $TD_{10}$  is an approximation, i.e. it is 'arbitarily' terminated at N<sub>10</sub>, the values obtained by this formula deviate by 11% for –**CLO** and 5% for **FAU** but the differences are generally below 3%. It seem that for very open structures, 10 steps are not sufficient for a satifactory convergence. The correlation factor between the exact topological density TD and the framework density FD is 0.82.

#### Origin of 3-letter codes and type material names

The derivation of the 3-letter codes for the zeolite minerals is fairly obvious, because the code generally consists of the first 3 letters of the mineral name. For the synthetic materials this is sometimes more obscure. One reason for this is that numbers are frequently included to distinguish different products from a particular lab, and these numbers cannot be transferred directly to the framework code. To help the reader better understand the origin of the codes, a table that includes all framework type codes derived from synthetic type materials is given in Appendix D. In this table, the letters taken for the code are written in bold. Also, an attempt has been made to decipher the origin of the mnemonic sometimes used in the designations of these materials.

## Isotypic material index

All materials are listed in alphabetical order in this index. To make the index as informative as possible, all reported materials and designations have been included in this section, provided the framework type assignment appears to be reasonably well established. Even a number of occasionally used, but discredited, names of mineral species have been included for the same reason. A full list of obsolete and discredited zeolite mineral names can be found in a report of the subcommittee on zeolites of the International Mineralogical Association<sup>(17)</sup>. Moreover, the inclusion of a synthetic material's designation in this index must not be interpreted to mean that the designation has been formally recognized or generally accepted. References are to be found on the respective framework type data sheets.

## References

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# FRAMEWORK TYPE DATA SHEETS

(arranged by 3-letter code in alphabethical order)



framework viewed along [010]

Idealized cell constants:	orthorhombic, Imma, $a = 9.9$ Å, $b = 5.3$ Å, $c = 8.8$ Å										
Coordination sequences and vertex symbols:	T <sub>1</sub> (8, m) 4 10 21 36 54 78	3 106 136 173 214	4·6·4·6·6·8 <sub>2</sub>								
Secondary building units:	8 or 6 or 4										
Loop configuration of T-Atoms:											
Isotypic framework structures:	*Li-A (Barrer and White) <sup>(1-3)</sup> [Be-As-O]- $ABW^{(4,5)}$ [Be-P-O]- $ABW^{(4,6)}$ [Ga-Si-O]- $ABW^{(7)}$ [Zn-As-O]- $ABW^{(4)}$ [Zn-P-O]- $ABW^{(4)}$	Cs- [Al-Ti-O]- <b>ABW</b> <sup>(11)</sup>  Li- [Al-Si-O]- <b>ABW</b> <sup>(12)</sup>  Li- [Zn-P-O]- <b>ABW</b> <sup>(13)</sup>  Li- [Al-Ge-O]- <b>ABW</b> <sup>(14)</sup>  Na- [Co-P-O]- <b>ABW</b> <sup>(15)</sup>  Rb- [Co-P-O]- <b>ABW</b> <sup>(8)</sup>									

|Rb-|[Al-Si-O]-**ABW**<sup>(9,10)</sup>

|Tl-|[Al-Si-O]-**ABW**<sup>(16)</sup>

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|Cs-|[Mg-P-O]-**ABW**<sup>(8)</sup> |Cs-|[Al-Si-O]-**ABW**<sup>(9,10)</sup>

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3.4

Crystal chemical data:	$\begin{split} & \text{Li}_{4}^{+}(\text{H}_{2}\text{O})_{4}  \text{ [Al}_{4}\text{Si}_{4}\text{ O}_{16}\text{]-}\textbf{ABW}\\ &\text{orthorhombic, Pna2}_{1}\text{, }a=10.31\text{ Å, }b=8.18\text{ Å, }c=5.00\text{ Å}^{\ (2)}\\ &(\text{Relationship to unit cell of Framework Type: }a'=a\text{, }b'=c\text{, }c'=b) \end{split}$					
Framework density:	19 T/1000Å <sup>3</sup>					
Channels:	[001] <b>8</b> 3.4 x 3.8*					
3.8						

8-ring viewed along [001]

3.4

# **References (cont.):**

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framework viewed along [001]

Idealized cell constants:	cubic, $\text{Im}\overline{3}\text{m}$ , $a = 9.9\text{\AA}$				
Coordination sequences and vertex symbols:	$T_{1} (16, 3m) \ 4  9 \ 19 \ 35 \ 52 \ 72 \ 100 \ 131 \ 163 \ 201 \qquad 4 \cdot 8_{2} \cdot 4 \cdot 8_{2} \cdot 4 \cdot 8_{2}$				
Secondary building units:	4-4 or 4				
Loop configuration of T-Atoms:					
Isotypic framework	*ACP-1 <sup>(1)</sup>				

# **References:**

structures:

(1) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, **388**, 735-741 (1997)

Crystal chemical data:	$ (C_2H_{10}N_2^{2^+})_4 (H_2O)_2 $ [Al <sub>0.88</sub> Co <sub>7.12</sub> P <sub>8</sub> O <sub>32</sub> ]-ACO C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> = ethylenediamine tetragonal, I $\overline{4}2m$ , a = 10.240Å, c = 9.652Å <sup>(1)</sup>					
Framework density:	15.8 T/1000Å <sup>3</sup>					
Channels:	$<\!\!100\!\!> 8 \ 2.8 \ \mathrm{x} \ 3.5^{**} \leftrightarrow [001] \ 8 \ 3.5 \ \mathrm{x} \ 3.5^{*}$					



8-ring viewed along <100>



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 13.7$ Å, $b = 12.6$ Å, $c = 18.5$ Å												
Coordination sequences and vertex symbols:	$\begin{array}{l} T_1  (16, 1) \\ T_2  (16, 1) \\ T_3  (16, 1) \end{array}$	4 4 4	9 9 9	17 17 17	29 29 29	45 45 45	64 65 65	85 88 87	111 113 113	143 143 143	177 178 176		$\begin{array}{c} 4 \cdot 4 \cdot 4 \cdot 8 \cdot 6 \cdot 8 \\ 4 \cdot 4 \cdot 4 \cdot 8 \cdot 6 \cdot 8 \\ 4 \cdot 4 \cdot 4 \cdot 8 \cdot 6 \cdot 8 \end{array}$
Secondary building units:	6-6 or 4-2	or 6	5 0	r 4									
Loop configuration of T-Atoms:		Γ <sub>1-3</sub>											

Isotypic framework structures: \*AlPO-18<sup>(1)</sup>

# **References:**

(1) Simmen, A., McCusker, L.B., Baerlocher, Ch. and Meier, W.M. Zeolites, 11, 654-661 (1991)

# **Type Material**

Crystal chemical data:	[Al <sub>24</sub> P <sub>24</sub> O <sub>96</sub> ]- <b>AEI</b> monoclinic, C12/c1 $a = 13.711$ Å, $b = 12.732$ Å, $c = 18.571$ Å, $\beta = 90.01^{\circ (1)}$
Framework density:	14.8 T/1000Å <sup>3</sup>
Channels:	$\{[100] \ 8 \ 3.8 \ x \ 3.8 \leftrightarrow [110] \ 8 \ 3.8 \ x \ 3.8 \leftrightarrow [001] \ 8 \ 3.8 \ x \ 3.8\}^{***}$



8-ring viewed along [100]



8-ring viewed along [110]



8-ring viewed along [001]



framework viewed along [100]

Idealized cell constants:	orthorhombic	e, Im	ma,	a = 8	3.3Å,	, b =	: 18.	7Å, c	c = 1	3.4Å	
Coordination sequences and vertex symbols:	$\begin{array}{ccc} T_1  (16, 1) & 4 \\ T_2  (16, 1) & 4 \\ T_3  (8, m) & 4 \end{array}$	11 11 12	21 22 24	37 38 40	59 58 59	85 85 84	114 115 115	150 148 150	189 188 186	232 234 230	$\begin{array}{l} 4{\cdot}6_2{\cdot}6{\cdot}6_3{\cdot}6_2{\cdot}6_3\\ 4{\cdot}6_2{\cdot}6{\cdot}6_3{\cdot}6_2{\cdot}6_3\\ 6{\cdot}6_2{\cdot}6_2{\cdot}6_2{\cdot}6_2{\cdot}6_2{\cdot}6_2 \end{array}$
Secondary building units:	6-2										
Loop configuration of T-Atoms:					<b>T</b> <sub>3</sub>						
Isotypic framework	*AlPO-11 <sup>(1,2)</sup>	1									

\*AlPO-11<sup>(1,2)</sup> MnAPO-11<sup>(3)</sup> SAPO-11 plus numerous compositional variants<sup>(4,5)</sup>

#### **References:**

structures:

- (1) Bennett, J.M., Richardson Jr., J.W., Pluth, J.J. and Smith, J.V. Zeolites, 7, 160-162 (1987)
- (2) Richardson Jr., J.W., Pluth, J.J. and Smith, J.V. Acta Crystallogr., B44, 367-373 (1988)
- (3) Pluth, J.J., Smith, J.V. and Richardson Jr., J.W. J. Phys. Chem., 92, 2734-2738 (1988)
- (4) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)
- (5) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In *Proc. 7th Int. Zeolite Conf.*, (eds. Y. Murakami, A. Iijima and J.W. Ward), pp. 103-112 (1986), Kodansha, Tokyo

Crystal chemical data:	$ [Al_{20}P_{20} O_{80}] \text{-} \textbf{AEL} $ orthorhombic, Ibm2, a = 13.534Å, b = 18.482Å, c = 8.370Å <sup>(2)</sup> (Relationship to unit cell of Framework Type: a' = c, b' = b, c' = a )
Framework density:	19.1 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 4.0 x 6.5*
6.5	

10-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmca, $a = 18.5$ Å, $b = 13.4$ Å, $c = 9.6$ Å					
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					
Secondary building units:	8 or 4					
Loop configuration of T-Atoms:						
Isotypic framework structures:	*AlPO-EN3 <sup>(1)</sup> JDF-2 <sup>(5)</sup> [Ga-P-O]-AEN <sup>(2)</sup> MSC-1 <sup>(6)</sup> AlPO-53(A) <sup>(3)</sup> UiO-12-500 <sup>(7)</sup> AlPO-53(B) <sup>(3)</sup> UiO-12-as <sup>(7)</sup>					

# **References:**

- (1) Parise, J.B. Stud. Surf. Sci. Catal., 24, 271-278 (1985)
- (2) Glasser, F.P., Howie, R.A. and Kan, Q.B. Acta Crystallogr., C50, 848-850 (1994)

CFSAPO-1A(4)

- (3) Kirchner, R.M., Grosse-Kunstleve, R.W., Pluth, J.J., Wilson, S.T., Broach, R.W. and Smith, J.V. *Microporous and Mesoporous Materials*, **39**, 319-332 (2000)
- (4) He, H. and Long, Y. J. Incl. Phenom., 5, 591-599 (1987)
- (5) Chippindale, A.M., Powell, A.V., Jones, R.H., Thomas, J.M., Cheetham, A.K., Huo, Q.S. and Xu, R.R. *Acta Crystallogr.*, **C50**, 1537-1540 (1994)
- (6) Simmen, A. Ph.D. Thesis, ETH, Zürich, Switzerland, (1992)
- (7) Kongshaug, K.O., Fjellvåg, H., Klewe, B. and Lillerud, K.P. *Microporous and Mesoporous Materials*, **39**, 333-339 (2000)

# **Type Material**

# AEN

Crystal chemical data:	$\begin{split}  (C_2H_8N_2)_4 \ (H_2O)_{16}  \ [Al_{24}P_{24} \ O_{96}]\text{-}AEN \\ C_2H_8N_2 &= ethylenediamine \\ orthorhombic, \ P2_12_12_1, \ a &= 10.292 \ \text{\AA}, \ b &= 13.636 \text{\AA}, \ c &= 17.344 \ \text{\AA}^{(1)} \\ (\text{Relationship to unit cell of Framework Type: }a' &= c, \ b' &= b, \ c' &= a) \end{split}$
Framework density:	19.7 T/1000Å <sup>3</sup>
Channels:	$[100] 8 3.1 x 4.3^* \leftrightarrow [010] 8 2.7 x 5.0^*$



8-ring viewed along [100]



8-ring viewed along [010]



- (1) Dessau, R.M., Schlenker, J.L. and Higgins, J.B. Zeolites, 10, 522-524 (1990)
- (2) Richardson Jr., J.W. and Vogt, E.T.C. Zeolites, **12**, 13-19 (1992)
- (3) Chu, C.T.W., Schlenker, J.L., Lutner, J.D. and Chang, C.D. U.S. Patent 5,091,073 (1992)
14-ring viewed along [001]

7.9

Crystal chemical data:	$[Al_{36}P_{36} O_{144}]-AET$ orthorhombic, Cmc2 <sub>1</sub> , a = 33.29Å, b = 14.76Å, c = 8.257Å <sup>(1)</sup>
Framework density:	17.7 T/1000Å <sup>3</sup>
Channels:	[001] <b>14</b> 7.9 x 8.7*
8.7	

7.9



- (1) Bariand, P., Cesbron, F. and Giraud, R. Bull. Soc. fr. Minéral. Cristallogr., 91, 34-42 (1968)
- (2) Merlino, S. and Mellini, M. Zeolite 1976, Program and Abstracts, Tucson, (1976)
- Pobedimskaya, E.A., Rastsvetaeva, R.k., Terenteva, L.E. and Saposhnikov, A.N. Dokl. Akad. Nauk SSSR, 320, 882-886 (1991)
- (4) Ballirano, P., Merlino, S., Bonaccorsi, E. and Maras, A. Eur. J. Mineral., 9, 21-31 (1997)

Afghanite

# **Type Material**

Α	FG
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Crystal chemical data:	$ Ca^{2+}_{9.8}Na^{+}_{22}Cl^{-}_{2}SO_{4}^{2-}_{5.3}CO_{3}^{2-}(H_{2}O)_{4}  [Al_{24}Si_{24}O_{96}]-AFG$ hexagonal , P6 <sub>3</sub> mc, a = 12.761Å, c = 21.416Å <sup>(3)</sup>
Framework density:	15.9 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [001] (bottom left: projection down [001])

Idealized cell constants:	hexagonal, P6/mcc, a = 13.8Å, c = $8.6Å$					
Coordination sequences and vertex symbols:	$T_{1}(24, 1)  4  11  21  35  53  77  105  137  172  212 \qquad \qquad 4 \cdot 6_{2} \cdot 6 \cdot 6_{3} \cdot 6_{2} \cdot 6_{3}$					
Secondary building units:	6 or 4					
Loop configuration of T-Atoms:						
Isotypic framework structures:	*AIPO-5 <sup>(1)</sup> CoAPO-5 <sup>(2)</sup> CrAPO-5 <sup>(3)</sup> SAPO-5 and numerous compositional variants <sup>(4,5)</sup> SSZ-24 <sup>(6)</sup> TPAF AIPO-5 <sup>(7)</sup>					

- (1) Bennett, J.M., Cohen, J.P., Flanigen, E.M., Pluth, J.J. and Smith, J.V. ACS Sym. Ser., 218, 109-118 (1983)
- (2) Chao, K.J., Sheu, S.P. and Sheu, H.S. J. Chem. Soc., Faraday Trans., 88, 2949-2954 (1992)
- (3) Radaev, S., Joswig, W. and Baur, W.H. J. Mater. Chem., 6, 1413-1418 (1996)
- (4) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)
- (5) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In Proc. 7th Int. Zeolite Conf., (eds. Y.
- Murakami, A. Iijima and J.W. Ward), pp. 103-112 (1986), Kodansha, Tokyo
- (6) Bialek, R., Meier, W.M., Davis, M. and Annen, M.J. *Zeolites*, **11**, 438-442 (1991)
- (7) Qiu, S., Pang, W., Kessler, H. and Guth, J.L. Zeolites, 9, 440-444 (1989)

Crystal chemical data:	$\begin{split}  (C_{12}H_{28}N^{+}) (OH^{-}) (H_{2}O)_{x}   [Al_{12}P_{12} O_{48}] - AFI \\ C_{12}H_{28}N^{+} &= tetrapropylammonium \\ hexagonal, P6cc, a &= 13.726\text{\AA}, c = 8.484\text{\AA}^{(1)} \end{split}$
Framework density:	17.3 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 7.3 x 7.3*



12-ring viewed along [001]



framework viewed normal to [010]

Idealized cell constants:	monoclinic,	C12/	m1,	<b>a</b> = 1	14.0Å	Å, b	= 13	.5Å,	c =	10.2Å,	$\beta = 10^{\circ}$	7.2°
Coordination sequences and vertex symbols:	$\begin{array}{l} T_1  (8, 1) \\ T_2  (8, 1) \\ T_3  (8, 1) \\ T_4  (8, 1) \end{array}$	4 9 4 9 4 9 4 10	19 18 17 21	33 31 30 35	51 49 49 50	76 72 75 71	98 99 102 100	123 130 125 132	162 160 157 164	203 198 202 198		$\begin{array}{c} 4{\cdot}4{\cdot}4{\cdot}8_{2}{\cdot}6{\cdot}8_{4}\\ 4{\cdot}4{\cdot}4{\cdot}8_{2}{\cdot}6{\cdot}6_{2}\\ 4{\cdot}6{\cdot}4{\cdot}8{\cdot}4{\cdot}8_{7}\\ 4{\cdot}4{\cdot}6{\cdot}8{\cdot}8{\cdot}8_{2}\end{array}$
Secondary building units:	4											
Loop configuration of T-Atoms:		,2			T <sub>3</sub>			 	- 4			
Isotypic framework structures:	*AlPO-14 <sup>(1)</sup> GaPO-14 <sup>(2)</sup>											

- (1) Broach, R.W., Wilson, S.T. and Kirchner, R.M. In *Proc. 12th Int. Zeolite Conf.*, (eds. M.M.J. Treacy, B.K. Marcus, M.E. Bisher and J.B. Higgins), pp. 1715-1722 (1999), MRS, Warrendale, PA
- (2) Parise, J.B. Acta Crystallogr., C42, 670-673 (1986)

Crystal chemical data:	
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$[Al_8P_8 O_{32}]-AFN$
triclinic, $P\overline{1}$ , $a = 9.704$ Å, $b = 9.736$ Å, $c = 10.202$ Å
$\alpha = 77.81^{\circ}, \beta = 77.50^{\circ}, \gamma = 87.69^{\circ}$ <sup>(1)</sup>

Framework density: 17.4 T/1000Å<sup>3</sup>

Channels:

 $\texttt{[100] 8 1.9 x 4.6*} \leftrightarrow \texttt{[010] 8 2.1 x 4.9*} \leftrightarrow \texttt{[001] 8 3.3 x 4.0*}$ 





8-ring viewed along [100]



8-ring viewed along [010]



8-ring viewed along [001]

AFO



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 9.8$ Å, $b = 25.6$ Å, $c = 8.3$ Å	
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$5_{3} \cdot 6_{2} \cdot 6_{3}$ $\cdot 6_{3} \cdot 6 \cdot 6_{3}$ $6_{3} \cdot 6_{2} \cdot 6_{3}$ $6_{2} \cdot 6_{2} \cdot 6_{2}$
Secondary building units:	2-6-2 or 4-1	
Loop configuration of T-Atoms:	T <sub>1-3</sub> T <sub>4</sub>	
Isotypic framework structures:	*AlPO-41 <sup>(1)</sup>	

### **References:**

(1) Kirchner, R.M. and Bennett, J.M. Zeolites, 14, 523-528 (1994)

Crystal chemical data:	[Al <sub>10</sub> P <sub>10</sub> O <sub>40</sub> ]- <b>AFO</b> monoclinic, P112 <sub>1</sub> , a = 9.718Å, b = 13.792Å, c = 8.359Å, $\gamma$ = 110.6° <sup>(1)</sup> (Relationship to unit cell of Framework Type: a' = a, b' = b·sin( $\gamma$ )/2, c' = c or, as vectors, <b>a'</b> = <b>a</b> , <b>b'</b> = ( <b>b</b> - <b>a</b> )/2, <b>c'</b> = <b>c</b> )
Framework density:	19.1 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 4.3 x 7.0*



10-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhom	oic,	Pm	mn	(orig	gin cl	hoice	e 2),	a = 1	22.3	Å, b =	= 13.6Å, c = 7.0Å
<b>Coordination sequences</b>	T <sub>1</sub> (8, 1)	4	9	16	27	43	63	88	115	141	171	4.6.4.62.4.8
and vertex symbols:	T <sub>2</sub> (8, 1)	4	9	18	30	43	64	90	111	140	181	4·4·4·8·6 <sub>3</sub> ·8
	T <sub>3</sub> (8, 1)	4	9	18	29	42	66	93	112	139	177	4.4.4.12.6.6
	T <sub>4</sub> (8, 1)	4	10	17	28	47	65	86	117	144	169	4.6.4.6.6.12
Secondary building units:	6-2 or 4											
Loop configuration of T-Atoms:		- 1	Ē			T <sub>2-3</sub>		+	 T	4		
Isotypic framework structures:	*SAPO-40 AlPO-40 <sup>(4)</sup> CoAPSO-4 ZnAPSO-4	(1-3) $0^{(5)}$ $0^{(5)}$	)									

- (1) Estermann, M.A., McCusker, L.B. and Baerlocher, Ch. J. Appl. Crystallogr., 25, 539-543 (1992)
- (2) Dumont, N., Gabelica, Z., Derouane, E.G. and McCusker, L.B. Microporous Materials, 1, 149-160 (1993)
- (3) McCusker, L.B. and Baerlocher, Ch. Microporous Materials, 6, 51-54 (1996)
- (4) Ramaswamy, V., McCusker, L.B. and Baerlocher, Ch. *Microporous and Mesoporous Materials*, **31**, 1-8 (1999)
- (5) Lourenco, J.P., Ribeiro, M.F., Borges, C., Rocha, J., Onida, B., Garrone, E. and Gabelica, Z., **38**, 267-278 (2000)

# **Type Material**

# AFR

Crystal chemical data:	$\begin{split}  (C_{12}H_{28}N^{+})_{4} (OH)^{-}_{4}  \ [Si_{8}Al_{28}P_{28} \ O_{128}] \textbf{-AFR} \\ C_{12}H_{28}N^{+} &= tetra propylammonium \\ orthorhombic, \ Pccn, \ a &= 21.944 \text{\AA}, \ b &= 13.691 \text{\AA}, \ c &= 14.249 \text{\AA}^{(3)} \\ (\text{Relationship to unit cell of Framework Type: }a' &= a, \ b' &= b, \ c' &= 2c) \end{split}$
Framework density:	15.0 T/1000Å <sup>3</sup>
Channels:	$[001] \ 12 \ 6.7 \ \mathbf{x} \ 6.9^* \leftrightarrow [010] \ 8 \ 3.7 \ \mathbf{x} \ 3.7^*$



12-ring viewed along [001]



8-ring viewed along [010]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal,	P6	<sub>3</sub> /m	cm,	a = 1	13.1	Å, c =	= 25	.9Å			
Coordination sequences and vertex symbols:	$\begin{array}{l} T_1 (24,1) \\ T_2 (24,1) \\ T_3 (8,3) \end{array}$	4 4 4	9 9 9	17 16 18	28 25 30	42 39 43	60 61 62	83 86 85	111 109 105	138 134 135	166 163 180	$\begin{array}{c} 4{\cdot}4{\cdot}4{\cdot}8_{2}{\cdot}6_{2}{\cdot}8\\ 4{\cdot}4{\cdot}4{\cdot}6{\cdot}6{\cdot}12\\ 4{\cdot}8{\cdot}4{\cdot}8{\cdot}4{\cdot}8\end{array}$
Secondary building units:	6*1											
Loop configuration of T-Atoms:		Γ <sub>1,2</sub>		/		T <sub>3</sub>						
Isotypic framework structures:	*MAPSO-	46 <sup>(1</sup>	)									

(1) Bennett, J.M. and Marcus, B.K. Stud. Surf. Sci. Catal., 37, 269-279 (1988)

Crystal chemical data:	$\begin{split}  (C_6H_{16}N^+)_8 \ (H_2O)_{14}  \ [Mg_6Al_{22}P_{26}Si_2 \ O_{112}]\text{-}AFS \\ C_6H_{15}N = dipropylamine \\ trigonal, P3c1, a = 13.225\text{\AA}, c = 26.892\text{\AA}^{(1)} \end{split}$
Framework density:	13.7 T/1000Å <sup>3</sup>

Channels:

 $[001] \ \textbf{12} \ 7.0 \ge 7.0^* \leftrightarrow \bot [001] \ \textbf{8} \ 4.0 \ge 4.0^{**}$ 



12-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal,	P6 <sub>3</sub>	/m	mc,	a = 1	13.7Å	Å, c =	= 29	.4Å			
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1 (24,1) \\ T_2 (24,1) \\ T_3 (24,1) \end{array}$	4 4 4	9 9 9	17 17 17	29 29 29	45 45 45	64 64 65	85 86 88	110 113 113	140 144 141	173 178 175	4·4·4·8·6·8 4·4·4·8·6·8 4·4·4·8·6·8
Secondary building units:	6-6 or 6 c	or 4										
Loop configuration of T-Atoms:		- 1-3										
Framework description:	AABBCCA	AAC	CE	BB s	seque	ence	of 6-	ring	;S			
Isotypic framework structures:	*AlPO-52 <sup>(1</sup>	1,2)										

- (1) Bennett, J.M., Kirchner, R.M. and Wilson, S.T. Stud. Surf. Sci. Catal., 49, 731-739 (1989)
- (2) McGuire, N.K., Bateman, C.A., Blackwell, C.S., Wilson, S.T. and Kirchner, R.M. Zeolites, 15, 460-469 (1995)

Crystal	chemical	data:
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 $[Al_{36}P_{36} O_{144}] \text{-} \textbf{AFT} \\ trigonal, P\overline{3}1c, a = 13.715\text{\AA}, c = 29.676\text{\AA}^{~(2)}$ 

Framework density: 14.9 T/1000Å<sup>3</sup>

Channels:

 $\perp$  [001] **8** 3.2 x 3.8\*\*\*



GME cage 8-ring viewed normal to [001]



CHA cage 8-ring viewed normal to [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, $P6_3$ /mmc, a = 13.7Å, c = 19.7Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-6 or 6 or 4
Loop configuration of T-Atoms:	
Framework description:	AABBCCBB sequence of 6-rings
Isotypic framework structures:	*SAPO-56 <sup>(1)</sup> SSZ-16 <sup>(2)</sup>

- (1) Wilson, S.T., Broach, R.W., Blackwell, C.S., Bateman, C.A., McGuire, N.K. and Kirchner, R.M. *Microporous and Mesoporous Materials*, **28**, 125-137 (1999)
- (2) Lobo, R.F., Zones, S.I. and Medrud, R.C. Chem. Mater., 8, 2409-2411 (1996)

AFX
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Crystal chemical data:	$ H_{3}^{+} [Al_{23}Si_{5}P_{20} O_{96}]-AFX$
	trigonal, $P\overline{3}1c$ , a = 13.762Å, c = 19.949Å <sup>(2)</sup>

Framework density: 14.7 T/1000Å<sup>3</sup>

Channels:

⊥[001] **8** 3.4 x 3.6\*\*\*



8-ring viewed normal to [001]



framework viewed along [001] (bottom left: projection down [001])

Idealized cell constants:	trigonal, P3	<u>3</u> 1m	, a	= 12	2.3Å	, c =	8.6Å	1					
Coordination sequences and vertex symbols:	$T_1 (12, 1) T_2 (4, 3)$	4 4	8 9	14 16	25 23	39 34	53 57	71 82	96 98	124 115	152 141	4	4·4·8·4·12 4·8·4·8·4·8
Secondary building units:	4-4 or 4												
Loop configuration of T-Atoms:		1				T <sub>2</sub>							

Isotypic framework structures:

\*CoAPO-50<sup>(1,2)</sup> MgAPO-50<sup>(3)</sup>

- (1) Wilson, S.T. private communication
- (2) Bennett, J.M. and Marcus, B.K. Stud. Surf. Sci. Catal., 37, 269-279 (1988)
- (3) Akolekar, D.B. Zeolites, **15**, 583-590 (1995)

Crystal chemical data:	$ (C_6H_{16}N^+)_3 (H_2O)_7 $ [Co <sub>3</sub> Al <sub>5</sub> P <sub>8</sub> O <sub>32</sub> ]- <b>AFY</b> C <sub>6</sub> H <sub>15</sub> N = dipropylamine trigonal, P3, a = 12.747Å, c = 9.015Å <sup>(2)</sup>
Framework density:	12.6 T/1000Å <sup>3</sup>
Channels:	$[001] \ 12 \ 6.1 \ \mathbf{x} \ 6.1^* \leftrightarrow \perp [001] \ 8 \ 4.0 \ \mathbf{x} \ 4.3^{**}$
Stability:	Unstable to removal of template <sup>(1)</sup>



12-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 15.8$ Å, $b = 9.2$ Å, $c = 8.6$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4-2
Loop configuration of T-Atoms:	$- \prod_{T_1} \prod_{T_2}$
Isotypic framework structures:	*AlPO-H2 <sup>(1-2)</sup>

- (1) Li, H.X., Davis, M.E., Higgins, J.B. and Dessau, R.M. Chem. Commun., 403-405 (1993)
- (2) Kennedy, G.J., Higgins, J.B., Ridenour, C.F., Li, H.X. and Davis, M.E. Solid State Nucl. Mag. Res., 4, 173-178 (1995)

Crystal chemical data:	$ (H_2O)_8 $ [Al <sub>6</sub> P <sub>6</sub> O <sub>24</sub> ]- <b>AHT</b> monoclinic, P112 <sub>1</sub> , a = 9.486Å, b = 9.914Å, c = 8.126Å, $\gamma$ = 121.49° <sup>(1)</sup> (Relationship to unit cell of Framework Type: a'= a/2 sin( $\gamma$ ), b' = b, c' = c or, as vectors, <b>a'</b> = ( <b>a</b> - <b>b</b> )/2, <b>b'</b> = <b>b</b> , <b>c'</b> = <b>c</b> )
Framework density:	18.4 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 3.3 x 6.8*
Stability:	Transforms to AlPO <sub>4</sub> -tridymite on heating <sup>(2)</sup>



10-ring viewed along [001]



- (1) Taylor, W.H. Z. Kristallogr., 74, 1-19 (1930)
- (2) Knowles, C.R., Rinaldi, F.F. and Smith, J.V. Indian Mineral., 6, 127-(1965)
- (3) Ferraris, G., Jones, D.W. and Yerkess, J. Z. Kristallogr., 135, 240-252 (1972)
- (4) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
- (5) Artioli, G., Pluth, J.J. and Smith, J.V. Acta Crystallogr., C40, 214-217 (1984)
- (6) Bu, X., Feng, P., Gier, T.E., Zhao, D. and Stucky, G.D. J. Am. Chem. Soc., 120, 13389-13397 (1998)

Crystal chemical data:

 $|Na_{16}^{+}(H_2O)_{16}|$  [Al<sub>16</sub>Si<sub>32</sub> O<sub>96</sub>]-ANA cubic, Ia3d, a = 13.73Å <sup>(3)</sup>

Framework density:

Channels: irregular channels formed by highly distorted 8-rings

18.5 T/1000Å<sup>3</sup>





distorted 8-ring viewed along [110]

#### **References (cont.):**

- (7) Yelon, W.B., Xie, D., Newsam, J.M. and Dunn, J. Zeolites, 10, 553-558 (1990)
- (8) Heinrich, A.R. and Baerlocher, Ch. Acta Crystallogr., C47, 237-241 (1991)
- (9) Millini, R., Montanari, L. and Bellussi, G. Microporous Materials, 1, 9-15 (1993)
- (10) Wilson, S.T., Lok, B.M., Messina, C.A., Cannan, T.R. and Flanigen, E.M. J. Am. Chem. Soc., 104, 1146-1147 (1982)
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- (13) Ames, L.L. and Sand, L.B. Am. Mineral., 43, 476-480 (1958)
- (14) Torres-Martines, L.M., Gard, J.A., Howie, R.A. and West, A.R. J. Solid State Chem., 51, 100-103 (1984)
- (15) Kopp, O.C., Harris, L.A., Clark, G.W. and Yakel, H.L. Am. Mineral., 48, 100-109 (1963)
- (16) Wen-Hui, H., Saho-Hua, T., Kung-Hai, W., Chun-Lin, C. and Cheng Chi, Y. *Am. Mineral.*, **44**, 1327-1328 (1959)
- (17) McConnell, D. and Foreman Jr., D.W. Can. Mines, 12, 352- (1974)
- (18) Peacor, D.R. Z. Kristallogr., 127, 213-224 (1968)
- (19) Barrer, R.M. and White, E.A.D. J. Chem. Soc., 1561-1571 (1952)
- (20) Nel, H.J. Am. Mineral., 29, 443-451 (1944)
- (21) Ghobarkar, H. and Franke, W. Cryst. Res. Technol., 1071-1075 (1986)
- (22) Ghobarkar, H., Schaef, O. and Knauth, Pl Annal. Chimie, Science Matériaux, 24, 209-215 (1999)
- (23) Ghobarkar, H. Cryst. Res. Technol., K90-92 (1985)
- (24) Takeuchi, Y., Mazzi, F., Haga, N. and Galli, E. Am. Mineral., 64, 993-1001 (1979)



Loop configuration of T-Atoms:

$\Gamma_2$

Isotypic framework structures: \*AlPO-C<sup>(1,2)</sup> AlPO-H3<sup>(3)</sup>

- (1) Bennett, J.M., Dytrych, W.J., Pluth, J.J., Richardson Jr., J.W. and Smith, J.V. Zeolites, 6, 349-359 (1986)
- (2) Keller, E.B., Meier, W.M. and Kirchner, R.M. Solid State Ionics, 43, 93-102 (1990)
- (3) Pluth, J.J. and Smith, J.V. Acta Crystallogr., C42, 1118-1120 (1986)

# **Type Material**

Crystal chemical data:	$\begin{split} & [Al_{16}P_{16} \ O_{64}]\text{-}\textbf{APC} \\ & \text{orthorhombic, Pbca, } a = 19.821 \text{ Å, } b = 10.028 \text{ Å, } c = 8.936 \text{ Å}^{~(2)} \\ & (\text{Relationship to unit cell of Framework Type: } a'= b, b'= c, c'=a) \end{split}$
Framework density:	18.0 T/1000Å <sup>3</sup>
Channels:	$[001]  8  3.4 \ge 3.7^* \leftrightarrow [100]  8  2.0 \ge 4.7^*$
Stability:	Transforms to AlPO <sub>4</sub> -D at ca 250°C $^{(2)}$





8-ring viewed along [001]



distorted 8-ring viewed along [100]



framework viewed along [100]

Idealized cell constants:	orthorhombic, Cmca, $a = 8.7$ Å, $b = 20.1$ Å, $c = 10.2$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	8 or 6-2 or 4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*AlPO-D <sup>(1)</sup>

(1) Keller, E.B., Meier, W.M. and Kirchner, R.M. Solid State Ionics, 43, 93-102 (1990)

# **Type Material**

Crystal chemical data:	[Al <sub>16</sub> P <sub>16</sub> O <sub>64</sub> ]- <b>APD</b> (forms irreversibly from AlPO <sub>4</sub> -C at around 200°C) orthorhombic, Pca2 <sub>1</sub> , a = 19.187Å, b = 8.576Å, c = 9.804Å <sup>(1)</sup> (Relationship to unit cell of Framework Type: a' = b, b' = a, c' = c)
Framework density:	19.8 T/1000Å <sup>3</sup>
Channels:	$[010] 8 2.3 x 6.0^* \leftrightarrow [201] 8 1.3 x 5.8^*$



distorted 8-ring viewed along [010]



distorted 8-ring along [201]



framework viewed along [100]

Idealized cell constants:	cubic, $Fm\overline{3}m$ , $a = 13.6$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$
Secondary building units:	4-1
Loop configuration of T-Atoms:	$\begin{array}{c c} & & \\ \hline & \\ \hline & \\ T_1 \end{array} \end{array} \begin{array}{c} & \\ T_2 \end{array}$
Framework description:	structural derivative of fluorite
Isotypic framework	*AlPO-16 <sup>(1)</sup>

**References:** 

structures:

(1) Bennett, J.M. and Kirchner, R.M. Zeolites, **11**, 502-506 (1991)

 $Octade casil^{(2)} \\$ 

(2) Caullet, P., Guth, J.L., Hazm, J., Lamblin, J.M. and Gies, H. *Eur. J. Solid State Inorg. Chem.*, **28**, 345-361 (1991)

Crystal chemical data:	$ (C_7H_{13}N)_4 (H_2O)_{16} $ [Al <sub>20</sub> P <sub>20</sub> O <sub>80</sub> ]-AST C <sub>7</sub> H <sub>13</sub> N = quinuclidine cubic, F23, a = 13.383Å <sup>(1)</sup>
Framework density:	16.7 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [001]

Idealized cell constants:	tetragonal, P4/mcc, $a = 8.7$ Å, $c = 13.9$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4-1
Loop configuration of T-Atoms:	$\begin{array}{c c} & & \\ \hline \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ &$
Isotypic framework structures:	*ASU-7 <sup>(1)</sup>

(1) Li, H. and Yaghi, O.M. J. Am. Chem. Soc., 120, 10569-10570 (1998)

Crystal chemical data:	$ (C_2H_7N)_2 (H_2O)_2 $ [Ge <sub>20</sub> O <sub>40</sub> ]-ASV C <sub>2</sub> H <sub>7</sub> N = dimethylamine tetragonal, P4/mcc, a = 8.780Å, c = 14.470Å <sup>(1)</sup>
Framework density:	17.9 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 4.1x 4.1*



12-ring along [001]



framework viewed along [001]

Idealized cell constants:	tetragonal, I4/mmm, a = 13.1Å, c = $5.3$ Å
Coordination sequences and vertex symbols:	$T_{1} (16, m)  4  10  21  36  54  78  106  136  173  214 \qquad \qquad 4 \cdot 6 \cdot 4 \cdot 6 \cdot 6 \cdot 8$
Secondary building units:	8 or 4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*MAPO-39 <sup>(1,2)</sup>

- (1) McCusker, L.B., Brunner, G.O. and Ojo, A.F. Acta Crystallogr., A46, C59 (1990)
- (2) Baur, W.H., Joswig, W., Kassner, D., Bieniok, A., Finger, G. and Kornatowski, J. Z. Kristallogr., 214, 154-159 (1999)

Crystal chemical data:	$ H_{n}^{+} $ [Mg <sub>n</sub> Al <sub>8-n</sub> P <sub>8</sub> O <sub>32</sub> ]-ATN tetragonal, I4/m, a = 13.209Å, c = 5.277Å <sup>(2)</sup>
Framework density:	18.0 T/1000Å <sup>3</sup>

Framework density:

Channels:

[001] **8** 4.0 x 4.0\*



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	trigonal, $R\overline{3}m$ , $a = 20.9$ Å, $c = 5.1$ Å
Coordination sequences and vertex symbols:	$T_{1}(36, 1)  4  11  22  37  59  85  114  147  184  230 \qquad \qquad 4 \cdot 6_{2} \cdot 6 \cdot 6_{2} \cdot 6 \cdot 6_{3}$
Secondary building units:	6 or 4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*AIPO-31 <sup>(1,2)</sup> SAPO-31 <sup>(3-5)</sup>

- (1) Bennett, J.M. and Kirchner, R.M. Zeolites, 12, 338-342 (1992)
- (2) Baur, W.H., Joswig, W., Kassner, D. and Kornatowski, J. Acta Crystallogr., B50, 290-294 (1994)
- (3) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)
- (4) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In *Proc. 7th Int. Zeolite Conf.*, (ed. eds. Y. Murakami, A. Iijima and J.W. Ward ), pp. pp. 103-112 (1986), Kodansha, Tokyo
- (5) Baur, W.H., Joswig, W., Kassner, D. and Kornatowski, J. Acta Crystallogr., B50, 290-294 (1994)

Crystal chemical data:	$[Al_{18}P_{18} O_{72}]$ - <b>ATO</b> trigonal, R $\overline{3}$ , a = 20.827Å, c = 5.003Å <sup>(1)</sup>
Framework density:	19.2 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 5.4 x 5.4*



12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, a = 13.2Å, b = 21.6Å, c = $5.3$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2 or 4-2 or 6 or 4
Loop configuration of T-Atoms:	T <sub>1-3</sub>
Isotypic framework	*MAPO-36 <sup>(1)</sup>

structures:

(1) Smith, J.V., Pluth, J.J. and Andries, K.J. Zeolites, 13, 166-169 (1993)
Crystal chemical data:	H <sup>+</sup>   [MgAl <sub>11</sub> P <sub>12</sub> O <sub>48</sub> ]- <b>ATS</b> monoclinic, C12/c1 $a = 13.148$ Å, $b = 21.577$ Å, $c = 5.164$ Å, $\beta = 91.84^{\circ}$	(1)
Framework density:	16.4 T/1000Å <sup>3</sup>	
Channels:	[001] <b>12</b> 6.5 x 7.5*	



12-ring viewed along [001]



framework viewed along [010]

Idealized cell constants:	orthorhombic, Pmma, $a = 10.0$ Å, $b = 7.5$ Å, $c = 9.4$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2 or 4-2 or 4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*AlPO-12-TAMU <sup>(1)</sup> AlPO-33 <sup>(2,3)</sup>

- (1) Rudolf, P.R., Saldarriaga-Molina, C. and Clearfield, A. J. Phys. Chem., 90, 6122-6125 (1986)
- (2) Smith, J.V., Pluth, J.J. and Bennett, J.M. private communication
- (3) Patton, R.L. and Gajek, R.T. U.S. Patent 4,473,663 (1984)

Crystal chemical data:	$ (C_4H_{12}N^+)_4 (OH)_4^-  [Al_{12}P_{12} O_{48}]$ - <b>ATT</b> $C_4H_{12}N^+ =$ tetramethylammonium orthorhombic, P2 <sub>1</sub> 2 <sub>1</sub> 2, a = 10.332Å, b = 14.640Å, c = 9.511Å <sup>(1)</sup> (Relationship to unit cell of Framework Type: a' = a, b' = 2b, c' = c)
Framework density:	16.7 T/1000Å <sup>3</sup>
Channels:	$[100] 8 4.2 \text{ x } 4.6^* \leftrightarrow [010] 8 3.8 \text{ x } 3.8^*$



8-ring viewed along [100]



complex 8-ring viewed along [010]



framework viewed along [100]

Idealized cell constants:	orthorhombic, Cmma, $a = 8.6$ Å, $b = 15.3$ Å, $c = 9.7$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4
Loop configuration of T-Atoms:	$T_1$ $T_2$
Isotynic framework	*Δ1PO-25 <sup>(1)</sup>

Isotypic framework \*AlPO-25<sup>(1)</sup> structures: [Ga-P-O]-ATV<sup>(2)</sup>

- (1) Richardson Jr., J.W., Smith, J.V. and Pluth, J.J. J. Phys. Chem., 94, 3365-3367 (1990)
- (2) Parise, J.B. Chem. Commun., 606-607 (1985)

# ATV

Crystal chemical data:	$ [Al_{12}P_{12} O_{48}] \text{-} \mathbf{ATV} $ orthorhombic, Acmm, a = 9.449Å, b = 15.203Å, c = 8.408Å <sup>(1)</sup> (Relationship to unit cell of Framework Type: a' = c, b' = b, c' = a)
Framework density:	19.9 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 3.0 x 4.9*
4.9	

8-ring viewed along [001]



framework viewed along [100]

Idealized cell constants:	orthorhombic,	, Cmca, $a = 9.1$	Å, $b = 15.0$ Å, $c = 19.2$ Å	
Coordination sequences and vertex symbols:	$\begin{array}{rrrr} T_1  (16, 1) & 4 \\ T_2  (16, 1) & 4 \\ T_3  (16, 1) & 4 \end{array}$	10203555102136539193554	781031331732177610814217321076102134172214	$\begin{array}{c} 4{\cdot}6_{2}{\cdot}4{\cdot}8_{3}{\cdot}6{\cdot}8_{2}\\ 4{\cdot}6{\cdot}4{\cdot}8_{2}{\cdot}6{\cdot}8\\ 4{\cdot}4{\cdot}4{\cdot}6{\cdot}8{\cdot}8_{3}\end{array}$
Secondary building units:	6			
Loop configuration of T-Atoms:	T <sub>1,2</sub>			

Isotypic framework structures: \*AlPO- $21^{(1,2)}$ [Ga-P-O]-AWO<sup>(3)</sup>

- (1) Bennett, J.M., Cohen, J.M., Artioli, G., Pluth, J.J. and Smith, J.V. Inorg. Chem., 24, 188-193 (1985)
- (2) Parise, J.B. and Day, C.S. Acta Crystallogr., C41, 515-520 (1985)
- (3) Parise, J.B. Chem. Commun., 606-607 (1985)

# AWO

Crystal chemical data:	$\begin{split}  H_{4}^{+}(C_{2}H_{7}N)_{10.66} & (C_{3}H_{8})_{5.33} & (OH)_{4}^{-}  [Al_{12}P_{12} O_{48}] \text{-AWO} \\ C_{2}H_{7}N &= \text{dimethylamine} , C_{3}H_{8} = \text{propane} \\ \text{monoclinic, } P12_{1}/a1 \\ a &= 10.330\text{\AA}, b = 17.524\text{\AA}, c = 8.676\text{\AA}, \beta = 123.37^{\circ (1)} \\ (\text{Relationship to unit cell of Framework Type:} \\ a' &= a, b' = c, c' = b/2\sin(\beta) \\ \text{or, as vectors, } a' &= a, b' = c, c' = (b - a)/2 ) \end{split}$
Framework density:	18.3 T/1000Å <sup>3</sup>
Channels:	[100] <b>8</b> 2.7 x 5.5*
Stability:	Transforms to AlPO-25 (ATV) upon calcination <sup>(2)</sup>







framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	tetragonal,	P4	/nm	m (o	origi	n cho	oice 2	2), a	= 13	3.6Å	$c = 7.6 \text{\AA}$	
Coordination sequences and vertex symbols:	T <sub>1</sub> (16, 1) T <sub>2</sub> (8, 2)	4 4	10 9	20 17	33 30	50 50	72 74	98 97	128 123	162 158	200 198	4·4·6·6·6·8 4·4·4·6·6·6
Secondary building units:	6 or 4											
Loop configuration of T-Atoms:		Г <sub>1</sub>	[			] T <sub>2</sub>						
	* 100 22	1)										

Isotypic framework structures: \*AlPO-22

#### **References:**

(1) Richardson Jr., J.W., Pluth, J.J. and Smith, J.V. Naturwiss., 76, 467-469 (1989)

# AWW

Crystal chemical data:	$\begin{split}  (C_{7}H_{14}N^{+})_{4} \ (HPO_{4}^{\ 2^{-}})_{2}  \ [Al_{24}P_{24} \ O_{96}]\text{-}AWW \\ C_{7}H_{13}N = quinuclidine \\ tetragonal, \ P4/ncc, \ a = 13.628\text{\AA}, \ c = 15.463\text{\AA}^{\ (1)} \\ (\text{Relationship to unit cell of Framework Type: }a'=a, \ b'=b, \ c'=2c) \end{split}$
Framework density:	16.7 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 3.9 x 3.9*



8-ring viewed along [001]



framework viewed along [010]

Idealized cell constants:	tetragonal,	P4	122 <b>,</b>	a =	12.6	5Å, c	c = 26.2Å	L			
Coordination sequences	T <sub>1</sub> (8, 1)	4	10	19	32	51	77 105	133	167	207	$4 \cdot 5 \cdot 4 \cdot 12_3 \cdot 5 \cdot 5$
and vertex symbols:	$T_2(8, 1)$	4	10	19	32	51	75 102	133	170	208	$4 \cdot 5 \cdot 4 \cdot 12_{6} \cdot 5 \cdot 5$
	$T_3(8, 1)$	4	10	21	32	49	76 109	137	170	207	$4 \cdot 6 \cdot 4 \cdot 12_3 \cdot 5 \cdot 5$
	$T_4(8, 1)$	4	10	21	32	49	74 105	139	173	204	4.6.4.12 <sub>6</sub> .5.5
	$T_5(8, 1)$	4	11	18	29	48	80 107	133	160	203	$4.5_{2}.5.5.5.6$
	$T_6(8, 1)$	4	11	18	29	48	77 106	134	160	204	$4.5_{2}.5.5.5.6$
	$T_7(8, 1)$	4	12	18	31	51	76 109	133	164	210	$5 \cdot 5 \cdot 5 \cdot 6 \cdot 5_2 \cdot 12_5$
	$T_8(4, 2)$	4	12	19	32	48	75 112	134	164	206	$5 \cdot 5 \cdot 5_2 \cdot 12_7 \cdot 6 \cdot 6$
	T <sub>9</sub> (4, 2)	4	12	17	30	54	77 106	134	160	212	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 12_3$
Secondary building units:	combination	ons	only	y							
Loop configuration of T-Atoms:			_				$\rightarrow$				
		T <sub>1-4</sub>				T <sub>5,6</sub>		Т	7-9		

Isotypic framework	*Beta <sup>(1,2)</sup>	CIT-6 <sup>(5)</sup>
structures:	[B-Si-O]-* <b>BEA</b> <sup>(3,4)</sup>	Tschernichite <sup>(6)</sup>
	[Ga-Si-O]- <b>*BEA</b> <sup>(4)</sup>	

- (1) Higgins, J.B., LaPierre, R.B., Schlenker, J.L., Rohrman, A.C., Wood, J.D., Kerr, G.T. and Rohrbaugh, W.J. *Zeolites*, **8**, 446-452 (1988)
- (2) Newsam, J.M., Treacy, M.M.J., Koetsier, W.T. and de Gruyter, C.B. *Proc. R. Soc. Lond. A*, **420**, 375-405 (1988)
- (3) Marler, B., Böhme, R. and Gies, H. In *Proc. 9th Int. Zeolite Conf.*, (eds. R. von Ballmoos, J.B. Higgins and M.M.J. Treacy), pp. 425-432 (1993), Butterworth-Heinemann, Boston

Crystal chemical data:	Na <sup>+</sup> <sub>7</sub>   [Al <sub>7</sub> Si <sub>57</sub> O <sub>128</sub> ]-* <b>BEA</b>
	tetragonal, P4 <sub>1</sub> 22, $a = 12.661$ Å, $c = 26.406$ Å <sup> (2)</sup>

Framework density: 15.1 T/1000Å<sup>3</sup>

Channels:

 ${<}100{>}\ \textbf{12}\ \textbf{6.6}\ \textbf{x}\ \textbf{6.7}^{**} \leftrightarrow [001]\ \textbf{12}\ \textbf{5.6}\ \textbf{x}\ \textbf{5.6}^{*}$ 



12-ring viewed along <100>



12-ring viewed along [001]

#### **References (cont.):**

- (4) Reddy, K.S.N., Eapen, M.J., Joshi, P.N., Mirajkar, S.P. and Shiralkar, V.P. J. Incl. Phenom. Mol. Recogn. Chem., 20, 197-210 (1994)
- (5) Takewaki, T., Beck, L.W. and Davis, M.E. Topics in Catalysis, 9, 35-42 (1999)
- (6) Boggs, R.C., Howard, D.G., Smith, J.V. and Klein, G.L. Am. Mineral., 78, 822-826 (1993)





framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 7.5$ Å, $b = 16.2$ Å, $c = 5.3$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	5-1
Loop configuration of T-Atoms:	T <sub>1,2</sub>
Isotypic framework	*Bikitaite <sup>(1,2)</sup>

structures:

(1) Kocman, V., Gait, R.I. and Rucklidge, J. Am. Mineral., 59, 71-78 (1974)

|Cs-|[Al-Si-O]-**BIK**<sup>(3)</sup> Triclinic bikitaite<sup>(4)</sup>

- (2) Ståhl, K., Kvick, Å. and Ghose, S. Zeolites, 9, 303-311 (1989)
- (3) Annehed, H. and Fälth, L. Z. *Kristallogr.*, **166**, 301-306 (1984)
- (4) Bissert, G. and Liebau, L. N. Jb. Miner. Mh., 241-252 (1986)

Crystal chemical data:	Li <sup>+</sup> <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>   [Al <sub>2</sub> Si <sub>4</sub> O <sub>12</sub> ]- <b>BIK</b> triclinic, P1, a = 8.607Å, b = 4.954Å, c = 7.597Å, $\alpha$ = 89.90°, $\beta$ = 114.44°, $\gamma$ = 89.99° <sup>(2)</sup> (Relationship to unit cell of Framework Type: a' = b/2 sin( $\beta$ ), b' = c, c' = a or, as vectors, <b>a'</b> = ( <b>b</b> - <b>a</b> )/2, <b>b'</b> = <b>c</b> , <b>c'</b> = <b>a</b> )
Framework density:	20.3 T/1000Å <sup>3</sup>
Channels:	[010] <b>8</b> 2.8 x 3.7*



8-ring viewed along [010]



framework viewed along [100] (bottom left: projection down [100])

Idealized cell constants:	orthorhon	ıbic	, Im	ma,	a =	20.0Å	Å, b	= 23	8.6Å,	c =	12.7Å	
<b>Coordination sequences</b>	T <sub>1</sub> (16, 1)	4	10	19	32	51	74	101	129	158	199	$4 \cdot 5 \cdot 4 \cdot 6 \cdot 5 \cdot 12_2$
and vertex symbols:	T <sub>2</sub> (16, 1)	4	10	20	32	48	74	104	131	159	195	$4 \cdot 5 \cdot 4 \cdot 6_2 \cdot 10 \cdot 12$
	T <sub>3</sub> (16, 1)	4	11	19	34	50	71	98	133	162	195	$4 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 10_3$
	T <sub>4</sub> (16, 1)	4	11	21	32	49	74	101	128	162	200	$4 \cdot 10_5 \cdot 5 \cdot 6_3 \cdot 5 \cdot 6_3$
	$T_5(16, 1)$	4	11	20	31	53	76	97	126	168	199	$4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10$
	$T_{6}(16, 1)$	4	11	18	31	52	75	100	126	158	206	$4 \cdot 5 \cdot 5 \cdot 6 \cdot 5 \cdot 6_2$
Secondary building units:	6 or 4											
Loop configuration of T-Atoms:		T <sub>1,2</sub>	_			] T <sub>3-6</sub>						
Isotypic framework structures:	*Boggsite	(1)										

(1) Pluth, J.J. and Smith, J.V. Am. Mineral., 75, 501-507 (1990)

Boggsite

### **Type Material**

Crystal chemical data:

$$\label{eq:ca2+7} \begin{split} |Ca^{2+}{}_7Na^{+}{}_4\ (H_2O)_{74}|\ [Al_{18}Si_{78}\ O_{192}]\text{-}BOG \\ \text{orthorhombic, Imma, } a = 20.236\text{\AA, } b = 23.798\text{\AA, } c = 12.798\text{\AA}^{(1)} \end{split}$$

Framework density: 15.6 T/1000Å<sup>3</sup>

Channels:

[100] **12** 7.0 x 7.0\*  $\leftrightarrow$  [010] **10** 5.5 x 5.8\*



12-ring viewed along [100]



10-ring viewed along [010]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal	, P∂	2m	, a =	13.	1Å, c	c = 11	3.0Å	1			
<b>Coordination sequences</b>	T <sub>1</sub> (12, 1)	4	9	17	28	42	60	84	113	140	169	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 6_2 \cdot 8$
and vertex symbols:	$T_2(12, 1)$	4	9	16	25	39	61	86	111	141	173	4.4.4.6.6.12
	$T_3(4, 3)$	4	9	18	30	43	62	85	105	135	180	4.8.4.8.4.8
Secondary building units:	6*1											
Loop configuration of T-Atoms:			Γ	/	$\frac{1}{2}$	]						

Isotypic framework structures:

\*Beryllophosphate- $H^{(1,2)}$ Linde  $Q^{(3)}$ STA- $5^{(4)}$ 

- (1) Harvey, G. Z. Kristallogr., 182, 123-124 (1988)
- (2) Harvey, G., Baerlocher, Ch. and Wroblewski, T. Z. Kristallogr., 201, 113-123 (1992)
- (3) Andries, K.J., Bosmans, H.J. and Grobet, P.J. Zeolites, 11, 124-131 (1991)
- (4) Patinec, V., Wright, P.A., Aitken, R.A., Lightfoot, P., Purdie, S.D.J., Cox, P.A., Kvick, A. and Vaughan, G. *Chem. Mater.*, **11**, 2456-2462 (1999)

Crystal chemical data:

 $\begin{array}{l} [K_{\ 7}^{+}Na_{\ 7}^{+}~(H_{2}O)_{20}]~[Be_{14}P_{14}~O_{56}]\text{-}BPH \\ trigonal,~P321,~a=12.582\text{\AA},~c=12.451\text{\AA}^{\ (2)} \end{array}$ 

Framework density: 16.4 T/1000Å<sup>3</sup>

Channels:

 $[001] \ \mathbf{12} \ 6.3 \ \mathbf{x} \ 6.3^* \leftrightarrow \perp [001] \ \mathbf{8} \ 2.7 \ \mathbf{x} \ 3.5^{**}$ 



12-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed along [100]

Idealized cell constants:	monoclinic, P2 <sub>1</sub> /m, a = 6.8Å, b = 17.1Å, c = 7.6Å, $\beta$ = 95.8°							
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$							
Secondary building units:	4							
Loop configuration of T-Atoms:	T <sub>1,2</sub> T <sub>3,4</sub>							
Isotypic framework structures:	*Brewsterite <sup>(1,2)</sup> Ba-dominant brewsterite <sup>(3)</sup> CIT-4 <sup>(4)</sup> Synthetic brewsterite <sup>(5)</sup>							

- (1) Perrotta, A.J. and Smith, J.V. Acta Crystallogr., 17, 857-862 (1964)
- (2) Schlenker, J.L., Pluth, J.J. and Smith, J.V. Acta Crystallogr., B33, 2907-2910 (1977)
- (3) Cabella, R., Lucchetti, G., Palenzona, A., Quartieri, S. and Vezzalini, G. *Eur. J. Mineral.*, **5**, 353-360 (1993)
- (4) Khodabandeh, S., Lee, G. and Davis, M.E. Microporous and Mesoporous Materials, 11, 87-95 (1997)
- (5) Ghobarkar, H. and Schaef, O. German Patent AZ 198 24 184.4-41 (1999)

Crystal chemical data:	$\begin{split} & (Ba^{2+},Sr^{2+})_2 \ (H_2O)_{10}  \ [Al_4Si_{12} \ O_{32}]\text{-}BRE \\ & \text{monoclinic, } P12_1/m1 \\ & a = 6.793\text{\AA}, \ b = 17.573\text{\AA}, \ c = 7.759\text{\AA}, \ \beta = 94.54^{\circ} \ ^{(2)} \end{split}$
Framework density:	17.3 T/1000Å <sup>3</sup>

Channels:

 $[100] \; \textbf{8} \; 2.3 \; \textbf{x} \; 5.0^* \leftrightarrow [001] \; \textbf{8} \; 2.8 \; \textbf{x} \; 4.1^*$ 



8-ring viewed along [100]



8-ring viewed along [001]



framework viewed along [001] (bottom left: projection down [001])

Idealized cell constants:	hexagonal, $P6_3/mmc$ , $a = 12.5$ Å, $c = 5.3$ Å							
Coordination sequences and vertex symbols:	T <sub>1</sub> (12, m) 4 10 20 34 54 78 10	04 134 168 210 4.6.4.6.6.6						
Secondary building units:	4-2 or 6 or 4							
Loop configuration of T-Atoms:								
Framework description:	AB sequence of 6-rings							
Isotypic framework structures:	*Cancrinite <sup>(1,2)</sup> [Al-Ge-O]-CAN <sup>(3)</sup> [Ga-Si-O]-CAN <sup>(4)</sup> [Zn-P-O]-CAN <sup>(5)</sup> Basic cancrinite <sup>(6,7)</sup> Cancrinite hydrate <sup>(8)</sup>	Davyne <sup>(9)</sup> ECR- $5^{(10)}$ Microsommite <sup>(11)</sup> Synthetic cancrinite <sup>(12)</sup> Tiptopite <sup>(13)</sup> Vishnevite <sup>(14)</sup>						
References:								

- (1) Pauling, L. Proc. Natl. Acad. Sci., 16, 453-459 (1930)
- (2) Jarchow, O. Z. Kristallogr., **122**, 407-422 (1965)
- (3) Belokoneva, E.L., Uvarova, T.G. and Dem'yanets, L.N. Sov. Phys. Crystallogr., 31, 516-519 (1986)
- (4) Newsam, J.M. and Jorgensen, J.D. Zeolites, **7**, 569-573 (1987)
- (5) Yakubovich, O.V., Karimova, O.V. and Mel'nikov, O.K. Crystallogr. Reports, 39, 564-568 (1994)
- (6) Barrer, R.M. and White, E.A.D. J. Chem. Soc., 1561-1571 (1952)
- (7) Bresciana Pahor, N., Calligaris, M., Nardin, G. and Randaccio, L. Acta Crystallogr., B38, 893-895 (1982)
- (8) Wyart, J. and Michel-Levy, M. Compt. Rend., 229, 131-(1949)
- (9) Hassan, I. and Grundy, H.D. Can. Mineral., 28, 341-349 (1990)
- (10) Vaughan, D.E.W. E. Patent A-190,90 (1986)

Cancrinite

Crystal chemical data:	$ Na_{6}^{+} Ca^{2+} CO_{3}^{2-} (H_{2}O)_{2}$ hexagonal, P6 <sub>3</sub> , a = 12.	$\begin{array}{l} [Al_{6}Si_{6} O_{24}]\text{-}CAN \\ 75\text{\AA}, c = 5.14\text{\AA}^{(2)} \end{array}$
Framework density:	16.6 T/1000Å <sup>3</sup>	
Channels:	[001] <b>12</b> 5.9 x 5.9*	
5.9	5.9	5.9 5.9 5.9 5.9

12-ring viewed along [001]

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- (11) Bonaccorsi, E., Comodi, P. and Merlino, S. Phys. Chem. Mineral., 22, 367-374 (1995)
- (12) Smolin, Y.I., Shepelev, Y.F., Butikova, I.K. and Kobyakov, I.B. Kristallografiya, 26, 63-66 (1981)
- (13) Peacor, D.R., Rouse, R.C. and Ahn, J.-H. Am. Mineral., 72, 816-820 (1987)
- (14) Hassan, I. and Grundy, H.D. Can. Mineral., 22, 333-340 (1984)



framework viewed along [100]

Idealized cell constants:	orthorhom	bic,	Cn	ncm	, a =	5.3	Å, b	= 14	.1Å,	<b>c</b> = 1	17.2Å		
Coordination sequences and vertex symbols:	$\begin{array}{l} T_{1} \left( 8,m\right) \\ T_{2} \left( 8,m\right) \\ T_{3} \left( 8,m\right) \end{array}$	4 4 4	12 12 12	23 26 23	41 43 43	70 64 72	97 101 95	125 138 128	174 165 177	224 215 225	264 284 259	5.5.5.5.6 5.6.5.6.6 5.6.5.6.5	$5 \cdot 8_2$ $\frac{1}{2} \cdot 8_2$ $5_2 \cdot 6$
Secondary building units:	5-1												
Loop configuration of T-Atoms:	_ <b>_</b>	Γ <sub>1-3</sub>											

Isotypic framework structures:

\*Cesium Aluminosilicate<sup>(1)</sup>

#### **References:**

(1) Araki, T. Z. Kristallogr., 152, 207-213 (1980)

4.7

Crystal chemical data:	$\begin{aligned} & \text{Cs}^{+}_{4}  \text{ [Al}_{4}\text{Si}_{20} \text{ O}_{48} \text{]-CAS} \\ &\text{orthorhombic, Ama2, a = 16.776\text{ Å}, b = 13.828\text{ Å}, c = 5.021\text{ Å}^{(1)} \\ &\text{(Relationship to unit cell of Framework Type: } \mathbf{a'} = -\mathbf{c}, b' = b, c' = a) \end{aligned}$
Framework density:	20.6 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 2.4 x 4.7*
2.	

8-ring viewed along [001]

4.

### Framework Type



framework viewed along [010]

Idealized cell constants:	orthorhomb	oic,	, Im	ma,	a =	14.0Å	Å, b	= 5.	3Å, (	c = 2	6.0Å		
Coordination sequences	T <sub>1</sub> (8, m)	4	10	21	36	56	84	114	143	182	231	4.6.4.6.5	i·6
and vertex symbols:	T <sub>2</sub> (8, m)	4	12	23	37	55	83	114	153	195	222	5.6.5.6.52	2·6
	T <sub>3</sub> (8, m)	4	12	22	37	57	84	114	156	184	222	5.6.5.6.5.	62
	T <sub>4</sub> (4, mm2)	4	12	24	36	54	79	118	153	190	234	5.5.5.5.14 <sub>20</sub>	) <sup>.*</sup>
	T <sub>5</sub> (4, mm2)	4	12	20	34	56	81	116	151	186	220	5.5.5.5.5	62
Secondary building units:	5-3												
Loop configuration of T-Atoms:		1	_			- T <sub>2-5</sub>							
Isotypic framework structures:	*CIT-5 <sup>(1,2)</sup>												

- (1) Wagner, P., Yoshikawa, M., Lovallo, M., Tsuji, K., Taspatsis, M. and Davis, M.E. Chem. Commun., 2179-2180 (1997)
- (2) Yoshikawa, M., Wagner, P., Lovallo, M., Tsuji, K., Takewaki, T., Chen, C.Y., Beck, L.W., Jones, C., Tsapatsis, M., Zones, S.I. and Davis, M.E. J. Phys. Chem. B, **102**, 7139-7147 (1998)

CIT-5

Crystal chemical data:	[Si <sub>32</sub> O <sub>64</sub> ]-CFI orthorhombic, Pmn2 <sub>1</sub> , a = 13.674Å, b = 5.022Å, c = 25.488Å $^{(2)}$
Framework density:	18.3 T/1000Å <sup>3</sup>
Channels:	[010] <b>14</b> 7.2 x 7.5*
r 6-6	



14-ring viewed along [010]



framework viewed along [001]

Idealized cell constants:	monoclin	ic, C	212/1	m1,	a =	15.54	Å, b	= 16	.9Å,	$\mathbf{c} = \hat{c}$	7.3Å,	$\beta = 96.1$	0		
Coordination sequences	T <sub>1</sub> (8, 1)	4	11	22	34	50	76	111	142	165	199		4·8·6 <sub>3</sub> ·	8·6 <sub>3</sub> ·8	
and vertex symbols:	$T_{2}(8, 1)$	4	10	19	33	55	79	100	129	172	216		4.6.4.	6 <sub>2</sub> .6.6	
	$T_3(8, 1)$	4	9	18	34	55	76	97	131	177	217		4.4.4.	6.6.62	
	$T_4(8, 1)$	4	9	18	34	55	75	98	133	177	216		$4 \cdot 6_3 \cdot 4 \cdot$	6 <sub>3</sub> .4.8	
	T <sub>5</sub> (4, 2)	4	10	18	32	58	80	96	124	176	228	4	$4 \cdot 4 \cdot 6_2 \cdot 6_2 \cdot$	10.10	
Secondary building units:	4														
Loop configuration of T-Atoms:		] T <sub>1</sub>				] T <sub>2</sub>			]	Г <sub>3</sub>					] T <sub>5</sub>

Isotypic framework structures:

\*Co-Ga-Phosphate-5<sup>(1)</sup>



(1) Chippindale, A.M. and Cowley, A.R. Zeolites, 18, 176-181 (1997)

Crystal chemical data:	$ (C_{6}H_{14}N_{2}^{2+})_{2} [Co_{4}Ga_{5}P_{9}O_{36}]-CGF$
	$C_6H_{12}N_2 = DABCO$
	monoclinic, I12/a1
	$a = 15.002$ Å, $b = 17.688$ Å, $c = 15.751$ Å, $\beta = 97.24^{\circ (1)}$
	(Relationship to unit cell of Framework Type: $a' = 2c$ , $b' = b$ , $c' = a$ )
Framework density:	$17.4 \text{ T}/1000\text{\AA}^3$
Channels:	{[100] <b>10</b> 2.5 x 9.2* + <b>8</b> 2.1 x 6.7*} $\leftrightarrow$ [001] <b>8</b> 2.4 x 4.8*



10-ring viewed along [100]



8-ring viewed along [100]

See Appendix A for 8-ring viewed along [001]



framework viewed along [100]

Idealized cell constants:	orthorhombic, Pnma, $a = 8.4$ Å, $b = 14.1$ Å, $c = 15.9$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4
Loop configuration of T-Atoms:	T <sub>1-4</sub>
Isotypic framework structures:	*Co-Ga-Phosphate- $6^{(1)}$ [Zn-Ga-P-O]-CGS <sup>(1)</sup> TNU-1, [Ga-Si-O]-CGS <sup>(2)</sup> TsG-1, [Ga-Si-O]-CGS <sup>(3)</sup>

- (1) Cowley, A.R. and Chippindale, A.M. *Microporous and Mesoporous Materials*, 28, 163-172 (1999)
- (2) Hong, S.B., Kim, S.H., Kim, Y.G., Kim, Y.C., Barrett, P.A. and Camblor, M.A. J. Mater. Chem., 9, 2287-2289 (1999)
- (3) Lee, Y.J., Kim, S.J., Wu, G. and Parise, J.B. Chem. Mater., 11, 879-880 (1999)

Crystal chemical data:	$\begin{split}  (C_{7}H_{14}N^{+})_{4}  & [Co_{4}Ga_{12}P_{16} \ O_{64}]\text{-}CGS \\ C_{7}H_{13}N = quinuclidine \\ monoclinic, P12_{1}/c1 \\ a = 14.365\text{\AA}, \ b = 16.305\text{\AA}, \ c = 8.734\text{\AA}, \ \beta = 90.24^{\circ \ (1)} \\ (\text{Relationship to unit cell of Framework Type: }a' = b, \ b' = c, \ c' = a) \end{split}$
Framework density:	15.6 T/1000Å <sup>3</sup>
Channels:	{[001] <b>10</b> 3.5 x 8.1 $\leftrightarrow$ [100] <b>8</b> 2.5 x 4.6}***



10-ring viewed along [001]



8-ring viewed along [100]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , $a = 13.7$ Å, $c = 14.8$ Å							
Coordination sequences and vertex symbols:	$T_1(36, 1)$ 4 9 17 29 45 64	85 110 140 173	4-4-4-8-6-8					
Secondary building units:	6-6 or 6 or 4							
Loop configuration of T-Atoms:								
Framework description:	AABBCC sequence of 6-rings							
Isotypic framework structures:	*Chabazite <sup>(1,2)</sup> [Al-Co-P-O]-CHA <sup>(3)</sup> [Co-Al-P-O]-CHA <sup>(3,4)</sup> [Mg-Al-P-O]-CHA <sup>(4)</sup> AlPO-34 <sup>(5)</sup> CoAPO-44 <sup>(6)</sup> CoAPO-47 <sup>(6)</sup> Dehydrated Na-Chabazite <sup>(7)</sup> GaPO-34 <sup>(8)</sup> LZ-218 <sup>(9)</sup> Linde D <sup>(10,11)</sup>	Linde $R^{(12)}$ MeAPO-47 <sup>(6,13,14)</sup> MeAPSO-47 <sup>(6,13,14)</sup> Phi <sup>(11,15)</sup> SAPO-34 <sup>(16)</sup> SAPO-47 <sup>(17)</sup> Si-CHA <sup>(18)</sup> Willhendersonite <sup>(19)</sup> ZK-14 <sup>(20,21)</sup> ZYT-6 <sup>(22)</sup>						
Alternate designation:	Herschelite (discredited)							

Chabazite

**Type Material** 

### CHA

Crystal chemical data:

 $|Ca^{2+}_{6} (H_{2}O)_{40}|$  [Al<sub>12</sub>Si<sub>24</sub> O<sub>72</sub>]-CHA rhombohedral, R $\overline{3}m$ , a = 9.42Å,  $\alpha$  = 94.47° <sup>(2)</sup>

Framework density: 14.5 T/1000Å<sup>3</sup>

**Channels:** 

 $\perp$  [001] **8** 3.8 x 3.8\*\*\* (variable due to considerable flexibility of framework)



8-ring viewed normal to [001]

- (1) Dent, L.S. and Smith, J.V. Nature, 181, 1794-1796 (1958)
- (2) Smith, J.V., Rinaldi, R. and Dent Glasser, L.S. Acta Crystallogr., 16, 45-53 (1963)
- (3) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
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- (6) Bennett, J.M. and Marcus, B.K. Stud. Surf. Sci. Catal., 37, 269-279 (1988)
- (7) Mortier, W.J., Pluth, J.J. and Smith, J.V. Mater. Res. Bull., 12, 241-250 (1977)
- (8) Schott-Darie, C., Kessler, H., Soulard, M., Gramlich, V. and Benazzi, E. Stud. Surf. Sci. Catal., 84, 101-108 (1994)
- (9) Breck, D.W. and Skeels, G.W. U.S. Patent 4,333,859 (1982)
- (10) Breck, D.W. and Acara, N.A. U.S. Patent 2,950,952 (1960)
- (11) Lillerud, K.P., Szostak, R. and Long, A. J. Chem. Soc., Faraday Trans., 90, 1547-1551 (1994)
- (12) Milton, R.M. Brit. Patent 841,812 (1960)
- (13) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)
- (14) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In *Proc. 7th Int. Zeolite Conf.*, (eds. Y. Murakami, A. Iijima and J.W. Ward), pp. 103-112 (1986), Kodansha, Tokyo
- (15) Grose, R.W. and Flanigen, E.M. U.S. Patent 4,124,686 (1978)
- (16) Lok, B.M., Messina, C.A., Patton, R.L., Gajek, R.T., Cannan, T.R. and Flanigen, E.M. J. Am. Chem. Soc., **106**, 6092-6093 (1984)
- (17) Pluth, J.J. and Smith, J.V. J. Phys. Chem., 93, 6516-6520 (1989)
- (18) Díaz-Cabañas, M.J., Barrett, P.A. and Camblor, M.A. Chem. Commun., 1881-1882 (1998)
- (19) Tillmanns, E., Fischer, R.X. and Baur, W.H. N. Jb. Miner. Mh., 547-558 (1984)
- (20) Kuehl, G.H. private communication
- (21) Kuehl, G.H. In Molecular Sieves, (ed. R.M. Barrer), pp. 85-91 (1968), Soc. Chem. Indus., London
- (22) Ito, M., Shimoyama, Y., Saito, Y., Tsurita, Y. and Otake, M. Acta Crystallogr., C41, 1698-1700 (1985)



framework viewed along [100]

Idealized cell constants:	orthorhombic, Pbcn, $a = 5.0$ Å, $b = 31.2$ Å, $c = 9.0$ Å
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	5-2
Loop configuration of T-Atoms:	$T_{1,2}$ $T_3$ $T_4$
Isotypic framework structures:	*Chiavennite <sup>(1)</sup>

(1) Tazzoli, V., Domeneghetti, M.C., Mazzi, F. and Cannillo, E. Eur. J. Mineral., 7, 1339-1344 (1995)

Chiavennite

## **Type Material**

# -CHI

Crystal chemical data:	$ Ca^{2+}_{4} Mn^{2+}_{4} (H_{2}O)_{8} $ [Be <sub>8</sub> Si <sub>20</sub> O <sub>52</sub> (OH) <sub>8</sub> ]CHI orthorhombic, Pnab, a = 8.729Å, b = 31.326Å, c = 4.903Å <sup>(1)</sup> (Relationship to unit cell of Framework Type: a' = -c, b' = b, c' = a)
Framework density:	20.9 T/1000Å <sup>3</sup>
Channels:	[001] <b>9</b> 3.9 x 4.3*
4.3	4.3 3.9 2.2 3.9 2.2 3.9

9-ring viewed along [001]



framework viewed along [001] (bottom left: projection down [001])

Idealized cell constants:	cubic, $Pm\overline{3}m$ , $a = 25.8$ Å											
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1 \ (48, 1) \\ T_2 \ (48, 1) \\ T_3 \ (48, 1) \\ T_4 \ (24, m) \\ T_5 \ (24, m) \end{array}$	4 4 4 3	9 9 8 9 5	16 17 13 16 10	23 27 22 23 18	31 37 34 32 29	44 47 44 45 45	59 56 55 58 56	74 66 72 76 65	91 80 94 98 86	109 99 117 118 110	$\begin{array}{c} 4{\cdot}6{\cdot}4{\cdot}6{\cdot}4{\cdot}12\\ 4{\cdot}6{\cdot}4{\cdot}6{\cdot}4{\cdot}8\\ 4{\cdot}6{\cdot}4{\cdot}6{\cdot}4{\cdot}20_8\\ 4{\cdot}6{\cdot}4{\cdot}6{\cdot}4{\cdot}8\\ 4{\cdot}4{\cdot}4{\cdot}4{\cdot}4{\cdot}4{\cdot}\end{array}$
Secondary building units:	4-4 or 4											
Loop configuration of T-Atoms:		- 1-4				T <sub>5</sub>						
Isotypic framework structures:	*Cloverite <sup>(</sup>	1)										

(1) Estermann, M., McCusker, L.B., Baerlocher, Ch., Merrouche, A. and Kessler, H. *Nature*, **352**, 320-323 (1991)

Crystal chemical data:	$\begin{split} & (C_{7}H_{14}N^{+})_{24} _{8} \ [F_{24} \ Ga_{96}P_{96} \ O_{372}(OH)_{24}]_{8}^{-} \ \textbf{-CLO} \\ &C_{7}H_{13}N = quinuclidine \\ & \text{cubic, } Fm \ \overline{3}c, \ a = 51.712 \ \text{\AA}^{\ (1)} \\ & (\text{Relationship to unit cell of Framework Type: }a' = 2a) \end{split}$
Framework density:	11.1 T/1000Å <sup>3</sup>
Channels:	<100> <b>20</b> 4.0 x 13.2***   <100> <b>8</b> 3.8 x 3.8***



20-ring viewed along <100>



8-ring viewed along <100>



framework viewed along [001]

Idealized cell constants:	monoclinic	e, C2/m	n, a = 22	.7Å,	b = 13.4	Å, c = 12	$.6\text{\AA}, \beta = 69.5^{\circ}$	)
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1 \left( 8, 1 \right) \\ T_2 \left( 8, 1 \right) \\ T_3 \left( 8, 1 \right) \\ T_4 \left( 8, 1 \right) \\ T_5 \left( 8, 1 \right) \\ T_6 \left( 8, 1 \right) \\ T_7 \left( 8, 1 \right) \end{array}$	$\begin{array}{rrrr} 4 & 10 \\ 4 & 11 \\ 4 & 10 \\ 4 & 10 \\ 4 & 10 \\ 4 & 11 \\ 4 & 11 \end{array}$	1932183121321932193218281932	50 52 47 51 51 49 49	7310177987410574100741017710375105	132 164 126 164 134 159 130 165 130 164 126 155 131 159	199 205 196 203 203 201 196	$\begin{array}{c} 4{\cdot}5{\cdot}4{\cdot}10_4{\cdot}5{\cdot}6_2\\ 4{\cdot}5{\cdot}5{\cdot}6{\cdot}5{\cdot}10_2\\ 4{\cdot}6{\cdot}4{\cdot}10_4{\cdot}5{\cdot}6_2\\ 4{\cdot}4{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_7\\ 4{\cdot}4{\cdot}5{\cdot}6_2{\cdot}5{\cdot}12_4\\ 4{\cdot}5_2{\cdot}5{\cdot}6_2{\cdot}6{\cdot}6_2\\ 4{\cdot}6_2{\cdot}5{\cdot}6{\cdot}5{\cdot}10_2 \end{array}$
Secondary building units:	5-2							
Loop configuration of T-Atoms:		- - 1,3		] T <sub>2,6,7</sub>		 T <sub>4,5</sub>		

Isotypic framework<br/>structures:\*CIT-1<sup>(1)</sup><br/>SSZ-26 (contains major structural units of CON)<sup>(1,2)</sup><br/>SSZ-33 (contains major structural units of CON)<sup>(1,2)</sup>

- (1) Lobo, R.F. and Davis, M.E. J. Am. Chem. Soc., 117, 3764-3779 (1995)
- (2) Lobo, R.F., Pan, M., Chan, I., Li, H.X., Medrud, R.C., Zones, S.I., Crozier, P.A. and Davis, M.E. *Science*, **262**, 1543-1546 (1993)
| Crystal chemical data: | H <sup>+</sup> <sub>2</sub>   [B <sub>2</sub> Si <sub>54</sub> O <sub>112</sub> ]-CON<br>monoclinic, C12/m1<br>$a = 22.624$ Å, $b = 13.350$ Å, $c = 12.364$ Å, $\beta = 68.91^{\circ (1)}$ |
|------------------------|--|
| Framework density:     | 16.1 T/1000Å <sup>3</sup>  |
| Channels:              | [001] <b>12</b> 6.4 x 7.0* ↔ [100] <b>12</b> 7.0 x 5.9* ↔ [010] <b>10</b> 5.1 x 4.5*   |



12-ring viewed along [001]



12-ring viewed along [100]

See Appendix A for 10-ring viewed along [010]



framework viewed normal to [001] (top left: projection down [001])

hexagonal	hexagonal, $P6_122$ , $a = 9.4$ Å, $c = 15.3$ Å										
$\begin{array}{l} T_1  (12,  1) \\ T_2  (6,  2) \\ T_3  (6,  2) \end{array}$	4 4 4	9 10 8	18 20 16	32 33 33	54 56 52	83 85 73	113 114 112	149 144 160	191 192 190	234 242 214	$\begin{array}{c} 4{\cdot}4{\cdot}4{\cdot}8_{6}{\cdot}8{\cdot}8\\ 4{\cdot}4{\cdot}8_{3}{\cdot}8_{3}{\cdot}8_{6}{\cdot}8_{6}\\ 4{\cdot}4{\cdot}4{\cdot}4{\cdot}8{\cdot}8\end{array}$
4	$\Gamma_1$	[			T <sub>2</sub>				3		
	hexagonal, $T_1 (12, 1)$ $T_2 (6, 2)$ $T_3 (6, 2)$ 4	hexagonal, P6 $T_1 (12, 1) = 4$ $T_2 (6, 2) = 4$ $T_3 (6, 2) = 4$ 4 $T_1$	hexagonal, $P6_122_2$ $T_1 (12, 1)  4  9$ $T_2 (6, 2)  4  10$ $T_3 (6, 2)  4  8$ 4 $T_1$	hexagonal, $P6_122$ , a = $T_1 (12, 1)$ 4 9 18 $T_2 (6, 2)$ 4 10 20 $T_3 (6, 2)$ 4 8 16 4 $T_1$	hexagonal, $P6_122$ , $a = 9.44$ $T_1 (12, 1)$ 4 9 18 32 $T_2 (6, 2)$ 4 10 20 33 $T_3 (6, 2)$ 4 8 16 33 4 $T_1$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = $T_1 (12, 1)$ 4 9 18 32 54 $T_2 (6, 2)$ 4 10 20 33 56 $T_3 (6, 2)$ 4 8 16 33 52 4 $T_1$ $T_2$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = 15 $T_1 (12, 1)$ 4 9 18 32 54 83 $T_2 (6, 2)$ 4 10 20 33 56 85 $T_3 (6, 2)$ 4 8 16 33 52 73 4 $T_1 T_1 T_2$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = 15.3Å $T_1 (12, 1)$ 4 9 18 32 54 83 113 $T_2 (6, 2)$ 4 10 20 33 56 85 114 $T_3 (6, 2)$ 4 8 16 33 52 73 112 4 $T_1 = T_1$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = 15.3Å $T_1 (12, 1)$ 4 9 18 32 54 83 113 149 $T_2 (6, 2)$ 4 10 20 33 56 85 114 144 $T_3 (6, 2)$ 4 8 16 33 52 73 112 160 4 $T_1 T_1 T_2 T_2 T_2$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = 15.3Å $T_1 (12, 1)$ 4 9 18 32 54 83 113 149 191 $T_2 (6, 2)$ 4 10 20 33 56 85 114 144 192 $T_3 (6, 2)$ 4 8 16 33 52 73 112 160 190 4 $T_1 \qquad T_1 \qquad T_2 \qquad T_3 \qquad T_3$	hexagonal, P6 <sub>1</sub> 22, a = 9.4Å, c = 15.3Å $T_1 (12, 1)$ 4 9 18 32 54 83 113 149 191 234 $T_2 (6, 2)$ 4 10 20 33 56 85 114 144 192 242 $T_3 (6, 2)$ 4 8 16 33 52 73 112 160 190 214 4 $T_1 = T_1$ $T_2 = T_3$

Isotypic framework structures: \*Chiral Zincophosphate<sup>(1,2)</sup>

- (1) Rajic, N., Logar, N.Z. and Kaucic, V. Zeolites, 15, 672-678 (1995)
- (2) Harrison, W.T.A., Gier, T.E., Stucky, G.D., Broach, R.W. and Bedard, R.A. *Chem. Mater.*, **8**, 145-151 (1996)

Crystal chemical data:	$ Na^{+}_{12} (H_2O)_{12}  [Zn_{12}P_{12} O_{48}]$ -CZP
	hexagonal, P6 <sub>1</sub> 22, a = 10.480Å, c = 15.089Å $^{(2)}$

Framework density: 16.7 T/1000Å<sup>3</sup>

Channels:

[001] **12** 3.8 x 7.2\* (highly distorted 12-ring)



distorted 12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 18.6Å, b = 7.5Å, c = 10.4Å, $\beta$ = 108.9°	
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$5 \cdot 5 \cdot 5_2 \cdot 8 \cdot 10_2$ $5 \cdot 5 \cdot 5_2 \cdot 5 \cdot 8$ $4 \cdot 5_2 \cdot 5 \cdot 8 \cdot 5 \cdot 8$ $4 \cdot 5_2 \cdot 5 \cdot 8 \cdot 5 \cdot 8$
Secondary building units:	5-1	
Loop configuration of T-Atoms:	T <sub>1,2</sub> T <sub>3,4</sub>	
Isotypic framework structures:	*Dachiardite <sup>(1,2)</sup>	
Alternate designation:	Svetlozarite (discredited) <sup>(3)</sup>	

- (1) Gottardi, G. and Meier, W.M. Z. Kristallogr., 119, 53-64 (1963)
- (2) Vezzalini, G. Z. Kristallogr., 166, 63-71 (1984)
- (3) Gellens, L.R., Price, G.D. and Smith, J.V. Mineral. Mag., 45, 157-161 (1982)

# DAC

Crystal chemical data:	$\begin{split} & (Ca^{2+}{}_{0.5},K^{+},Na^{+})_{5} \ (H_{2}O)_{12}  \ \text{[Al}_{5}Si_{19} \ O_{48}\text{]-DAC} \\ &\text{monoclinic, C12/m1} \\ &a = 18.676 \text{\AA}, \ b = 7.518 \text{\AA}, \ c = 10.246 \text{\AA}, \ \beta = 107.87^{\circ} \ ^{(2)} \end{split}$
Framework density:	17.5 T/1000Å <sup>3</sup>
Channels:	$[010] \ 10 \ 3.4 \ge 5.3^* \leftrightarrow [001] \ 8 \ 3.7 \ge 4.8^*$



10-ring viewed along [010]



8-ring viewed along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , a = 13.8Å, c = 40.8Å											
Coordination sequences and vertex symbols:	T <sub>1</sub> (36, 1) T <sub>2</sub> (18, m)	4 4	11 12	23 22	39 37	62 59	91 93	124 127	159 158	203 193	251 251	4.5.5.5.5.8 5.5.5.5.5.5
	$\begin{array}{l} T_3 (18,m) \\ T_4 (18,m) \\ T_5 (18,2) \\ T_6 (6,2) \\ T_7 (6,2) \end{array}$	4 4 4 4	12 12 10 12 12	25 24 21 24 24	40 40 37 39 33	61 63 62 57 60	86 87 94 93 97	119 121 124 121 136	164 165 158 157 150	212 208 196 210 192	253 255 252 240 264	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 6$ $5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 8$ $4 \cdot 4 \cdot 5 \cdot 5 \cdot 5 \cdot 6 \cdot 8$ $5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5$ $5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 5$
Secondary building units:	5-1											



Isotypic framework	*Deca-dodecasil 3R <sup>(1)</sup>
structures:	Sigma-1 <sup>(2)</sup>
	ZSM-58 <sup>(3,4)</sup>

Crystal chemical data:	$ (C_{10}H_{17}N)_6 (N_2)_9 $ [Si <sub>120</sub> O <sub>240</sub> ]- <b>DDR</b> C <sub>10</sub> H <sub>17</sub> N = 1-aminoadamantane trigonal, R $\overline{3}m$ , a = 13.860Å, c = 40.891Å <sup>(1)</sup>
Framework density:	17.6 T/1000Å <sup>3</sup>
Channels:	⊥ [001] <b>8</b> 3.6 x 4.4**
	A A



8-ring viewed normal to [001]

- (1) Gies, H. Z. Kristallogr., 175, 93-104 (1986)
- (2) Stewart, A., Johnson, D.W. and Shannon, M.D. Stud. Surf. Sci. Catal., 37, 57-64 (1988)
- (3) Valyocsik, E.W. U.S. Patent 4,698,217 (1987)
- (4) Ernst, S., Chen, C.Y., Lindner, D. and Weitkamp, J. In *Zeolites for the Nineties, Recent Progress Reports Abstracts*, (eds. J.C. Jansen, L. Moscou and M.F.M. Post), pp. 55-56 (1989), 8th IZC, Amsterdam



(1) Wright, P.A., Jones, R.H., Natarajan, S., Bell, R.G., Chen, J.S., Hursthouse, M.B. and Thomas, J.M. *Chem. Commun.*, 633-635 (1993)

Crystal chemical data:	$\begin{split}  (C_{16}H_{38}N_2^{2+})_7 & (H_2O)_{40}  \ [Mg_{14}Al_{52}P_{66} \ O_{264}]\text{-}\textbf{DFO} \\ C_{16}H_{38}N_2^{2+} &= \text{decamethonium} \\ \text{hexagonal, P6/mmm, a} &= 22.351\text{\AA, c} = 21.693\text{\AA}^{(1)} \end{split}$
Framework density:	14.1 T/1000Å <sup>3</sup>
Channels:	{[001] <b>12</b> 7.3 x 7.3 $\leftrightarrow \perp$ [001] <b>8</b> 3.4 x 5.6}*** $\leftrightarrow$ {[001] <b>12</b> 6.2 x 6.2 $\leftrightarrow$ $\perp$ [001] <b>10</b> 5.4 x 6.4}***
Stability:	Transforms to AlPO <sub>4</sub> -5 and AlPO <sub>4</sub> -tridymite on heating to 500°C $^{(1)}$



12-ring viewed along [001]



8-ring viewed normal to [001]

See Appendix A for 2nd 12-ring viewed along [001] and 10-ring viewed normal to [001]



framework viewed along 001]

Idealized cell constants:	tetragonal, $P4_2$ /mmc, a = 7.1Å, c = 9.0Å								
Coordination sequences and vertex symbols:	$T_{1}(8, m)  4 \ 10 \ 21 \ 36 \ 55 \ 79 \ 106 \ 138 \ 175 \ 215 \qquad 4 \cdot 4 \cdot 6_{2} \cdot 8_{3} \cdot 6_{2} \cdot 8_{3}$								
Secondary building units:	4								
Loop configuration of T-Atoms:									
Isotypic framework structures:	*DAF- $2^{(1)}$ ACP- $3^{(2)}$ UCSB- $3GaGe^{(3)}$ UCSB- $3ZnAs^{(2)}$ UiO- $20^{(4)}$								

- (1) Chen, J., Jones, R.H., Natarajan, S., Hursthouse, M.B. and Thomas, J.M. Angew. Chem., Int. Ed., 33, 639-640 (1994)
- (2) Bu, X., Feng, P., Gier, T.E. and Stucky, G.D. J. Solid State Chem., 136, 210-215 (1998)
- (3) Bu, X., Feng, P., Gier, T.E., Zhao, D. and Stucky, G.D. J. Am. Chem. Soc., 120, 13389-13397 (1998)
- (4) Kongshaug, K.O., Fjellvag, H. and Lillerud, K.P. Chem. Mater., 12, 1095-1099 (2000)

Crystal chemical data:	$\begin{split}  (C_2H_{10}N_2^{2^+})_2  & [Co_4P_4 O_{16}]\text{-}DFT \\ C_2H_8N_2 &= \text{ethylenediamine} \\ \text{monoclinic, I112/b} \\ a &= 14.719\text{\AA, b} = 14.734\text{\AA, c} = 17.891\text{\AA, } \gamma = 90.02^{\circ \ (1)} \\ (\text{Relationship to unit cell of Framework Type: a' = 2a, b' = 2b, c' = 2c)} \end{split}$
Framework density:	16.5 T/1000Å <sup>3</sup>
Channels:	$[001]$ 8 4.1 x 4.1* $\leftrightarrow$ $[100]$ 8 1.8 x 4.7* $\leftrightarrow$ $[010]$ 8 1.8 x 4.7*



8-ring viewed along [001]



8-ring viewed along [100]



8-ring viewed along [010]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6/mmm, a = 14.2Å, c = 11.5Å												
<b>Coordination sequences</b>	T <sub>1</sub> (12, m)	4	12	23	41	64	92	128	167	207	259	5.5.	5.5.5.6
and vertex symbols:	T <sub>2</sub> (12, m)	4	11	24	41	63	91	128	171	214	259	4.5.	5.6.5.6
	T <sub>3</sub> (6, mm2)	4	12	25	42	68	90	122	167	210	268	5.5.5	5.5.5.6
	T <sub>4</sub> (4, 3m)	4	12	24	36	61	101	133	156	204	256	5.5.5	5.5.5.5
Secondary building units:	combinatio	ns	only	/									

Loop configuration of **T-Atoms:** 



Isotypic framework structures: \*Dodecasil 1H<sup>(1)</sup>

#### **References:**

(1) Gerke, H. and Gies, H. Z. Kristallogr., 166, 11-22 (1984)

# Crystal chemical data: $|C_5H_{11}N (N_2)_5|$ [Si34 O68]-DOH<br/> $C_5H_{11}N = piperidine$ <br/>hexagonal, P6/mmm, a = 13.783Å, c = 11.190Å (1)Framework density:18.5 T/1000Å<sup>3</sup>Channels:apertures formed by 6-rings only



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 18.9$ Å, $b = 23.4$ Å, $c = 8.5$ Å											
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1  (16, 1) \\ T_2  (16, 1) \\ T_3  (16, 1) \\ T_4  (8, m) \\ T_5  (8, m) \end{array}$	4 4 4 4	10 10 12 12 12	20 20 24 22 23	34 35 38 33 37	54 54 55 53 52	77 77 76 80 74	107 106 105 109 107	140 138 143 143 143	175 177 184 179 183	218 221 223 217 223	$\begin{array}{c} 4{\cdot}6{\cdot}4{\cdot}6_{2}{\cdot}5{\cdot}6\\ 4{\cdot}6{\cdot}4{\cdot}6_{2}{\cdot}5{\cdot}6\\ 5{\cdot}6_{2}{\cdot}6{\cdot}6_{2}{\cdot}6{\cdot}6_{2}\\ 5{\cdot}6{\cdot}5{\cdot}6{\cdot}6{\cdot}6{\cdot}6_{2}\\ 5{\cdot}6_{2}{\cdot}5{\cdot}6_{2}{\cdot}6_{2}{\cdot}6_{2}{\cdot}6_{2}\end{array}$
Secondary building units:	5-3											
Loop configuration of T-Atoms:		-1,2	_			T <sub>3-5</sub>						
Isotypic framework structures:	*UTD-1F <sup>(1</sup> UTD-1 <sup>(2)</sup>	)										

- (1) Wessels, T., Baerlocher, C., McCusker, L.B. and Creyghton, E.J. J. Am. Chem. Soc., **121**, 6242-6247 (1999)
- (2) Lobo, R.F., Tsapatsis, M., Freyhardt, C.C., Khodabandeh, S., Wagner, P., Chen, C.Y., Balkus, K.J., Zones, S.I. and Davis, M.E. *J. Am. Chem. Soc.*, **119**, 8474-8484 (1997)

# DON

Crystal chemical data:	$ ((Cp^*)_2Co)_2^+ F_{1.5}^-(OH)_{0.5} $ [Si <sub>64</sub> O <sub>128</sub> ]- <b>DON</b> Cp* = pentamethylcyclopentadiene monoclinic, P1c1, a = 14.970Å, b = 8.476Å, c = 30.028Å, $\beta$ = 102.65° <sup>(1)</sup>
Framework density:	17.2 T/1000Å <sup>3</sup>
Channels:	[010] <b>14</b> 8.1 x 8.2*



14-ring viewed along [010]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /mmc, a = 13.2Å, c = 15.0Å									
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5-8 5-8								
Secondary building units:	6 or 4									
Loop configuration of T-Atoms:										
Framework description:	ABBACC sequence of 6-rings									
Isotypic framework structures:	*TMA-E (Aiello and Barrer) <sup>(1,2)</sup> Bellbergite <sup>(3)</sup>									

- (1) Aiello, R. and Barrer, R.M. J. Chem. Soc. (A), 1470-1475 (1970)
- (2) Meier, W.M. and Groner, M. J. Solid State Chem., 37, 204-218 (1981)
- (3) Rüdinger, B., Tillmanns, E. and Hentschel, G. Miner. Petrol., 48, 147-152 (1993)

Crystal chemical data:	$ (C_4H_{12}N^+)_2Na^+_7 (H_2O)_{26}  [Al_9Si_{27} O_{72}]-EAB$ $C_4H_{12}N^+ =$ tetramethylammonium hexagonal, P6 <sub>3</sub> /mmc, a = 13.28Å, c = 15.21Å <sup>(2)</sup>
Framework density:	15.5 T/1000Å <sup>3</sup>
Channels:	⊥ [001] <b>8</b> 3.7 x 5.1**



8-ring viewed normal to [001]



framework viewed normal to [001]

Idealized cell constants:	tetragonal, $P\overline{4}m2$ , $a = 6.9$ Å, $c = 6.4$ Å									
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$								
Secondary building units:	4=1									
Loop configuration of T-Atoms:										
Isotypic framework structures:	*Edingtonite <sup>(1-3)</sup> [Co-Al-P-O]- <b>EDI</b> <sup>(4)</sup> [Co-Ga-P-O]- <b>EDI</b> <sup>(4)</sup>	Linde F <sup>(7)</sup> Synthetic edingtonite <sup>(8)</sup> Tetragonal edingtonite <sup>(9)</sup>								

Zeolite  $N^{(10)}$  (not to be confused

with Linde N)

#### **References:**

(1) Taylor, W.H. and Jackson, R. Z. Kristallogr., 86, 53-64 (1933)

K-F<sup>(5,6)</sup>

- (2) Galli, E. Acta Crystallogr., B32, 1623-1627 (1976)
- (3) Kvick, Å. and Smith J.V. J. Chem. Phys., 79, 2356-2362 (1983)
- (4) Bu, X., Gier, T.E., Feng, P. and Stucky, G.D. Chem. Mater., 10, 2546-2551 (1998)
- (5) Barrer, R.M. and Baynham, J.W. J. Chem. Soc., 2882-2891 (1956)
- (6) Baerlocher, Ch. and Barrer, R.M. Z. *Kristallogr.*, **140**, 10-26 (1974)
- (7) Sherman, J.D. ACS Sym. Ser., 40, 30-42 (1977)
- (8) Ghobarkar, H. and Schaef, O. Cryst. Res. Technol., 32, 653-657 (1997)
- (9) Mazzi, F., Galli, E. and Gottardi, G. N. Jb. Miner. Mh., 373-382 (1984)
- (10) Christensen, A.N. and Fjellvåg, H. Acta Chemica Scand., 51, 969-973 (1997)

Crystal chemical data:	$\begin{aligned} & \text{Ba}^{2+}_{2}(\text{H}_{2}\text{O})_{8}  \text{ [Al}_{4}\text{Si}_{6}\text{ O}_{20}\text{]-EDI} \\ &\text{orthorhombic, P2}_{1}2_{1}2, a = 9.550\text{ Å, } b = 9.665\text{ Å, } c = 6.523\text{ Å}^{(2)} \\ &(\text{Relationship to unit cell of Framework Type:} \\ &a' = a \cdot \text{sqrt}(2), b' = b \cdot \text{sqrt}(2), c' = c \\ &\text{or, as vectors, } a' = a + b, b' = b - a, c' = c) \end{aligned}$
Framework density:	16.6 T/1000Å <sup>3</sup>
Channels:	<110> 8 2.8 x 3.8** $\leftrightarrow$ [001] 8 2.0 x 3.1* (variable due to considerable flexibility of the framework)



8-ring viewed along <110>



8-ring viewed along [001] (variable)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /mmc, a = 17.2Å, c = 28.1Å												
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1 (24,1) \\ T_2 (24,1) \\ T_3 (24,1) \\ T_4 (24,1) \end{array}$	4 4 4 4	9 1 9 1 9 1 9 1 9 1	6 25 6 25 6 25	37 37 37 37	53 53 53 53	73 73 73 73	96 96 97 96	121 121 124 120	148 148 152 145	4·4·4·6·6·12 4·4·4·6·6·12 4·4·4·6·6·12 4·4·4·6·6·12		
Secondary building units:	6-6 or 6 or 4												
Loop configuration of T-Atoms:		-1-4											
Framework description:	structural derivative of hexagonal diamond and tridymite, respetively												
Isotypic framework structures:	*EMC-2 <sup>(1,2)</sup> CSZ-1 (EMT-FAU structural intermediate) <sup>(3)</sup> ECR-30 (EMT-FAU structural intermediate) <sup>(4)</sup> ZSM-20 (EMT-FAU structural intermediate) <sup>(5)</sup> ZSM-3 (EMT-FAU structural intermediate) <sup>(6)</sup>												
Alternate designation:	Breck struc BSS (impro hexagonal	ture oper) fauja	six site	(imp	oper)	1							

Crystal chemical data:	$\begin{split} & Na^{+}_{21} (C_{12}H_{24}O_{6})_{4}  \ [Al_{21}Si_{75} \ O_{192}]\text{-}EMT \\ &C_{12}H_{24}O_{6} = 18\text{-}crown\text{-}6 \\ &hexagonal, P6_{3}/mmc, \ a = 17.374\text{\AA}, \ c = 28.365\text{\AA}^{\ (2)} \end{split}$
Framework density:	12.9 T/1000Å <sup>3</sup>
Channels:	$[001] \ 12 \ 7.3 \ \mathbf{x} \ 7.3^* \leftrightarrow \perp [001] \ 12 \ 6.5 \ \mathbf{x} \ 7.5^{**}$



12-ring viewed along [001]



12-ring viewed normal to [001]

- (1) Delprato, F., Delmotte, L., Guth, J.L. and Huve, L. Zeolites, 10, 546-552 (1990)
- (2) Baerlocher, Ch., McCusker, L.B. and Chiappetta, R. Microporous Materials, 2, 269-280 (1994)
- (3) Barrett, M.G. and Vaughan, D.E.W. UK Patent GB 2,076,793 (1981)
- (4) Vaughan, D.E.W. *E. Patent* 0,351,461 (1989)
- (5) Newsam, J.M., Treacy, M.M.J., Vaughan, D.E.W., Strohmaier, K.G. and Mortier, W.J. *Chem. Commun.*, 493-495 (1989)
- (6) Kokotailo, G.T. and Ciric, J. Adv. Chem. Ser., 101, 109-121 (1971)



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 9.1Å, b = 17.5Å, c = 10.4Å, $\beta$ = 124.9°
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	5-1
Loop configuration of T-Atoms:	$T_1$ $T_{2,3}$
Isotypic framework structures:	*Epistilbite <sup>(1-4)</sup> Synthetic epistilbite <sup>(5)</sup>

- (1) Kerr, I.S. Nature, 202, 589 (1964)
- (2) Perrotta, A.J. Mineral. Mag., 36, 480-490 (1967)
- (3) Alberti, A., Galli, E. and Vezzalini, G. Z. Kristallogr., **173**, 257-265 (1985)
- (4) Yang, P. and Armbruster, T. Eur. J. Mineral., 8, 263-271 (1996)
- (5) Ghobarkar, H. Cryst. Res. Technol., 151-1573 (1984)

## **Epistilbite**

## **Type Material**

Crystal chemical data:

$$\begin{split} |Ca^{2+}{}_3\ (H_2O)_{16}|\ [Al_6Si_{18}\ O_{48}]\text{-}EPI \\ monoclinic,\ C2/m,\ a=9.08\text{\AA},\ b=17.74\text{\AA},\ c=10.25\text{\AA},\ \beta=124.54^{\circ\ (2)} \end{split}$$

Framework density:

17.6 T/1000Å<sup>3</sup>

Channels:

 $[100] \ \textbf{10} \ \textbf{3.4} \ \textbf{x} \ \textbf{5.6}^* \leftrightarrow [001] \ \textbf{8} \ \textbf{3.7} \ \textbf{x} \ \textbf{4.5}^*$ 



10-ring viewed along [100] associated



with second 10-ring along [100]



8-ring viewed along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, $P6_3$ /mmc, a = 13.1Å, c = 15.2Å								
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$								
Secondary building units:	6 or 4								
Loop configuration of T-Atoms:									
Framework description:	AABAAC sequence of 6-rings								
Isotypic framework structures:	*Erionite <sup>(1-3)</sup> AlPO-17 plus numerous compositional variants <sup>(4-6)</sup> LZ-220 <sup>(7)</sup> Linde T ( <b>ERI-OFF</b> structural intermediate) <sup>(8)</sup>								

- (1) Staples, L.W. and Gard, J.A. Mineral. Mag., 32, 261-281 (1959)
- (2) Kawahara, A. and Curien, H. Bull. Soc. fr. Minéral. Cristallogr., 92, 250-256 (1969)
- (3) Gard, J.A. and Tait, J.M. In *Proc. 3rd Int. Conf. Molecular Sieves*, (ed. J.B. Uytterhoeven), pp. 94-99 (1973), Leuven University Press, Leuven
- (4) Pluth, J.J., Smith, J.V. and Bennett, J.M. Acta Crystallogr., C42, 283-286 (1986)
- (5) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)

**Erionite** 

8-ring viewed normal to [001]

5.1

Crystal chemical data:	$ (Ca^{2+},Na^{+}_{2})_{3.5} K^{+}_{2} (H_{2}O)_{27}  [Al_{9}Si_{27} O_{72}]-ERI$ hexagonal, P6 <sub>3</sub> /mmc, a = 13.27Å, c = 15.05Å <sup>(3)</sup>								
Framework density:	15.7 T/1000Å <sup>3</sup>								
Channels:	$\perp$ [001] <b>8</b> 3.6 x 5.1***								
3.6									

5.1

#### **References (cont.):**

- (6) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In *Proc. 7th Int. Zeolite Conf.*, (eds. Y. Murakami, A. Iijima and J.W. Ward), pp. 103-112 (1986), Kodansha, Tokyo
- (7) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (8) Breck, D.W. Zeolite Molecular Sieves, p. 173 (1974), Wiley, New York



framework viewed along [010]

Idealized cell constants:	orthorhor	nbic	, Pn	ma,	a = 1	9.7Å,	, b =	12.2	2Å, c	c = 22	2.8Å	
Coordination sequences and vertex symbols:	$T_{1} (8, 1) T_{2} (8, 1) T_{3} (8, 1) T_{4} (8, 1) T_{5} (8, 1) $	4 4 4 4	10 10 10 10	20 20 21 21 22	35 36 36 36 36	56 58 57 56 56	82 82 82 82 78	111 109 111 113 110	143 144 145 145 148	180 186 183 180 184	228 230 231 224 225	$4 \cdot 5 \cdot 4 \cdot 5 \cdot 6 \cdot 8$ $4 \cdot 4 \cdot 5 \cdot 6 \cdot 6 \cdot 8$ $4 \cdot 4 \cdot 5 \cdot 8 \cdot 6 \cdot 6$ $4 \cdot 4 \cdot 5 \cdot 6 \cdot 6 \cdot 8$ $4 \cdot 6 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
Secondary building units:	T <sub>6</sub> (8, 1) 6-2	4	11	20	37	54	82	112	142	182	226	4.5.5.5.6.6
Loop configuration of T-Atoms:		] T <sub>1</sub>	[			T <sub>2-4</sub>	_			- 5,6		
Isotypic framework structures:	*ERS-7 <sup>(1</sup>	,2)										

- (1) Campbell, B.J., Bellussi, G., Carluccio, L., Perego, G., Cheetham, A.K., Cox, D.E. and Millini, R. *Chem. Commun.*, 1725-1726 (1998)
- (2) Millini, R., Perego, G., Carluccio, L., Bellussi, G., Cox, D.E., Campbell, B.J. and Cheetham, A.K. In *Proc. 12th Int. Zeolite Conf.*, (eds. M.M.J. Treacy, B.K. Marcus, M.E. Bisher and J.B. Higgins), pp. 541-548 (1999), MRS, Warrendale, PA

ERS-7

# **Type Material**

Crystal chemical data:	$ H^{+}_{5.06}Na^{+}_{0.07} $ [Al <sub>5.13</sub> Si <sub>42.87</sub> O <sub>96</sub> ]-ESV orthorhombic, Pnma, a = 9.780Å, b = 12.412Å, c = 22.861Å <sup>(2)</sup>						
Framework density:	17.3 T/1000Å <sup>3</sup>						
Channels:	[010] <b>8</b> 3.5 x 4.7*						
3.5	4.7						

8-ring viewed along [010]



framework viewed along [100]

Idealized cell constants:	orthorhom	bic	, Cn	nma	, a =	13.9	$\partial \mathbf{A}, \mathbf{b} = 2$	2.9Å	, c =	20.6	Å
<b>Coordination sequences</b>	T <sub>1</sub> (16, 1)	4	11	21	36	59	92 129	167	197	246	$4 \cdot 6 \cdot 5 \cdot 5 \cdot 5_2 \cdot 10$
and vertex symbols:	T <sub>2</sub> (16, 1)	4	12	25	41	64	88 122	160	202	256	5.6.5.6.5.6
	T <sub>3</sub> (16, 1)	4	12	23	38	60	89 124	159	194	248	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
	T <sub>4</sub> (16, 1)	4	12	22	39	59	91 124	160	206	257	$5 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10$
	T <sub>5</sub> (8, m)	4	12	20	31	61	88 120	159	197	248	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 6_2$
	T <sub>6</sub> (8, m)	4	12	20	34	57	92 131	164	202	236	$5 \cdot 5_2 \cdot 5 \cdot 5_2 \cdot 12_2 \cdot *$
	T <sub>7</sub> (8, m)	4	12	24	39	60	91 126	161	195	243	$5 \cdot 6 \cdot 5 \cdot 6 \cdot 5 \cdot 6_2$
	T <sub>8</sub> (8, m)	4	12	24	36	56	90 127	157	197	236	5.5.5.5.12 <sub>4</sub> .*
	T <sub>9</sub> (8, m)	4	11	23	45	67	88 115	162	218	261	4.6.5.5.5.5
	$T_{10}(8, m)$	4	11	24	39	68	92 118	156	213	268	4.10.5.5.5.5

Secondary building units: combinations only

Loop configuration of T-Atoms:



Isotypic framework	$*EU-1^{(1,2)}$
structures:	TPZ-3 <sup>(3)</sup>
	ZSM-50 <sup>(4)</sup>

- (1) Casci, J.L., Lowe, B.M. and Whittam, T.V. U.S. Patent 4,537,754, (1985)
- (2) Briscoe, N.A., Johnson, D.W., Shannon, M.D., Kokotailo, G.T. and McCusker, L.B. Zeolites, 8, 74-76 (1988)
- (3) Sumitani, K., Sakai, T., Yamasaki, Y. and Onodera, T. E. Patent EP 51318 (1982)
- (4) Rohrbaugh, W.J. private communication

# EUO

Crystal chemical data:

 $|Na^{+}_n~(H_2O)_{26}|$  [Al\_nSi\_{112-n}~O\_{224}]-EUO , n<19, typically  $n\sim3.6$  orthorhombic, Cmma,  $a=13.695 \text{\AA},~b=22.326 \text{\AA},~c=20.178 \text{\AA}^{~(2)}$ 

Framework density: 18.2 T/1000Å<sup>3</sup>

Channels:

10.2 1/1000/1

[100] **10** 4.1 x 5.4\* (with large side pockets)



10-ring viewed along [100]



- (1) Bergerhoff, G., Baur, W.H. and Nowacki, W. N. Jb. Miner. Mh., 193-200 (1958)
- (2) Baur, W.H. Am. Mineral., **49**, 697-704 (1964)

Crystal chemical data:	$ (Ca^{2+},Mg^{2+}Na^{+}_{2})_{29} (H_{2}O)_{240}  [Al_{58}Si_{134} O_{384}]-FAU cubic, Fd\overline{3}m, a = 24.74 \text{\AA}^{(2)}$
Framework density:	12.7 T/1000Å <sup>3</sup>
Channels:	<111> <b>12</b> 7.4 x 7.4***



12-ring viewed along <111>

#### **References (cont.):**

- (3) Barrer, R.M., Baynham, J.W., Bultitude, F.W. and Meier, W.M. J. Chem. Soc., 195-208 (1959)
- (4) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
- (5) Gier, T.E. and Stucky, G.D. Zeolites, 12, 770-775 (1992)
- (6) Barrett, M.G. and Vaughan, D.E.W. UK Patent GB 2,076,793 (1981)
- (7) Vaughan, D.E.W. E. Patent 0,351,461 (1989)
- (8) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (9) Milton, R.M. U.S. Patent 2,882,244 (1959)
- (10) Olson, D.H. J. Phys. Chem., 74, 2758-2764 (1970)
- (11) Breck, D.W. U.S. Patent 3,130,007 (1964)
- (12) Costenoble, M.L., Mortier, W.J. and Uytterhoeven, J.B. J. Chem. Soc., Faraday Trans. 1, 72, 1877-1883 (1976)
- (13) Lok, B.M., Messina, C.A., Patton, R.L., Gajek, R.T., Cannan, T.R. and Flanigen, E.M. J. Am. Chem. Soc., 106, 6092-6093 (1984)
- (14) Hriljac, J.J., Eddy, M.M., Cheetham, A.K., Donohue, J.A. and Ray, G.J. J. Solid State Chem., 106, 66-72 (1993)
- (15) Newsam, J.M., Treacy, M.M.J., Vaughan, D.E.W., Strohmaier, K.G. and Mortier, W.J. Chem. Commun., 493-495 (1989)
- (16) Kokotailo, G.T. and Ciric, J. Adv. Chem. Ser., 101, 109-121 (1971)



<b>Coordination sequences</b>	$T_1$ (16, 1)	4	12	21	39	66	95	126	169	221	265	5.5.5.5.5.5.8
and vertex symbols:	$T_2(8, m)$	4	12	27	43	62	97	139	172	206	264	$5 \cdot 8 \cdot 5 \cdot 8 \cdot 5_2 \cdot 6$
-	$T_{3}(8, m)$	4	12	20	35	67	104	121	157	223	276	$5 \cdot 5_2 \cdot 5 \cdot 5_2 \cdot 10_2 \cdot 12_2$
	T <sub>4</sub> (4, 2mm)	4	12	23	40	66	96	131	164	214	272	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 6$

Secondary building units: 5-1

Loop configuration of T-Atoms:

T<sub>1-4</sub>

Isotypic framework structures: \*Ferrierite<sup>(1)</sup> [Ga-Si-O]-**FER**<sup>(2)</sup> [Si-O]-**FER**<sup>(3,4)</sup> FU-9<sup>(5)</sup> ISI-6<sup>(6)</sup>  $\begin{array}{l} Monoclinic \ ferrierite^{(7)}\\ NU-23^{(8)}\\ Sr-D^{(9)}\\ ZSM-35^{(10)} \end{array}$ 

- (1) Vaughan, P.A. Acta Crystallogr., **21**, 983-990 (1966)
- (2) Jacob, N.E., Joshi, P.N., Shaikh, A.A. and Shiralkar, V.P. Zeolites, 13, 430-434 (1993)
- (3) Gies, H. and Gunawardane, R.P. Zeolites, 7, 442-445 (1987)
- (4) Morris, R.E., Weigel, S.J., Henson, N.J., Bull, L.M., Janicke, M.T., Chmelka, B.F. and Cheetham, A.K. *J. Am. Chem. Soc.*, **116**, 11849-11855 (1994)
- (5) Seddon, D. and Whittam, T.V. E. Patent B-55,529 (1985)
- (6) Morimoto, N., Takatsu, K. and Sugimoto, M. U.S. Patent 4,578,259 (1986)
- (7) Gramlich-Meier, R., Gramlich, V. and Meier, W.M. Am. Mineral., 70, 619-623 (1985)

Ferrierite

## **Type Material**

## **FER**

Crystal chemical data:

$$\begin{split} |Mg^{2+}{}_{2}Na^{+}{}_{2}\ (H_{2}O)_{18}|\ [Al_{6}Si_{30}\ O_{72}]\text{-}\textbf{FER}\\ orthorhombic,\ Immm,\ a=19.156\text{\AA},\ b=14.127\text{\AA},\ c=7.489\text{\AA}^{\ (1)} \end{split}$$

Framework density: 17.8 T/1000Å<sup>3</sup>

**Channels:** 

[001] **10** 4.2 x 5.4\*  $\leftrightarrow$  [010] **8** 3.5 x 4.8\*



10-ring viewed along [001]



8-ring viewed along [010]

**References (cont.):** 

- (8) Whittam, T.V. *E. Patent A-103*,981 (1984)
- (9) Barrer, R.M. and Marshall, D.J. J. Chem. Soc., 2296-2305 (1964)
- (10) Plank, C.J., Rosinski, E.J. and Rubin, M.K. U.S. Patent 4,016,245 (1977)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $P\overline{3}m1$ , a = 12.7Å, c = 25.3Å											
Coordination sequences and vertex symbols:	$T_{1} (12, 1) T_{2} (12, 1) T_{3} (12, 1) T_{4} (12, 1) T_{5} (6, 2) T_{6} (6, 2)$	4 4 4 4 4 4	10 10 10 10 10 10	20 20 20 20 20 20 20	34 34 34 34 34 34	52 52 52 53 52 52 54	74 74 74 76 74 78	100 101 101 102 100 104	130 133 133 132 130 134	165 168 168 166 164 168	205 206 206 206 202 202	$4 \cdot 4 \cdot 6 \cdot 6 \cdot 6 \cdot 6$ $4 \cdot 4 \cdot 6 \cdot 6 \cdot 6 \cdot 6$ $4 \cdot 6 \cdot 4 \cdot 6 \cdot 6 \cdot 6$ $4 \cdot 4 \cdot 6 \cdot 6 \cdot 6 \cdot 6$ $4 \cdot 4 \cdot 6 \cdot 6 \cdot 6 \cdot 6$
Secondary building units:	6											
Loop configuration of T-Atoms:		Γ <sub>1,2,</sub>	4-6			 T <sub>3</sub>						
Framework description:	ABCABA	CA	BC	sequ	ienc	e of 6	5-rir	ngs				
Isotypic framework structures:	*Franzinit	e <sup>(1)</sup>										

(1) Ballirano, P., Bonaccorsi, E., Maras, A. and Merlino, S. Can. Mineral., 38, 657-668 (2000)

Franzinite	Type Material					
Crystal chemical data:	$ (Na,K)^{+}_{30} Ca^{2+}_{10} (SO_4)^{2-}_{10} (H_2O)_2  [Al_{30}Si_{30} O_{120}]$ - <b>FRA</b> trigonal, P321, a = 12.916Å, c = 26.543Å <sup>(1)</sup>					
Framework density:	15.6 T/1000Å <sup>3</sup>					
Channels:	apertures formed by 6-rings only					



- **References:**
- (1) Fischer, K. and Schramm, V. Adv. Chem. Ser. , 101, 250-258 (1971)
- (2) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
- (3) Feng, P., Bu, X., Gier, T.E. and Stucky, G.D. Microporous and Mesoporous Materials, 23, 221-229 (1998)
- (4) Cowley, A.R. and Chippindale, A.M. Chem. Commun., 673-674 (1996)
- (5) Yuan, H.M., Chen, J.S., Zhu, G.S., Li, J.Y., Yu, J.H., Yang, G.D. and Xu, R. *Inorg. Chem.*, **39**, 1476-1479 (2000)
#### **Type Material**

Crystal chemical data:	$ Ca^{2+}_{4} (H_{2}O)_{16}  [Al_{8}Si_{8} O_{32}]$ - <b>GIS</b> monoclinic, P112 <sub>1</sub> /a $a = 9.843$ Å, $b = 10.023$ Å, $c = 10.616$ Å, $\gamma = 92.417^{\circ (1)}$ (Relationship to unit cell of Framework Type: $a' = a, b' = b, c' = c$ )
Framework density:	15.3 T/1000Å <sup>3</sup>
Channels:	{[100] <b>8</b> 3.1 x 4.5 $\leftrightarrow$ [010] <b>8</b> 2.8 x 4.8}*** (variable due to considerable flexibility of the framework)



8-ring viewed along [100]

See Appendix A for 8-ring viewed along [010]

#### **References** (cont.):

- (6) Cho, H.H., Kim, S.H., Kim, Y.G., Kim, Y.C., Koller, H., Camblor, M.A. and Hong, S.B. *Chem. Mater.*, **12**, 2292-2300 (2000)
- (7) Chippindale, A.M., Cowley, A.R. and Peacock, K.J. *Microporous and Mesoporous Materials*, **24**, 133-141 (1998)
- (8) Kniep, R., Schäfer, G., Engelhardt, H. and Boy, I. Angew. Chem. Int. Ed., 38, 3642-3644 (1999)
- (9) Alberti, A. and Vezzalini, G. Acta Crystallogr., B35, 2866-2869 (1979)
- (10) Artioli, G. Am. Mineral., 77, 189-196 (1992)
- (11) Artioli, G. and Marchi, M. Powder Diffraction, 14, 190-194 (1999)
- (12) McCusker, L.B., Baerlocher, Ch. and Nawaz, R. Z. Kristallogr., 171, 281-289 (1985)
- (13) Håkansson, U., Fälth, L. and Hansen, S. Acta Crystallogr., C46, 1363-1364 (1990)
- (14) Albert, B.R., Cheetham, A.K., Stuart, J.A. and Adams, C.J. *Microporous and Mesoporous Materials*, **21**, 133-142 (1998)
- (15) Pluth, J.J., Smith, J.V. and Bennett, J.M. J. Am. Chem. Soc., 111, 1692-1698 (1989)
- (16) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. Pure Appl. Chem., 58, 1351-1358 (1986)
- (17) Flanigen, E.M., Lok, B.M., Patton, R.L. and Wilson, S.T. In *Proc. 7th Int. Zeolite Conf.*, (eds. Y. Murakami, A. Iijima and J.W. Ward), pp. 103-112 (1986), Kodansha, Tokyo
- (18) Baerlocher, Ch. and Meier, W.M. Z. Kristallogr., 135, 339-354 (1972)
- (19) Hansen, S., Håkansson, U. and Fälth, L. Acta Crystallogr., C46, 1361-1362 (1990)
- (20) Helliwell, M., Kaucic, V., Cheetham, G.M.T., Harding, M.M., Kariuki, B.M. and Rizkallah, P.J. Acta Crystallogr., B49, 413-420 (1993)
- (21) Schropfer, L and Joswig, W. Eur. J. Mineral., 9, 53-65 (1997)
- (22) Ghobarkar, H. and Schaef, O. Mater. Res. Bull., 34, 517-525 (1999)
- (23) Baerlocher, Ch. and Meier, W.M. Helv. Chim. Acta, 53, 1285-1293 (1970)



framework viewed along [001]

Idealized cell constants:	hexagonal, $P6_3$ /mmc, a = 13.7Å, c = 9.9Å
Coordination sequences and vertex symbols:	$T_{1}(24, 1)  4  9  17  29  45  65  89  116  144  175 \qquad \qquad 4 \cdot 4 \cdot 4 \cdot 8 \cdot 6 \cdot 8$
Secondary building units:	6-6 or 8 or 4-2 or 6 or 4
Loop configuration of T-Atoms:	
Framework description:	AABB sequence of 6-rings
Isotypic framework structures:	*Gmelinite <sup>(1)</sup> K-rich gmelinite <sup>(2)</sup> Synthetic fault-free gmelinite <sup>(3)</sup>
Alternate designation:	sarcolite (discredited)

- (1) Fischer, K. N. Jb. Miner. Mh., 1-13 (1966)
- (2) Vezzalini, G., Quartieri, S. and Passaglia, E. N. Jb. Miner. Mh., 504-516 (1990)
- (3) Daniels, R.H., Kerr, G.T. and Rollmann, L.D. J. Am. Chem. Soc., 100, 3097-3100 (1978)

Gmelinite

## **Type Material**

Crystal chemical data:

$$\begin{split} |(Ca^{2+},Na^{+}_{2})_{4}~(H_{2}O)_{24}|~[Al_{8}Si_{16}~O_{48}]\text{-}GME \\ hexagonal,~P6_{3}/mmc,~a=13.75\text{\AA},~c=10.05\text{\AA}^{~(1)} \end{split}$$

Framework density: 14.6 T/1000Å<sup>3</sup>

Channels:

 $[001] \ \mathbf{12} \ 7.0 \ge 7.0^* \leftrightarrow \perp [001] \ \mathbf{8} \ 3.6 \ge 3.9^{**}$ 



12-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed along [001]

Idealized cell constants:	orthorhom	bic,	Cn	nmn	1, a =	= 16.	9Å,	b = 2	20.4	Å, c =	= 5.3Å			
<b>Coordination sequences</b>	T <sub>1</sub> (8, 1)	4	12	21	39	63	85	117	154	192	242		5.6.5.6.5 <sub>2</sub> .6	5
and vertex symbols:	$T_2(8, 1)$	4	12	25	38	57	86	119	158	194	233	5	·6·5·6·6·12	6
	$T_3(8, 1)$	4	11	22	38	58	86	121	156	191	229		4.62.5.6.5.6	5
	$T_4(8, 1)$	4	11	22	38	63	91	115	147	195	244		$4 \cdot 6_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$	5
Secondary building units:	5-3													
Loop configuration of T-Atoms:														
	, I	$\Gamma_{1,2}$				T <sub>3,4</sub>								

Isotypic framework \*GUS-1<sup>(1)</sup>

**References:** 

(1) Plévert, J., Kubota, Y., Honda, T., Okubo, T. and Sugi, Y. Chem. Commun., 2363-2364 (2000)

GUS-1

# **Type Material**

Crystal chemical data:	[Si <sub>32</sub> O <sub>64</sub> ]-GON orthorhombic, C222, a = 16.421Å, b = 20.054Å, c = $5.046Å^{(1)}$
Framework density:	19.3 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 5.4 x 6.8*



12-ring viewed along [001]



8-ring viewed along [001]



framework viewed along [110]

Idealized cell constants:	orthorhombic, C222 <sub>1</sub> , $a = 8.7$ Å, $b = 11.0$ Å, $c = 17.5$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2
Loop configuration of T-Atoms:	T <sub>1,3</sub> T <sub>2,4,5</sub>
Isotypic framework structures:	*Goosecreekite <sup>(1)</sup>

#### **References:**

(1) Rouse, R.C. and Peacor, D.R. Am. Mineral., 71, 1494-1501 (1986)

# **Type Material**

# G00

Crystal chemical data:	$\begin{split}  Ca^{2+}_{2} (H_{2}O)_{10}  & [Al_{4}Si_{12} O_{32}] \text{-} \textbf{GOO} \\ \text{monoclinic, } P12_{1}1, a &= 7.401\text{ Å}, b = 17.439\text{ Å}, c = 7.293\text{ Å}, \beta = 105.44^{\circ (1)} \\ (\text{Relationship to unit cell of Framework type:} \\ a' &= a/2\cos(\beta'/2), b' = c, c' = a/2\cos(\beta'/2) \\ \text{or, as vectors, } a' &= (a + b)/2, b' = c, c' = (a - b)/2) \end{split}$
Framework density:	17.6 T/1000Å <sup>3</sup>
Channels:	$[100] 8 2.8 \ge 4.0^* \leftrightarrow [010] 8 2.7 \ge 4.1^* \leftrightarrow [001] 8 2.9 \ge 4.7^*$



8-ring viewed along [100]



8-ring viewed along [010]



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 17.5Å, b = 17.6Å, c = 7.4Å, $\beta$ = 116.1°
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4-4=1
Loop configuration of T-Atoms:	$\begin{array}{ c c c c c }\hline \hline \\ \hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \hline \\ \\ \\ \hline \\$
Isotypic framework structures:	*Heulandite <sup>(1,2)</sup> Clinoptilolite <sup>(3)</sup> Dehydrated Ca,NH <sub>4</sub> -Heulandite <sup>(4)</sup> LZ-219 <sup>(5)</sup>
Alternate designation:	stilbite (mistake in older literature)

- (1) Merkle, A.B. and Slaughter, M. Am. Mineral., 52, 273-276 (1967)
- (2) Alberti, A. Tschermaks Min. Petr. Mitt., 18, 129-146 (1972)
- (3) Koyama, K. and Takeuchi, Y. Z. Kristallogr., 145, 216-239 (1977)
- (4) Mortier, W.J. and Pearce, J.R. Am. Mineral., **66**, 309-314 (1981)
- (5) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)

### Heulandite

#### **Type Material**

## HEU

Crystal chemical data:

$$\begin{split} |Ca^{2+}_{~4}~(H_2O)_{24}|~[Al_8Si_{28}~O_{72}]\text{-}\textbf{HEU} \\ monoclinic,~Cm,~a = 17.718\text{\AA},~b = 17.897\text{\AA},~c = 7.428\text{\AA},~\beta = 116.42^{\circ}~^{(2)} \end{split}$$

Framework density: 17.1 T/1000Å<sup>3</sup>

Channels:

{[001] **10** 3.1 x 7.5\* + **8** 3.6 x 4.6\*}  $\leftrightarrow$  [100] **8** 2.8x 4.7\* (variable due to considerable flexibility of the framework)



10-ring viewed along [001]



8-ring, also along [001]



8-ring viewed along [100]



- Barrett, P.A., Camblor, M.A., Corma, A., Jones, R.H. and Villaescusa, L.A. *Chem. Mater.*, 9, 1713-1715 (1997)
- (2) Valyocsik, E.W. WOP 9511196 (1995)
- (3) Chen, C.Y., Finger, L.W., Medrud, R.C., Crozier, P.A., Chan, I.Y., Harris, T.V. and Zones, S.I. *Chem. Commun.*, 1775-1776 (1997)

Crystal chemical data:	[Si <sub>32</sub> O <sub>64</sub> ]- <b>IFR</b> monoclinic, I12/m1 $a = 18.652$ Å, $b = 13.496$ Å, $c = 7.631$ Å, $\beta = 101.98^{\circ (1)}$ (Relationship to unit cell of Framework Type: as vectors, $\mathbf{a'} = \mathbf{a} + \mathbf{c}$ , $\mathbf{b'} = \mathbf{b}$ , $\mathbf{c'} = -\mathbf{c}$ )
Framework density:	17 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 6.2 x 7.2*



12-ring viewed along [001]

# Framework Type



framework viewed along [100]

Idealized cell constants:	tetragonal,	tetragonal, P4 <sub>2</sub> /mmc, a = 12.9Å, c = 25.7Å										
Coordination sequences and vertex symbols:	$T_{1} (16, 1) T_{2} (16, 1) T_{3} (16, 1) $	4 4 4	12 9 9	17 18 18	30 32 32	48 50 50	72 71 72	99 96 97	128 129 128	160 167 167	199 200 203	$5 \cdot 5 \cdot 5_2 \cdot 12_5 \cdot 6 \cdot 6 \\ 4 \cdot 5 \cdot 4 \cdot 6 \cdot 4 \cdot 12_7 \\ 4 \cdot 5 \cdot 4 \cdot 6 \cdot 4 \cdot 12_4$
	$T_4 (8, m)$ $T_5 (8, m)$	4 4	11 11	20 20	28 28	42 41	74 70	110 105	132 131	150 154	195 188	$4 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$ $4 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
Secondary building units:	6-2											
Loop configuration of T-Atoms:		- 1		/		T <sub>2,3</sub>				Γ <sub>4,5</sub>		
Isotypic framework structures:	*ITQ-7 <sup>(1)</sup>											

#### **References:**

(1) Villaescusa, L.A., Barrett, P.A. and Camblor, M.A. Angew. Chem., Int. Ed., 38, 1997-2000 (1999)

## **Type Material**

Crystal chemical data:	[Si <sub>64</sub> O <sub>128</sub> ]- <b>ISV</b>
	tetragonal, P4 <sub>2</sub> /mmc, a = 12.853 Å, c = 25.214Å $^{(1)}$

Framework density: 15.4 T/1000Å<sup>3</sup>

Channels:

 ${<}100{>}\,\mathbf{12}\;6.1\ge 6.5^{**} \leftrightarrow [001]\;\mathbf{12}\;5.9\ge 6.6^*$ 



12-ring viewed along <100>



12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 20.8$ Å, $b = 9.8$ Å, $c = 20.0$ Å	
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5.8 5.8 5.5 5.5
Secondary building units:	4	
Loop configuration of T-Atoms:	$\begin{array}{c c} & & \\ \hline \\ \hline \\ T_1 \end{array} \end{array} \begin{array}{c} \hline \\ T_2 \end{array} \begin{array}{c} \hline \\ T_{3,4} \end{array}$	
Isotypic framework structures:	*ITQ-3 <sup>(1)</sup>	

(1) Camblor, M.A., Corma, A., Lightfoot, P., Villaescusa, L.A. and Wright, P.A. Angew. Chem., Int. Ed., 36, 2659-2661 (1997)

## ITQ-3

# Type Material

Crystal chemical data:	[Si <sub>64</sub> O <sub>128</sub> ]- <b>ITE</b> orthorhombic, Cmcm, a = 20.622Å, b = 9.724Å, c = 19.623Å <sup>(1)</sup>
Framework density:	16.3 T/1000Å <sup>3</sup>

**Channels:** 

 $[010] \ \mathbf{8} \ 3.8 \ \mathrm{x} \ 4.3^* \leftrightarrow [001] \ \mathbf{8} \ 2.7 \ \mathrm{x} \ 5.8^*$ 



8-ring viewed along [010]







framework viewed along [100]

Idealized cell constants:	orthorhomb	oic,	Pm	ıma,	a =	5.3Å	., b =	= 7.5	Å, c	= 8.	2Å		
Coordination sequences and vertex symbols:	T <sub>1</sub> (4, m) T <sub>2</sub> (2, mm2)	4 4	10 12	21 24	39 36	61 56	81 86	107 118	148 146	192 176	228 228	4.6 6.	$5_2 \cdot 4 \cdot 6_2 \cdot 6 \cdot 8_2$ $6 \cdot 6 \cdot 6 \cdot 6_2 \cdot 6_2$
Secondary building units:	6												

Loop configuration of T-Atoms:



Isotypic framework structures: \*Na-J (Barrer and White)<sup>(1)</sup> Nepheline hydrate<sup>(2)</sup> (not related to nepheline) Synthetic |Na-|[Al-Si-O]-JBW<sup>(3)</sup>

- (1) Hansen, S. and Fälth, L. Zeolites, **2**, 162-166 (1982)
- (2) Rheinhardt, A., Hellner, E. and Ahsbahs, H. Fortsch. Mineral., 60, 175-176 (1982)
- (3) Ragimov, K.G., Chiragove, M.I., Mustafaev, N.M. and Mamedov, Kh.S. Sov. Phys. Dokl., 23, 697-698 (1978)

# JBW

Crystal chemical data:	$\begin{split} & \text{Na}_{3}^{+}(\text{H}_{2}\text{O})_{1.5}  \text{ [Al}_{3}\text{Si}_{3}\text{ O}_{12} \text{]-JBW} \\ &\text{orthorhombic, Pna2}_{1}, a = 16.426\text{\AA}, b = 15.014\text{\AA}, c = 5.224\text{\AA}^{(1)} \\ &(\text{Relationship to unit cell of Framework Type: a' = 2c, b' = 2b, c' = a)} \end{split}$
Framework density:	18.6 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 3.7 x 4.8*
4.8	

8-ring along [001]



framework viewed along [001]

Idealized cell constants:	cubic, $\text{Im}\overline{3}\text{m}$ , a = 18.6Å
Coordination sequences and vertex symbols:	$T_{1}(96, 1)  4  9  17  29  45  64  86  112  141  173 \qquad \qquad 4 \cdot 4 \cdot 4 \cdot 8 \cdot 6 \cdot 8$
Secondary building units:	6-6 or 6-2 or 8 or 6 or 4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*ZK-5 <sup>(1)</sup> (Cs,K)-ZK-5 <sup>(2,3)</sup> $P^{(4)}$ $Q^{(4)}$

- (1) Meier, W.M. and Kokotailo, G.T. Z. Kristallogr., **121**, 211-219 (1965)
- (2) Robson, H.E. U.S. Patent 3,720,753 (1973)
- (3) Parise, J.B., Shannon, R.D., Prince, E. and Cox, D.E. Z. Kristallogr., 165, 175-190 (1983)
- (4) Barrer, R.M. and Robinson, D. Z. Kristallogr., 135, 374-390 (1972)

Crystal chemical data:

$$\label{eq:1.1} \begin{split} &|Na^{+}_{30}\;(H_{2}O)_{98}|\;[Al_{30}Si_{66}\;O_{192}]\text{-}\textbf{KFI}\\ &\text{cubic, }Im\overline{3}m,\;a=18.75\text{\AA}^{\ (1)} \end{split}$$

Framework density:  $14.6 \text{ T}/1000 \text{\AA}^3$ 

Channels:

<100> **8** 3.9 x 3.9\*\*\* | <100> **8** 3.9 x 3.9\*\*\*



8-ring viewed along <100>



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 14.6Å, b = 12.9Å, c = 7.6Å, $\beta$ = 111.2°
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2 or 6
Loop configuration of T-Atoms:	T <sub>1-3</sub>
Isotypic framework structures:	*Laumontite <sup>(1-4)</sup> [Co-Ga-P-O]-LAU <sup>(5,6)</sup> [Fe-Ga-P-O]-LAU <sup>(6)</sup> [Mn-Ga-P-O]-LAU <sup>(6)</sup> Synthetic laumontite <sup>(8)</sup>
Alternate designation:	Leonhardite <sup>(7)</sup> (discredited)

- (1) Bartl, H. and Fischer, K. N. Jb. Miner. Mh., 33-42 (1967)
- (2) Amirov, S.T., Ilyukhin, V.V. and Belov, N.V. Dokl. Akad. Nauk SSSR, 174, 667- (1967)
- (3) Schramm, V. and Fischer Adv. Chem. Ser. , 101, 259-265 (1971)
- (4) Artioli, G. and Ståhl, K. Zeolites, 17, 249-255 (1993)
- (5) Chippindale, A.M. and Walton, R.I. Chem. Commun., 2453-2454 (1994)
- (6) Bond, A.D., Chippindale, A., Cowley, A.R., Readman, J.E. and Powell, A.V. Zeolites, 19, 326-333 (1997)
- (7) Lapham, D.L. Am. Mineral., 48, 683-689 (1963)
- (8) Ghobarkar, H. and Schaef, O. *Microporous and Mesoporous Materials*, 23, 55-60 (1998)

Crystal chemical data:	$ Ca^{2+}_{4}(H_2O)_{16} $ [Al <sub>8</sub> S monoclinic, Am, a = (Relationship to unit	<sup>1</sup> <sub>16</sub> O <sub>48</sub> ]- <b>LAU</b> 7.549Å, b = 14.740Å, c = 13.072Å, $\gamma$ = 111.9° <sup>(3)</sup> cell of Framework Type: a' = c, b' = a, c' = b, $\gamma' = \beta$ )
Framework density:	17.8 T/1000Å <sup>3</sup>	
Channels:	[100] <b>10</b> 4.0 x 5.3* (	contracts upon dehydration)
	<b>b o d</b>	h



10-ring viewed along [100]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , a = 13.2Å, c = 22.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6
Loop configuration of T-Atoms:	
Framework description:	AABCCABBC sequence of 6-rings
Isotypic framework structures:	*Levyne <sup>(1,2)</sup> NU-3 <sup>(6)</sup> AlPO-35 <sup>(3)</sup> SAPO-35 <sup>(7)</sup> CoDAF-4 <sup>(4)</sup> ZK-20 <sup>(8)</sup> LZ-132 <sup>(5)</sup>
Alternate designation:	Levynite (obsolete)

- (1) Barrer, R.M. and Kerr, I.S. Trans. Faraday Soc., 55, 1915-1923 (1959)
- (2) Merlino, S., Galli, E. and Alberti, A. Tschermaks Min. Petr. Mitt., 22, 117-129 (1975)
- (3) Zhu, G.S., Xiao, F.S., Qiu, S.L., Hun, P.C., Xu, R.R., Ma, S.J. and Terasaki, O. *Microporous Materials*, **11**, 269-273 (1997)
- (4) Barrett, P.A. and Jones, R.H. Phys. Chem. Chem. Phys., 2, 407-412 (2000)

Levyne

Crystal chemical data:	$ Ca^{2+}{}_{9}(H_{2}O)_{50} $ [Al <sub>18</sub> Si <sub>36</sub> O <sub>108</sub> ]-LE trigonal, R $\overline{3}$ m, a = 13.338Å, c =	23.014Å <sup>(2)</sup>
Framework density:	15.2 T/1000Å <sup>3</sup>	
Channels:	⊥ [001] <b>8</b> 3.6 x 4.8**	
3.6	4.8	3.6

8-ring viewed normal to [001]

#### **References (cont.):**

- (5) Tvaruzkova, Z., Tupa, M., Kiru, P., Nastro, A., Giordano, G. and Trifiro, F. Int. Zeolite Sym., Wurzburg, Extended Abstracts (1988)
- (6) McCusker, L.B. Mater. Sci. Forum, 133-136, 423-433 (1993)
- (7) Lok, B.M., Messina, C.A., Patton, R.L., Gajek, R.T., Cannan, T.R. and Flanigen, E.M. J. Am. Chem. Soc., 106, 6092-6093 (1984)
- (8) Kerr, G.T. U.S. Patent 3,459,676 (1969)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, $P\overline{6}m2$ , a = 12.3Å, c = 15.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6
Loop configuration of T-Atoms:	T <sub>1,3,4</sub> T <sub>2</sub>
Framework description:	ABABAC sequence of 6-rings
Isotypic framework structures:	*Liottite <sup>(1,2)</sup>

- (1) Merlino, S. and Orlandi, P. Am. Mineral., 62, 321-326 (1977)
- (2) Ballirano, P., Merlino, S. and Bonaccorsi, E. Can. Mineral., 34, 1021-1030 (1996)

Crystal chemical data:	$ Ca^{2+}_{8}(K^{+},Na^{+})_{16} (SO_{4}^{2-})_{5}Cl_{4}^{-} $ [Al <sub>18</sub> Si <sub>18</sub> O <sub>72</sub> ]-LIO hexagonal, P $\overline{6}$ , a = 12.870Å, c = 16.096Å <sup>(2)</sup>
Framework density:	17.6 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, $P6_3$ /mmc, a = 12.6Å, c = 10.3Å	
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
Secondary building units:	6-2 or 6	
Loop configuration of T-Atoms:		
Framework description:	ABAC sequence of 6-rings	
Isotypic framework structures:	*Losod <sup>(1,2)</sup> [Al-Ge-O]-LOS <sup>(3)</sup>  Li- [Be-P-O]-LOS <sup>(4)</sup> Bystrite <sup>(5)</sup>	

- (1) Sieber, W. and Meier, W.M. Helv. Chim. Acta, 57, 1533-1549 (1974)
- (2) Schicker, P. Ph.D. Thesis, ETH, Zürich, Switzerland, (1988)
- (3) Sokolov, Yu.A., Maksimov, B.A., Ilyukhin, V.V. and Belov, N.V. Sov. Phys. Dokl., 23, 789-791 (1978)
- (4) Harrison, W.T.A., Gier, T.E. and Stucky, G.D. Zeolites, 13, 242-248 (1993)
- (5) Pobedimskaya, E.A., Terent'eva, L.F., Sapozhnikov, A.N., Kashaev, A.A. and Dorokhova, G.I. Sov. Phys. Dokl., **36**, 553-555 (1991)

# **Type Material**

Crystal chemical data:	$ Na_{12}^{+}(H_2O)_{18} $ [A1 <sub>12</sub> Si <sub>12</sub> O <sub>48</sub> ]-LOS hexagonal, P6 <sub>3</sub> mc, a = 12.906Å, c = 10.541Å <sup>(2)</sup>
Framework density:	15.8 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed normal to [001]

Idealized cell constants:	tetragonal, P4 <sub>2</sub> /mmc, $a = 7.2$ Å, $c = 20.9$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	combinations only
Loop configuration of T-Atoms:	$\square_{T_1} \qquad \square_{T_2} \qquad \square_{T_3}$

Isotypic framework structures:

\*Lovdarite<sup>(1,2)</sup> Synthetic lovdarite<sup>(3)</sup>

- (1) Merlino, S. Acta Crystallogr. (Suppl.), A37, C189 (1981)
- (2) Merlino, S. Eur. J. Mineral., 2, 809-817 (1990)
- (3) Ueda, S., Koizumi, M., Baerlocher, Ch., McCusker, L.B. and Meier, W.M. *Preprints of Poster Papers, 7th Int. Zeolite Conf.*, pp. 23-24 (1986), Jap. Assoc. Zeolite, Tokyo

Lovdarite

# **Type Material**

# LOV

Crystal chemical data:	$ K_{4}^{+}Na_{12}^{+}(H_{2}O)_{18} $ [Be <sub>8</sub> Si <sub>28</sub> O <sub>72</sub> ]-LOV orthorhombic, Pma2, a = 39.576Å, b = 6.931Å, c = 7.153Å <sup>(2)</sup> (Relationship to unit cell of Framework Type: a' = 2c, b' = c' = a)
Framework density:	18.3 T/1000Å <sup>3</sup>
Channels:	$[010] 9 3.2 \ge 4.5^* \leftrightarrow [001] 9 3.0 \ge 4.2^* \leftrightarrow [100] 8 3.6 \ge 3.7^*$



9-ring viewed along [010]



9-ring viewed along [001]







framework viewed along [001]

Idealized cell constants:	cubic, $Pm\overline{3}m$ , a = 11.9Å	
Coordination sequences and vertex symbols:	$T_1(24, m)$ 4 9 17 28 42 60	81 105 132 162 4.6.4.6.4.8
Secondary building units:	8 or 4-4 or 6-2 or 4-2 or 4	
Loop configuration of T-Atoms:		
Isotypic framework structures:	*Linde Type $A^{(1,2)}$ [Al-Ge-O]-LT $A^{(3)}$ [Ga-P-O]-LT $A^{(4)}$ Alpha <sup>(5)</sup> LZ-215 <sup>(6)</sup>	N-A <sup>(7)</sup> SAPO-42 <sup>(8)</sup> ZK-21 <sup>(9)</sup> ZK-22 <sup>(9)</sup> ZK-4 <sup>(10)</sup>

- (1) Reed, T.B. and Breck, D.W. J. Am. Chem. Soc., 78, 5972-5977 (1956)
- (2) Gramlich, V. and Meier, W.M. Z. Kristallogr., 133, 134-149 (1971)
- (3) Barrer, R.M., Baynham, J.W., Bultitude, F.W. and Meier, W.M. J. Chem. Soc., 195-208 (1959)
- (4) Simmen, A., Patarin, J. and Baerlocher, Ch. In *Proc. 9th Int. Zeolite Conf.*, (eds. R. von Ballmoos, J.B. Higgins and M.M.J. Treacy), pp. 433-440 (1993), Butterworth-Heinemann, Boston
- (5) Wadlinger, R.L., Rosinski, E.J. and Plank, C.J. U.S. Patent 3,375,205 (1968)
- (6) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (7) Barrer, R.M. and Denny, P.J. J. Chem. Soc., 971-982 (1961)
- (8) Lok, B.M., Messina, C.A., Patton, R.L., Gajek, R.T., Cannan, T.R. and Flanigen, E.M. J. Am. Chem. Soc., 106, 6092-6093 (1984)
- (9) Kuehl, G.H. Inorg. Chem., 10, 2488-2495 (1971)
- (10) Kerr, G.T. Inorg. Chem., 5, 1537-1539 (1966)

## **Type Material**

# Crystal chemical data: $|Na^+_{12} (H_2O)_{27}|_8 [Al_{12}Si_{12} O_{48}]_8 - LTA$ cubic, Fm 3c, a = 24.61Å (2) (Relationship to unit cell of Framework Type: a' = b' = c' = 2a) Framework density: 12.9 T/1000Å<sup>3</sup> Channels: <100> 8 4.1 x 4.1\*\*\*



8-ring viewed along <100>



framework viewed normal to [001]

Idealized cell constants:	hexagonal, P6/mmm, a = $18.1$ Å, c = $7.6$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	8 or 6
Loop configuration of T-Atoms:	$ \begin{array}{c c} \hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $
Isotypic framework structures:	*Linde Type $L^{(1)}$ (K,Ba)-G, $L^{(2)}$ Gallosilicate $L^{(3,4)}$

- (1) Barrer, R.M. and Villiger, H. Z. Kristallogr., **128**, 352-370 (1969)
- (2) Baerlocher, Ch. and Barrer, R.M. Z. Kristallogr., 136, 245-254 (1972)

LZ-212<sup>(5)</sup> Perlialite<sup>(6,7)</sup>

- (3) Wright, P.A., Thomas, J.M., Cheetham, A.K. and Nowak, A.K. Nature, 318, 611-614 (1985)
- (4) Newsam, J.M. Mater. Res. Bull., 21, 661-672 (1986)
- (5) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (6) Menshikov, Y.P. Zap. Vses. Mineral. O-va, 113, 607-612 (1984)
- (7) Artioli, G. and Kvick, Å. Eur. J. Mineral., 2, 749-759 (1990)

## **Type Material**

Framework density: 16.3 T/1000Å<sup>3</sup>

Channels:

[001] **12** 7.1 x 7.1\*



12-ring viewed along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	cubic, $Fd\overline{3}m$ , a = 35.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2 or 6 or 4
Loop configuration of T-Atoms:	$ \begin{array}{c c} & & & \\ \hline & & \\ & & $
Isotypic framework structures:	*Linde Type $N^{(1)}$ NaZ-21 <sup>(2)</sup>

- (1) Fälth, L. and Andersson, S. Z. Kristallogr., 160, 313-316 (1982)
- (2) Shepelev, Yu.F., Smolin, Yu.I., Butikova, I.K. and Tarasov, V.I. *Dokl. Akad. Nauk SSSR*, **272**, 1133-1137 (1983)

LTN
-----

Crystal chemical data:	$ Na^{+}_{384} (H_{2}O)_{518}  [Al_{384}Si_{384} O_{1536}]-LTN$ cubic, Fd3, a = 36.93Å <sup>(1)</sup>
Framework density:	15.2 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /mmc, a = 18.1Å, c = 7.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	5-1 or 4-2 or 4
Loop configuration of T-Atoms:	T <sub>1,2</sub>
Isotypic framework structures:	*Mazzite <sup>(1,2)</sup> [Ga-Si-O]-MAZ <sup>(3)</sup> $LZ-202^{(4)}$

- (1) Galli, E. Cryst. Struct. Comm., 3, 339-344 (1974)
- (2) Galli, E. Rend. Soc. Ital. Mineral. Petrol., 31, 599-612 (1975)
- (3) Newsam, J.M., Jarman, R.H. and Jacobson, A.J. Mater. Res. Bull., 20, 125-136 (1985)
- (4) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (5) Galli, E. Cryst. Struct. Comm., 3, 339-344 (1974)
- (6) Rubin, M.K., Plank, C.J. and Rosinski, E.J. U.S. Patent 4,021,447 (1977)

 $\begin{array}{c} Omega^{(5)} \\ ZSM-4^{(6)} \end{array}$
Crystal chemical data:	$ (Na_{2}^{+},K_{2}^{+},Ca^{2+},Mg^{2+})_{5} (H_{2}G^{+})_{5} (H_{2}G^{+}) (H_{2}G^{+})_{5} (H_{2}G^{+}) (H_{2}$
	have a constant $P6 / mmc = 1$

$$\begin{split} |(Na^{\scriptscriptstyle +}_{\scriptscriptstyle 2},\!K^{\scriptscriptstyle +}_{\scriptscriptstyle 2},\!Ca^{2\scriptscriptstyle +},\!Mg^{2\scriptscriptstyle +})_5\,(H_2O)_{28}|\,[Al_{10}Si_{26}\,O_{72}]\text{-}\textbf{MAZ} \\ hexagonal,\,P6_3\!/mmc,\,a=18.392\text{\AA},\,c=7.646\text{\AA}^{(2)} \end{split}$$

16.1 T/1000Å<sup>3</sup> Framework density:

Channels:





12-ring viewed along [001]



limiting 8-ring along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /m, a = 13.1Å, c = 15.6Å										
Coordination sequences and vertex symbols:	$T_{1} (12, 1) T_{2} (12, 1) T_{3} (6, m) T_{4} (4, 3)$	4 4 4 4	9 10 10 9	18 17 16 18	30 30 26 30	46 46 46 39	63 67 66 67	94 12 91 12 94 12 98 12	25 152 23 153 14 158 21 147	183 190 194 189	4·4·4·12·5·7 4·5·4·7·5·12 3·7·5·5·5·5 4·7·4·7·4·7
Secondary building units:	combinatio	ons	only	/							
Loop configuration of T-Atoms:		ſ <sub>1</sub>				T <sub>2</sub>			∠ T <sub>3</sub>	Ź	

Isotypic framework \*Z structures:

\*ZSM-18<sup>(1)</sup>

### **References:**

(1) Lawton, S.L. and Rohrbaugh, W.J. Science, 247, 1319-1321 (1990)

Crystal	chemical	data:
---------	----------	-------

$$\begin{split} |Na^{+}_{n}~(H_{2}O)_{28}|~[Al_{n}Si_{34\text{-}n}~O_{68}]\text{-}\textbf{MEI},~n=2.1~\text{-}~5.7\\ hexagonal,~P6_{3}/m,~a=13.175\text{\AA},~c=15.848\text{\AA}^{~(1)} \end{split}$$

Framework density: 14.3 T/1000Å<sup>3</sup>

Channels:

 $[001] \ \mathbf{12} \ 6.9 \ge 6.9^* \leftrightarrow \perp [001] \ \mathbf{7} \ 3.2 \ge 3.5^{**}$ 



12-ring viewed along [001]



7-ring viewed normal to [001]



framework viewed along [100]

Idealized cell constants:	tetragonal, I $\overline{4}$ m2, a = 20.3Å, c = 13.5Å										
Coordination sequences	T <sub>1</sub> (16, 1)	4	12	21	36	63	88 121	153	192	249	5.5.5.5.5.6
and vertex symbols:	T <sub>2</sub> (16, 1)	4	11	23	38	61	93 121	153	198	246	$4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10_2$
	T <sub>3</sub> (16, 1)	4	12	23	38	62	91 116	155	203	244	$5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 5 \cdot 10_3$
	$T_4(16, 1)$	4	12	23	38	59	87 122	158	198	243	$5 \cdot 6_2 \cdot 5 \cdot 10_2 \cdot 5_2 \cdot 6$
	$T_5(16, 1)$	4	11	22	36	57	90 127	157	194	244	$4 \cdot 5 \cdot 5 \cdot 6 \cdot 5 \cdot 8_2$
	$T_{6}(8, 2)$	4	11	23	38	57	88 126	158	191	236	$4 \cdot 5_2 \cdot 6_2 \cdot 6_2 \cdot 10 \cdot 10$
	$T_7(8, 2)$	4	12	21	40	63	83 124	155	197	244	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 10_2$

Secondary building units: 5-1



Isotypic framework	*ZSM-11 <sup>(1-3)</sup>	SSZ-46 <sup>(6,7)</sup>
structures:	Bor-D ( <b>MFI/MEL</b> intergrowth) <sup>(4)</sup>	Silicalite 2 <sup>(8)</sup>
	Boralite D <sup>(5)</sup>	TS-2 <sup>(9)</sup>

- (1) Kokotailo, G.T., Chu, P., Lawton, S.L. and Meier, W.M. Nature, 275, 119-120 (1978)
- (2) Fyfe, C.A., Gies, H., Kokotailo, G.T., Pasztor, C., Strobl, H. and Cox, D.E. J. Am. Chem. Soc., 111, 2470-2474 (1989)
- (3) van Koningsveld, H., den Exter, M.J., Koegler, J.H., Laman, C.D., Njo, S.L. and Graafsma, H. In Proc. 12th Int. Zeolite Conf., (eds. M.M.J. Treacy, B.K. Marcus, M.E. Bisher and J.B. Higgins), pp. 2419-2424 (1999), MRS, Warrendale, PA
- (4) Perego, G. and Cesari, M. J. Appl. Crystallogr., 17, 403-410 (1984)
- (5) Taramasso, M., Manara, G., Fattore, V. and Notari, B. GB Patent 2,024,790, (1980)
- Terasaki, O., Ohsuna, T., Sakuma, H., Watanabe, D., Nakagawa, Y. and Medrud, R.C. Chem. Mater., 8, (6) 463-468 (1996)
- (7) Nakagawa, Y. and Dartt, C. U.S. Patent 5,968,474 (1999)

Crystal chemical data:	$\begin{split}  Na_{n}^{^{+}}(H_{2}O)_{16}  \; \text{[Al}_{n}Si_{96\text{-}n}\;O_{192}\text{]-MEL},  n < 16 \\ \text{tetragonal}, \; I\overline{4}m2,  a = 20.12\text{\AA},  c = 13.44\text{\AA}^{\;(1)} \end{split}$
Framework density:	17.6 T/1000Å <sup>3</sup>

Channels:

<100>10 5.3 x 5.4\*\*\*



10-ring viewed along <100>

### **References (cont.):**

- (8) Bibby, D.M., Milestone, N.B. and Aldridge, L.P. *Nature*, 280, 664-665 (1979)
  (9) Reddy, J.S. and Kumar, R. *Zeolites*, 12, 95-100 (1992)



framework viewed along [001] (top left: projection down [001])

Idealized cell constants:	cubic, $Pm\overline{3}n$ , $a = 13.7$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	combinations only
Loop configuration of T-Atoms:	T <sub>1-3</sub>
Isotypic framework structures:	*Melanophlogite <sup>(1)</sup> Synthetic melanophlogite <sup>(2)</sup>

(1) Gies, H. Z. Kristallogr., 164, 247-257 (1983)

(2) Gies, H., Gerke, H. and Liebau, F. N. Jb. Miner. Mh., 119-124 (1982)

Crystal chemical data:	$ (CH_4, N_2, CO_2)_x $ [Si <sub>46</sub> O <sub>92</sub> ]- <b>MEP</b> cubic, Pm $\overline{3}$ n, a = 13.436Å <sup>(1)</sup> (Data refer to structure at 200°; tetragonal at 25°C)
Framework density:	19 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [001]

Idealized cell constants:	tetragonal, I4/mmm, $a = 14.0$ Å, $c = 10.0$ Å							
Coordination sequences and vertex symbols:	T <sub>1</sub> (32, 1) 4 9 18 32 49 69	9 93 121 153 189	4·4·4·8 <sub>2</sub> ·8·8					
Secondary building units:	8-8 or 8 or 4							
Loop configuration of T-Atoms:								
Isotypic framework structures:	*Merlinoite <sup>(1,2)</sup> [Al-Co-P-O]- <b>MER</b> <sup>(3)</sup>  Ba- [Al-Si-O]- <b>MER</b> <sup>(4)</sup>  Ba-Cl- [Al-Si-O]- <b>MER</b> <sup>(5)</sup>	K-M <sup>(4,7)</sup> Linde W <sup>(4,8)</sup> Synthetic merlinoite <sup>(9)</sup> Zeolite W <sup>(10)</sup>						

(1) Passaglia, E., Pongiluppi, D. and Rinaldi, R. N. Jb. Miner. Mh., 355-364 (1977)

|NH<sub>4</sub>-|[Be-P-O]-MER<sup>(6)</sup>

- (2) Galli, E., Gottardi, G. and Pongiluppi, D. N. Jb. Miner. Mh., 1-9 (1979)
- (3) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
- (4) Gottardi, G. and Galli, E. Natural Zeolites, p. 157 (1985), Springer-Verlag, Berlin
- (5) Solov'eva, L.P., Borisov, S.V. and Bakakin, V.V. Sov. Phys. Crystallogr., 16, 1035-1038 (1972)
- (6) Bu, X., Gier, T.E. and Stucky, G.D. Microporous and Mesoporous Materials, 26, 61-66 (1998)
- (7) Barrer, R.M. and Baynham, J.W. J. Chem. Soc., 2882-2891 (1956)
- (8) Sherman, J.D. ACS Sym. Ser., 40, 30-42 (1977)
- (9) Barrett, P.A., Valencia, S. and Camblor, M.A. J. Mater. Chem., 8, 2263-2268 (1998)
- (10) Bieniok, A., Bornholdt, K., Brendel, U. and Baur, W.H. J. Mater. Chem., 6, 271-275 (1996)

Merlinoite

## **Type Material**

# MER

Crystal chemical data:	$\begin{split}  K_{5}^{+}Ca^{2+}{}_{2}(H_{2}O)_{24}   [Al_{9}Si_{23}  O_{64}]\text{-MER} \\ \text{orthorhombic, Immm, } a = 14.116\text{\AA, } b = 14.229\text{\AA, } c = 9.946\text{\AA}^{(2)} \\ (\text{Relationship to unit cell of Framework Type: } a' = b' = a, c' = c) \end{split}$
Framework density:	16 T/1000Å <sup>3</sup>
Channels:	$[100] 8 3.1 x 3.5^* \leftrightarrow [010] 8 2.7 x 3.6^* \leftrightarrow [001] {8 3.4 x 5.1^* + 8 3.3 x 3.3^*}$



8-ring viewed along [100]



8-ring viewed along [010]



8-ring viewed along [001]

See Appendix A for 2nd 8-ring viewed along [001]



framework viewed along [010]

Idealized cell constants:	orthorhom	bic,	Pnr	na,	a = 2	20.1	Å, $b = 19.7$ Å, $c = 13.1$ Å
<b>Coordination sequences</b>	T <sub>1</sub> (8, 1)	4	12	22	41	61	88 125 159 198 250 5·5·5·10 <sub>2</sub> ·5 <sub>2</sub> ·
and vertex symbols:	$T_2(8, 1)$	4	12	22	39	64	91 117 158 209 247 5·5·5·5 <sub>2</sub> ·5·10
	$T_3(8, 1)$	4	12	23	37	62	91 120 157 206 250 5·5·5·5 <sub>2</sub> ·5·10
	$T_4(8, 1)$	4	12	21	36	61	90 122 159 196 251 $5 \cdot 5 \cdot 5_2 \cdot 5_2 \cdot 5 \cdot $
	$T_5(8, 1)$	4	12	24	38	63	93 123 157 206 247 5·5·5·6 <sub>2</sub> ·5·10
	$T_{6}(8, 1)$	4	12	22	40	61	88       124       156       197       253 $5 \cdot 5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 10^{-1000}$
	T <sub>7</sub> (8, 1)	4	12	24	38	56	90 132 164 193 241 $5 \cdot 6_2 \cdot 5_2 \cdot 6_2 \cdot 10 \cdot 10^{-10}$
	$T_8(8, 1)$	4	12	21	37	63	90 121 155 201 253 5.5.5.5.
	T <sub>9</sub> (8, 1)	4	11	23	39	62	93 119 153 204 254 $4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10^{-10}$
	$T_{10}(8, 1)$	4	11	22	36	61	93 120 154 200 255 $4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10^{-10}$
	$T_{11}(8, 1)$	4	12	22	38	59	92 125 159 202 250 5.5.5.6.5.6
	$T_{12}(8, 1)$	4	12	23	38	59	$89 \ 126 \ 161 \ 196 \ 246 \qquad 5 \cdot 6_2 \cdot 5 \cdot 10_2 \cdot 5_2 \cdot 6_2$
Secondary building units:	5-1						
					_		



Isotypic framework	*ZSM-5 <sup>(1-3)</sup>
structures:	(See Appendix A for additional structures and references)

- (1) Kokotailo, G.T., Lawton, S.L., Olson, D.H. and Meier, W.M. Nature, 272, 437-438 (1978)
- (2) Olson, D.H., Kokotailo, G.T., Lawton, S.L. and Meier, W.M. J. Phys. Chem., 85, 2238-2243 (1981)
- (3) van Koningsveld, H., van Bekkum, H. and Jansen, J.C. Acta Crystallogr., B43, 127-132 (1987)

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ZSM-5

# **Type Material**

# MFI

Crystal chemical data:

$$\begin{split} |Na^{+}_n~(H_2O)_{16}|~[Al_nSi_{96\text{-}n}~O_{192}]\text{-}MFI,~n<27\\ \text{orthorhombic,~Pnma,~a}=20.07\text{\AA},~b=19.92\text{\AA},~c=13.42\text{\AA}^{~(2)} \end{split}$$

Framework density: 17.9 T/1000Å<sup>3</sup>

Channels:

 $\{[100] \ \mathbf{10} \ 5.1 \ x \ 5.5 \leftrightarrow [010] \ \mathbf{10} \ 5.3 \ x \ 5.6\}^{***}$ 



10-ring viewed along [100]



10-ring viewed along [010]



framework viewed along [010]

Idealized cell constants:	orthorhombic, Imm2, $a = 7.5$ Å, $b = 14.4$ Å, $c = 19.0$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units: Loop configuration of T-Atoms:	5-1 $T_{1,3-5,7-8}$ $T_2$ $T_6$
Isotypic framework structures:	*ZSM-57 <sup>(1)</sup>

(1) Schlenker, J.L., Higgins, J.B. and Valyocsik, E.W. Zeolites, 10, 293-296 (1990)

Crystal chemical data:

 $|H^{+}_{1.5}| \text{ [Al}_{1.5}\text{Si}_{34.5} \text{ O}_{72} \text{]-MFS}$  orthorhombic, Imm2, a = 7.451Å, b = 14.171Å, c = 18.767Å  $^{(1)}$ 

Framework density:

18.2 T/1000Å<sup>3</sup>

Channels:

 $[100] \ \textbf{10} \ \textbf{5.1} \ \textbf{x} \ \textbf{5.4}^* \leftrightarrow [010] \ \textbf{8} \ \textbf{3.3} \ \textbf{x} \ \textbf{4.8}^*$ 



10-ring viewed along [100]



8-ring viewed along [010]



structures:

### **References:**

(1) Rouse, R.C., Dunn, P.J., Grice, J.D., Schlenker, J.L. and Higgins, J.B. Am. Mineral., 75, 1415-1420 (1990)

### **Montesommaite**

## **Type Material**

# MON

Crystal chemical data:

$$\label{eq:constraint} \begin{split} |(K^+,Na^+)_{4.5}~(H_2O)_5|~[Al_{4.5}Si_{11.5}~O_{32}]\text{-}MON \\ tetragonal,~I4_1/amd,~a=7.141\text{\AA},~c=17.307\text{\AA}^{~(1)} \end{split}$$

Framework density: 1

Channels:

18.1 T/1000Å<sup>3</sup>

[100]**8** $3.2 x 4.4^* \leftrightarrow [001]$ **8** $3.6 x 3.6^*$ 



8-ring viewed along [100]



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	orthorhom	bic, (	Cmcm	n, a =	= 18.3	$^{3}$ Å, b = 2	0.5Å	, c =	7.5Å	L .
<b>Coordination sequences</b>	T <sub>1</sub> (16, 1)	4 1	2 22	38	60	88 115	155	204	242	$5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 8 \cdot 12$
and vertex symbols:	T <sub>2</sub> (16, 1)	4 1	2 20	37	64	87 114	154	198	241	$5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 5 \cdot 8$
	T <sub>3</sub> (8, m)	4 1	1 24	39	54	86 126	156	195	242	$4 \cdot 5_2 \cdot 5 \cdot 8_2 \cdot 5 \cdot 8_2$
	T <sub>4</sub> (8, m)	4 1	1 24	39	60	92 122	148	195	250	$4 \cdot 5_2 \cdot 5 \cdot 8 \cdot 5 \cdot 8$

**Secondary building units:** 5-1

Loop configuration of T-Atoms:		
	T <sub>1,2</sub>	T <sub>3,4</sub>

Isotypic framework structures:	*Mordenite <sup>(1)</sup> [Ga-Si-O]- <b>MOR</b> <sup>(2)</sup> Ca-Q <sup>(3)</sup> LZ-211 <sup>(4)</sup> Large port mordenite <sup>(5)</sup> Maricopaite (interrupted framework) <sup>(6)</sup> Na-D <sup>(7)</sup>
Alternate designation:	Ptilolite (discredited) Arduinite (discredited) Flokite (discredited)

- (1) Meier, W.M. Z. Kristallogr., **115**, 439-450 (1961)
- (2) Eapen, M.J., Reddy, K.S.N., Joshi, P.N. and Shiralkar, V.P. J. Incl. Phenom., 14, 119-129 (1992)

**Mordenite** 

### **Type Material**

## MOR

Crystal chemical data:

$$\label{eq:1.1} \begin{split} & |Na^{+}_{8}~(H_{2}O)_{24}|~[Al_{8}Si_{40}~O_{96}]\text{-}\textbf{MOR} \\ & \text{orthorhombic, Cmcm, }a=18.1\text{\AA}, ~b=20.5\text{\AA}, ~c=7.5\text{ \AA}^{~(1)} \end{split}$$

Framework density: 17.2 T/1000Å<sup>3</sup>

**Channels:** 

 $[001] \mathbf{12} 6.5 \ge 7.0^* \leftrightarrow \{[010] \mathbf{8} 3.4 \ge 4.8 \leftrightarrow [001] \mathbf{8} 2.6 \ge 5.7\}^*$ 



12-ring viewed along [001]



*limiting 8 ring along [001] between 12-ring channels* 

See Appendix A for 8-ring viewed along [010]

### **References (cont.):**

- (3) Koizumi, M. and Roy, R. J. Geol., 68, 41-53 (1960)
- (4) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (5) Sand, L.B. In Molecular Sieves, (ed. R.M. Barrer), pp. 71-77 (1968), Soc. Chem. Indus., London
- (6) Rouse, R.C. and Peacor, D.R. Am. Mineral., 79, 175-184 (1994)
- (7) Barrer, R.M. and White, E.A.D. J. Chem. Soc., 1561-1571 (1952)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , a = 17.2Å, c = 19.8Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	2-6-2
Loop configuration of T-Atoms:	$\begin{array}{ c c c }\hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$
Isotypic framework structures:	*MCM-61 <sup>(1,2)</sup>

- (1) Valyosik, E.W. U.S. Patent 5,670,131 (1997)
- (2) Shantz, D.F., Burton, A. and Lobo, R.F. Microporous and Mesoporous Materials, 31, 61-73 (1999)

<b>MSO</b>	
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Crystal chemical data:	$\begin{split}  K^{+}_{2.1} C_{12} H_{24} O_6  \; [Si_{27.9} Al_{2.1} \; O_{60}]\text{-}\textbf{MSO} \\ C_{12} H_{24} O_6 = 18\text{-}crown\text{-}6 \\ rhombohedral, \; &R\;\overline{3}m\;, \; a = 11.841 \text{\AA}, \; \alpha = 93.29^{\circ \;(2)} \\ (hexagonal \; setting: \; a = 17.220 \text{\AA}, \; c = 19.296 \text{\AA}) \end{split}$
Framework density:	18.2 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [001]

Idealized cell constants:	monoclini	c, C	12/1	m1,	a =	9.6Å	, b =	= 30.4	4Å, c	c = 7	.2Å, $\beta = 90.5^{\circ}$	
Coordination sequences	T <sub>1</sub> (8, 1)	4	11	24	45	77	109	137	174	224	280	4.5.5.6.5.8
and vertex symbols:	T <sub>2</sub> (8, 1)	4	12	24	42	70	95	136	184	227	277	$5.5_{2}.5.6.5.8$
	$T_3(8, 1)$	4	12	27	47	69	99	142	184	227	281	5.6.5.7.5.8
	$T_4(8, 1)$	4	12	26	45	64	96	134	186	230	290	5.6.5.6.5.6
	$T_5(8, 1)$	4	12	24	42	64	93	133	179	234	290	$5 \cdot 6 \cdot 5 \cdot 6_2 \cdot 5 \cdot 7$
	$T_{6}(4, 2)$	4	12	21	44	74	106	138	172	226	284	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5_2 \cdot 6$
Secondary building units:	5-5=1											
Loop configuration of T-Atoms:		т	_			- T						
	I	<b>1</b> 1				1 <sub>2-6</sub>						

Isotypic framework	*MCM-35 <sup>(1</sup>
structures:	UTM-1 <sup>(2)</sup>

- (1) Barrett, P.A., Díaz-Cabañas, M.J. and Camblor, M.A. Chem. Mater., 11, 2919-2927 (1999)
- (2) Plévert, J., Yamamoto, K. Chiari, G. and Tatsumi, T. J. Phys. Chem. B, 103, 8647-8649 (1999)

Crystal chemical data:	[Si <sub>44</sub> O <sub>88</sub> ]- <b>MTF</b> monoclinic, C12/m1 a = 9.500 Å, b = 30.710Å, c = 7.313Å, β = 91.71° <sup>(1)</sup>
Framework density:	20.6 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 3.6 x 3.9*
2	



8-ring viewed along [001]



framework viewed along [111] (bottom left: projection down [110])

Idealized cell constants:	cubic, $Fd\overline{3}m$ (origin choice 2), $a = 19.9$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	combinations only
Loop configuration of T-Atoms:	
Isotypic framework structures:	$*ZSM-39^{(1)}$ CF-4 <sup>(2)</sup> Dodecasil-3C <sup>(3)</sup> Holdstite <sup>(4)</sup>

- (1) Schlenker, J.L., Dwyer, F.G., Jenkins, E.E., Rohrbaugh, W.J., Kokotailo G.T. and Meier, W.M. *Nature*, **294**, 340-342 (1981)
- (2) Long, Y., He, H., Zheng, P., Guang, W. and Wang, B. J. Incl. Phenom., 5, 355-362 (1987)
- (3) Gies, H. Z. Kristallogr., 167, 73-82 (1984)
- (4) Smith, J.V. and Blackwell, C.S. *Nature*, **303**, 223-225 (1983)

Crystal chemical data:	$\begin{split}  (C_8H_{20}N^+)_n \ (OH)^n  \ [Si_{136} \ O_{272}]\text{-MTN} \\ C_8H_{20}N^+ &= tetraethylammonium \\ cubic, \ Fd \ \overline{3}m, \ a &= 19.36 \ A^{(1)} \end{split}$
Framework density:	18.7 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [100]

Idealized cell constants:	orthorhom	oic.	, Prr	nmn	(orig	gin cl	hoic	e 1),	a =	5.3Å	, b = 1	22.0Å, c	= 11.4Å	
<b>Coordination sequences</b>	T <sub>1</sub> (4, m)	4	12	23	43	66	92	130	170	213	261		5.5.5.5.6.	102
and vertex symbols:	T <sub>2</sub> (4, m)	4	12	24	40	64	96	136	167	207	258	4	$5_2 \cdot 6_2 \cdot 6 \cdot 6_2 \cdot 6$	5·6 <sub>2</sub>
	$T_3(4, m)$	4	12	22	40	67	97	124	165	219	265		$5.5.5.5.6_2$	102
	$T_4$ (4, m)	4	12	22	40	65	98	132	159	206	278		5.5.5.5.6	$5_2 \cdot *$
	$T_{5}(4, m)$	4	12	24	41	62	97	129	170	212	262	4	$5_2 \cdot 6_2 \cdot 6 \cdot 6_2 \cdot 6$	5.6 <sub>2</sub>
	$T_6(2, mm2)$	4	12	22	42	66	94	126	164	220	270		5.5.5.5.62	102
	T <sub>7</sub> (2, mm2)	4	12	24	44	66	88	132	174	214	258		5.5.5.5.10	) <sub>2</sub> .*
Secondary building units:	5-1													
Loop configuration of T-Atoms:		1-7												
Isotypic framework structures:	*ZSM-23 <sup>(1)</sup> EU-13 <sup>(4)</sup> ISI-4 <sup>(5)</sup> KZ-1 <sup>(6)</sup>	-3)												

- (1) Schlenker, J.L., Higgins, J.B. and Cox, D.E. private communication
- (2) Rohrman Jr., A.C., LaPierre, R.B., Schlenker, J.L., Wood, J.D., Valyocsik, E.W., Rubin, M.K., Higgins, J.B. and Rohrbaugh, W.J. *Zeolites*, **5**, 352-354 (1985)

Crystal chemical data:	$\begin{split} & Na^{+}_{n}~(H_{2}O)_{4} ~[Al_{n}Si_{24\text{-}n}~O_{48}]\text{-}\textbf{MTT},~n<2\\ &\text{orthorhombic},~Pmn2_{1},~a=21.5\text{\AA},~b=11.1\text{\AA},~c=5.0~\text{\AA}^{~(1)} \end{split}$
Framework density:	20.1 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 4.5 x 5.2*
4.5	4.5

10-ring viewed along [001]

5.2

#### **References (cont.):**

- (3) Marler, B., Deroche, C., Gies, H., Fyfe, C.A., Grondey, H., Kokotailo, G.T., Feng, Y., Ernst, S., Weitkamp, J. and Cox, D.E. J. Appl. Crystallogr., **26**, 636-644 (1993)
- (4) Araya, A. and Lowe, B.M. U.S. Patent 4,581,211 (1986)
- (5) Kakatsu, K. and Kawata, N. Eur. Pat. Appl. EPA 102,497 (1984)

5.2

(6) Parker, L.M. and Bibby, D.M. Zeolites, **3**, 8-11 (1983)



framework viewed along [010]

Idealized cell constants:	monoclini	c, C	22/m	ı, a =	= 25	.6Å, 1	b = 5	5.3Å	, c =	12.1	Å, β	= 109.3°
Coordination sequences	T <sub>1</sub> (4, m)	4	11	22	38	60	88	113	147	190	243	$4 \cdot 6_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
and vertex symbols:	T <sub>2</sub> (4, m)	4	11	22	38	60	86	115	147	191	238	$4 \cdot 6_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
	T <sub>3</sub> (4, m)	4	12	21	37	62	84	119	147	188	239	$5 \cdot 6 \cdot 5 \cdot 6 \cdot 5_2 \cdot 6$
	$T_4$ (4, m)	4	12	23	37	59	85	120	154	184	231	$5 \cdot 6 \cdot 5 \cdot 6 \cdot 6 \cdot 6_2$
	T <sub>5</sub> (4, m)	4	12	21	37	58	87	119	154	182	227	$5 \cdot 6_2 \cdot 5 \cdot 6_2 \cdot 5_2 \cdot 6$
	T <sub>6</sub> (4, m)	4	12	24	39	55	85	122	156	188	225	$5 \cdot 6_2 \cdot 5 \cdot 6_2 \cdot 6_2 \cdot 12_6$
	T <sub>7</sub> (4, m)	4	12	23	38	59	83	115	155	192	233	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 6 \cdot 12_6$

Secondary building units:	5-2	
Loop configuration of T-Atoms:	T <sub>1,2</sub> T <sub>3-7</sub>	
Isotypic framework structures:	*ZSM- $12^{(1,2)}$ [Ga-Si-O]- <b>MTW</b> <sup>(3)</sup> CZH- $5^{(4)}$ NU- $13^{(5)}$	TPZ-12 <sup>(6)</sup> Theta-3 <sup>(7)</sup> VS-12 <sup>(8)</sup>

5.6

### MTW

Crystal chemical data:	$\begin{split} & Na_{n}^{+}(H_{2}O)_{8}  \; [Al_{n}Si_{56\text{-}n}\;O_{112}]\text{-}MTW,  n < 5 \\ &\text{monoclinic, C12/c1} \\ &a = 24.863\text{\AA},  b = 5.012\text{\AA},  c = 24.328\text{\AA},  \beta = 107.72^{\circ}  ^{(2)} \end{split}$
Framework density:	19.4 T/1000Å <sup>3</sup>
Channels:	[010] <b>12</b> 5.6 x 6.0*
5.9	6.0

5.6

#### **References:**

 LaPierre, R.B., Rohrman Jr., A.C., Schlenker, J.L., Wood, J.D., Rubin, M.K. and Rohrbaugh, W.J. Zeolites, 5, 346-348 (1985)

12-ring viewed along [010]

- (2) Fyfe, C.A., Gies, H., Kokotailo, G.T., Marler, B. and Cox, D.E. J. Phys. Chem., 94, 3718-3721 (1990)
- (3) Zhi, Y.X., Tuel, A., Bentaarit, Y. and Naccache, C. Zeolites, 12, 138-141 (1992)
- (4) Hickson, D.A. UK Pat. Appl. GB 2079735A (1981)
- (5) Whittam, T.V. Eur. Pat. Appl. EPA 0059059 (1982)
- (6) Sumitani, K., Sakai, T., Yamasaki, Y. and Onodera, T. U.S. Patent 4,557,919 (1985)
- (7) Barlow, T.M. E. Patent A-162,719 (1985)
- (8) Reddy, K.M., Moudrakovski, I. and Sayari, A. Chem. Commun., 1491-1492 (1994)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal,	P6	/mn	nm,	a =	14.4	Å, c	= 25	.2Å			
Coordination sequences	T <sub>1</sub> (12, .m.)	4	10	20	32	52	76	111	146	185	225	$4_2 \cdot 6 \cdot 5 \cdot 5 \cdot 5 \cdot 5$
and vertex symbols:	T <sub>2</sub> (12, .m.)	4	12	22	35	51	81	109	137	175	218	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 6 \cdot 10_2$
	T <sub>3</sub> (12, .m.)	4	10	21	40	62	78	95	128	177	228	$4 \cdot 5 \cdot 4 \cdot 5 \cdot 6 \cdot 10_2$
	T <sub>4</sub> (12,m)	4	11	18	32	52	78	107	147	187	215	$4 \cdot 10_2 \cdot 5_2 \cdot 6_2 \cdot 5_2 \cdot 6_2$
	T <sub>5</sub> (12,m)	4	11	22	32	53	79	113	144	176	220	$4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 6_2$
	T <sub>6</sub> (4, 3m)	4	10	20	34	54	87	114	139	188	244	$4 \cdot 10_4 \cdot 4 \cdot 10_4 \cdot 4 \cdot 10_4$
	T <sub>7</sub> (4, 3m)	4	10	16	30	49	77	100	138	181	214	$4 \cdot 6_2 \cdot 4 \cdot 6_2 \cdot 4 \cdot 6_2$
	T <sub>8</sub> (4, 3m)	4	12	22	31	52	74	112	142	166	204	$5 \cdot 6_2 \cdot 5 \cdot 6_2 \cdot 5 \cdot 6_2$
Secondary building units:	combinatio	ns	only	y								
Loop configuration of T-Atoms:											Γ	



Crystal chemical data:

 $|H^{+}_{2.4}Na^{+}_{3.1}|$  [Al<sub>0.4</sub>B<sub>5.1</sub>Si<sub>66.5</sub> O<sub>144</sub>]-MWW hexagonal, P6/mmm, a = 14.208Å, c = 24.945Å <sup>(4)</sup>

Framework density:

16.5 T/1000Å<sup>3</sup>

Channels:

 $\perp$  [001] **10** 4.0 x 5.5\*\* |  $\perp$  [001] **10** 4.1 x 5.1\*\*



10-ring viewed normal to [001] between layers



10-ring viewed normal to [001] within layers

Isotypic framework	*MCM-22 <sup>(1)</sup>	PSH-3 <sup>(5)</sup>
structures:	ERB-1 <sup>(2)</sup>	SSZ-25 <sup>(6)</sup>
	ITO-1 <sup>(3,4)</sup>	

- (1) Leonowicz, M.E., Lawton, J.A., Lawton, S.L. and Rubin, M.K. Science, 264, 1910-1913 (1994)
- (2) Belussi, G., Perego, G., Clerici, M.G. and Giusti, A. Eur. Pat. Appl. EPA 293032 (1988)
- (3) Camblor, M.A., Corell, C., Corma, A., Díaz-Cabañas, M.J., Nicolopoulos, S., González-Calbet, J.M. and Vallet-Regí, M. *Chem. Mater.*, **8**, 2415-2417 (1996)
- (4) Camblor, M.A., Corma, A., Díaz-Cabañas, M.J. and Baerlocher, Ch. J. Phys. Chem. B, 102, 44-51 (1998)
- (5) Puppe, L. and Weisser, J. U.S. Patent 4,439,409 (1984)
- (6) Zones, S.I. E. Patent 231,860 (1987)



framework viewed normal to [001]

Idealized cell constants:	tetragonal, $I4_1$ /amd (origin choice 2), a = 13.9Å, c =	: (
<b>Coordination sequences</b>	T <sub>1</sub> (16, m) 4 9 19 35 52 78 106 139 179 213	3
and vertex symbols:	$T_2(4, \overline{4}m2)$ 4 8 18 36 56 66 116 140 154 232	2

 $4 \cdot 8_2 \cdot 4 \cdot 8_2 \cdot 4_2 \cdot 8_4$  $4_2 \cdot 4_2 \cdot 8_4 \cdot 8_4 \cdot 8_4 \cdot 8_4$ 

**Secondary building units:** 4=1

Loop configuration of T-Atoms:



Isotypic framework structures: \*Natrolite<sup>(1,2)</sup> [Al-Ge-O]-**NAT**<sup>(3)</sup> [Ga-Si-O]-**NAT**<sup>(4)</sup> |Rb-|[Ga-Ge-O]-**NAT**<sup>(5)</sup> Gonnardite<sup>(6)</sup> High natrolite<sup>(7)</sup> Mesolite<sup>(8)</sup> Metanatrolite<sup>(9)</sup> Scolecite<sup>(10-12)</sup> Synthetic gonnardite<sup>(13)</sup> Synthetic mesolite<sup>(14)</sup> Synthetic natrolite<sup>(14)</sup> Synthetic scolecite<sup>(14)</sup>

= 6.4Å

### Alternate designation: Laubanite (discredited)

- (1) Pauling, L. Proc. Natl. Acad. Sci., 16, 453-459 (1930)
- (2) Meier, W.M. Z. Kristallogr., 113, 430-444 (1960)
- (3) Tripathi, A., Johnson, G.M., Kim, S.J. and Parise, J.B. J. Mater. Chem., 10, 451-455 (2000)
- (4) Xie, D., Newsam, J.M., Yang, J. and Yelong, W.B. In *MRS Sym. Proc.*, (eds. M.M.J. Treacy, J.M. White and J.M. Thomas), **111**, pp. 147-154 (1988), Materials Research Society, Pittsburgh, PA

## NAT

Crystal chemical data:	$ Na_{16}^{+}(H_2O)_{16} $ [Al <sub>16</sub> Si <sub>24</sub> O <sub>80</sub> ]-NAT orthorhombic, Fdd2, a = 18.30Å, b = 18.63Å, c = 6.60Å <sup>(2)</sup> (Relationship to unit cell of Framework Type: a' = b' = a·sqrt(2), c' = c or, as vectors, a' = a + b, b' = b - a, c' = c)
Framework density:	17.8 T/1000Å <sup>3</sup>
Channels:	<100> 8 2.6 x 3.9** $\leftrightarrow$ [001] 9 2.5 x 4.1* (variable due to considerable flexibility of framework)



8-ring viewed along <100>



9-ring viewed along [001] (variable)

### References (cont.):

- (5) Klaska, K.H. and Jarchow, O. Z. Kristallogr., **172**, 167-174 (1985)
- (6) Mazzi, F., Larsen, A.O., Gottardi, G. and Galli, E. N. Jb. Miner. Mh., 219-228 (1986)
- (7) Baur, W.H. and Joswig, W. N. Jb. Miner. Mh., 171-187 (1996)
- (8) Artioli, G., Smith, J.V. and Pluth, J.J. Acta Crystallogr., C42, 937-942 (1986)
- (9) Joswig, W. and Baur, W.H. N. Jb. Miner. Mh., 26-38 (1995)
- (10) Taylor, W.H. and Jackson, R. Z. Kristallogr., 86, 53-64 (1933)
- (11) Fälth, L. and Hansen, S. Acta Crystallogr., **B35**, 1877-1880 (1979)
- (12) Smith, J.V., Pluth, J.J., Artioli, G. and Ross, F.K. In *Proc. 6th Int. Zeolite Conf.*, (eds. D.H. Olson and A. Bisio), pp. 842-850 (1984), Butterworths, Guildford, Surrey
- (13) Ghobarkar, H. and Schaef, O. Zeolites, 19, 259-261 (1997)
- (14) Ghobarkar, H. and Schaef, O. Cryst. Res. Technol., 31, K67-69 (1996)



framework viewed along [010]

Idealized cell constants:	orthorhomb	ic,	, Fm	mm	i, a =	26.1	۱Å,	b = 1	3.9Å	Å, c =	= 22.9	РÅ
<b>Coordination sequences</b>	T <sub>1</sub> (32, 1)	4	11	21	36	58	89	123	157	187	237	$4 \cdot 6 \cdot 5 \cdot 5 \cdot 5_2 \cdot 10$
and vertex symbols:	T <sub>2</sub> (32, 1)	4	12	22	38	57	86	118	152	196	245	$5 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10$
	T <sub>3</sub> (16, m)	4	12	20	34	57	88	125	158	192	224	$5 \cdot 5_2 \cdot 5 \cdot 5_2 \cdot 12_2 \cdot *$
	T <sub>4</sub> (16, m)	4	12	20	31	57	84	118	150	187	237	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 5 \cdot 6_2$
	T <sub>5</sub> (16, m)	4	11	24	40	63	86	114	158	208	255	4.10.5.5.5.5
	T <sub>6</sub> (16, m)	4	12	22	35	55	83	119	151	184	237	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
	T <sub>7</sub> (8, mm2)	4	12	24	32	50	88	120	152	180	226	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 12_6 \cdot *$
Secondary building units:	5-3											
Loop configuration of T-Atoms:			_									
	T	1,5				T <sub>2-4,6</sub> ,	,7					
Isotypic framework	*NU-87 <sup>(1)</sup>											

structures:

\*NU-8/<sup>(1)</sup> Gottardiite<sup>(2)</sup>

- (1) Shannon, M.D., Casci, J.L., Cox, P.A. and Andrews, S.J. Nature, 353, 417-420 (1991)
- (2) Alberti, A., Vezzalini, G., Galli, E. and Quartieri, S. Eur. J. Mineral., 8, 69-75 (1996)

Crystal chemical data:	$\begin{aligned}  H_{4}^{+}(H_{2}O)_{n}  & [Al_{4}Si_{64} O_{136}] \text{-NES} \\ \text{monoclinic, } P12_{1}/c1 \\ a &= 14.324\text{\AA}, b = 22.376\text{\AA}, c = 25.092\text{\AA}, \beta = 151.51^{\circ (1)} \\ (\text{Relationship to unit cell of Framework Type:} \\ a' &= b/2 \sin\beta, b' = c, c' = a \\ \text{or, as vectors, } a' &= (b - a)/2, b' = c, c' = a) \end{aligned}$
Framework density:	17.7 T/1000Å <sup>3</sup>
Channels:	[100] <b>10</b> 4.8 x 5.7**



10-ring along [100]



framework viewed along [010]

Idealized cell constants:	orthorhombic, Fmmm, a = 22.9Å, b = 15.7Å, c = 13.9Å											
<b>Coordination sequences</b>	$T_1(32, 1)$	4	12	25	42	67	95	133	174	219	273	5.6.5.6.5.6
and vertex symbols:	T <sub>2</sub> (16, m)	4	12	24	39	64	99	130	174	217	262	$5 \cdot 6 \cdot 5 \cdot 6 \cdot 5 \cdot 6_2$
-	T <sub>3</sub> (16, m)	4	11	23	44	72	95	124	170	229	279	4.6.5.5.5.5
	$T_4$ (16, m)	4	12	24	41	65	97	133	173	212	267	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
	T <sub>5</sub> (8, 2mm)	4	12	24	40	62	92	142	166	214	262	$5 \cdot 5 \cdot 5 \cdot 5 \cdot 12_2 \cdot *$

Secondary building units: combinations only

Loop configuration of T-Atoms:



Isotypic framework	*Nonasil <sup>(1)</sup>
structures:	[B-Si-O]- <b>NON</b> <sup>(2)</sup>
	$ (Co(C_5H_5)_2)_4 F_4  [Si_{88}O_{176}]-NON^{(3)}$
	CF-3 <sup>(4)</sup>
	ZSM-51 <sup>(5)</sup>

- (1) Marler, B., Dehnbostel, N., Eulert, H.-H., Gies, H. and Liebau, F. J. Incl. Phenom., 4, 339-349 (1986)
- (2) Marler, B. and Gies, H. Zeolites, 15, 517-525 (1995)
- (3) Vandegoor, G., Freyhardt, C.C. and Behrens, P. Z. anorg. allg. Chemie, 621, 311-322 (1999)
- (4) Long, Y.-C., Zhong, W. and Shen, X. J. Incl. Phenom., 4, 121-127 (1986)
- (5) Rohrbaugh, W.J. private communication

Nonasil

# **Type Material**

# NON

Crystal chemical data:	$ (C_5H_{13}N)_4 $ [Si <sub>88</sub> O <sub>176</sub> ]-NON C <sub>5</sub> H <sub>13</sub> N = 2-aminopentane orthorhombic, Fmmm, a = 22.232Å, b = 15.058Å, c = 13.627Å	
Framework density:	19.3 T/1000Å <sup>3</sup>	
Channels:	apertures formed by 6-rings only	



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, $P\overline{6}m2$ , a = 13.1Å, c = 7.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6
Loop configuration of T-Atoms:	
Framework description:	AAB sequence of 6-rings
Isotypic framework structures:	*Offretite <sup>(1,2)</sup> LZ-217 <sup>(3)</sup> Linde T ( <b>ERI-OFF</b> structural intermediate) <sup>(4)</sup> Synthetic offretite <sup>(5)</sup>

- (1) Bennett, J.M. and Gard, J.A. Nature , 214, 1005-1006 (1967)
- (2) Gard, J.A. and Tait, J.M. Acta Crystallogr., B28, 825-834 (1972)
- (3) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023 (1985)
- (4) Breck, D.W. Zeolite Molecular Sieves, p. 173 (1974), Wiley, New York

TMA-O<sup>(6)</sup>

- (5) Ghobarkar, H. and Schaef, O. Cryst. Res. Technol., 31, K29-31 (1996)
- (6) Aiello, R., Barrer, R.M., Davies, J.A. and Kerr, I.S. Trans. Faraday Soc., 66, 1610-1617 (1970)
Offretite

## **Type Material**

Crystal chemical data:

 $\begin{array}{l} |(Ca^{2+},Mg^{2+})_{1.5}K^{+}~(H_{2}O)_{14}|~[Al_{4}Si_{14}~O_{36}]\text{-}OFF \\ hexagonal,~P\overline{6}m2,~a=13.291\text{\AA},~c=7.582\text{\AA}^{~(2)} \end{array}$ 

15.5 T/1000Å<sup>3</sup> Framework density:

**Channels:** 

 $[001] \ \mathbf{12} \ 6.7 \ x \ 6.8^* \leftrightarrow \perp [001] \ \mathbf{8} \ 3.6 \ x \ 4.9^{**}$ 



12-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed along [001]

Idealized cell constants:	tetragonal, I4/mmm, $a = 18.5$ Å, $c = 5.3$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2
Loop configuration of T-Atoms:	$\begin{array}{ c c c c c }\hline \hline \\ \hline \\ \hline \\ \hline \\ T_1 \end{array} \end{array} \begin{array}{ c c c }\hline \\ \hline \\ T_2 \end{array} \end{array} \begin{array}{ c c }\hline \\ \hline \\ \hline \\ T_3 \end{array}$
Isotypic framework structures:	*UiO-6 <sup>(1)</sup>

(1) Akporiaye, D.E., Fjellvåg, H., Halvorsen, E.N., Haug, T., Karlsson, A. and Lillerud, K.P. Chem. Commun., 1553-1554 (1996)

Crystal chemical data:	[Al <sub>16</sub> P <sub>16</sub> O <sub>64</sub> ]- <b>OSI</b> orthorhombic, Imm2, a = 18.355Å, b = 18.321Å, c = $5.053$ Å <sup>(1)</sup>
Framework density:	18.8 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 5.2 x 6.0*
6.0	5.2 6.0 5.2

12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	hexagonal,	P6 <sub>2</sub>	22,	a =	10.1	lÅ, c	= 7	.6Å					
Coordination sequences and vertex symbols:	T <sub>1</sub> (6, 2) T <sub>2</sub> (3, 222)	4 4	8 8	16 16	29 30	46 44	70 76	101 92	118 130	162 148	190 202	3.3.8. 3.3.8.8	$8 \cdot 8 \cdot 14_{10}$ $\cdot 14_7 \cdot 14_7$
Secondary building units:	3												
Loop configuration of T-Atoms:		1,2											
Isotypic framework	*OSB-1 <sup>(1)</sup>												

structures:

- **References:**
- (1) Kongshaug, K.O., Fjellvåg, H., Lillerud, K.P., Gier, T.E., Stucky, G.D. and Cheetham, A.K. *private communication*

Crystal chemical data:

$$\begin{split} |K_{\ 6}^{+}(H_{2}O)_{9}| \ [Be_{3}Si_{6}\ O_{18}] \text{-} \textbf{OSO} \\ trigonal, \ P3_{2}, \ a = 10.093 \text{\AA}, \ c = 7.626 \text{\AA}^{\ (1)} \end{split}$$

Framework density: 13.4 T/1000Å<sup>3</sup>

**Channels:** 

 $[001] \ \mathbf{14} \ 5.4 \ge 7.3^* \leftrightarrow \perp [001] \ \mathbf{8} \ 2.8 \ge 3.3^{**}$ 



puckered 14-ring viewed along [001]



8-ring viewed normal to [001]



framework viewed along [001]

Idealized cell constants:	monoclini	c, C	C2/c,	a =	20.	9Å, t	o = 9	.2Å,	c = 2	8.6Å	, $\beta = 89.7^{\circ}$	
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1  (8, 1) \\ T_2  (8, 1) \\ T_3  (8, 1) \\ T_4  (8, 1) \end{array}$	4 4 4 3	9 9 10 8	18 19 19 16	31 33 33 29	48 51 52 49	71 77 72 68	99 96 102 94	132 126 126 123	162 162 161 162	197 203 204 203	$\begin{array}{c} 4{\cdot}6{\cdot}6{\cdot}6{\cdot}6{\cdot}10_2\\ 4{\cdot}6{\cdot}4{\cdot}8_2{\cdot}6{\cdot}6_2\\ 4{\cdot}6_2{\cdot}4{\cdot}8_2{\cdot}8_2{\cdot}10\\ 6{\cdot}6_2}\end{array}$
Secondary building units:	4											
Loop configuration of T-Atoms:		$T_1$				] T <sub>2,3</sub>	_		T	4		
Isotypic framework structures:	*Partheite	(1)										

(1) Engel, N. and Yvon, K. Z. Kristallogr., 169, 165-175 (1984)

Partheite

# **Type Material**

# -PAR

Crystal chemical data:	$\begin{split} & Ca^{2+}{}_8\ (H_2O)_{16} \ [Al_{16}Si_{16}\ O_{60}(OH)_8]\text{PAR} \\ &monoclinic,\ C2/c,\ a=21.555\text{\AA},\ b=8.761\text{\AA},\ c=9.304\text{\AA},\ \beta=91.55^{\circ\ (1)} \end{split}$
Framework density:	18.2 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 3.5 x 6.9*
Stability:	Stable at 150°C, transforms at 400°C <sup>(1)</sup>



10-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	cubic, Im	<u>3</u> m, a	a =	34.8	3Å				
Coordination sequences	T <sub>1</sub> (96, 1)	4	9	18	31	47	68	91 117 151 188	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$
and vertex symbols:	T <sub>2</sub> (96, 1)	4	9	18	32	49	70	95 122 154 191	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$
	T <sub>3</sub> (96, 1)	4	9	18	32	49	69	94 123 153 186	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$
	T <sub>4</sub> (96, 1)	4	9	18	32	48	67	92 121 152 185	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$
	T <sub>5</sub> (96, 1)	4	9	18	31	47	68	92 119 152 188	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$
	T <sub>6</sub> (96, 1)	4	9	17	29	45	65	89 117 149 185	4.4.4.6.8.8
	T <sub>7</sub> (48, 2)	4	9	17	30	47	66	88 113 144 183	4.4.4.6.8.8
	T <sub>8</sub> (48, 2)	4	9	18	32	49	69	95 123 152 188	$4 \cdot 4 \cdot 4 \cdot 8_2 \cdot 8 \cdot 8$

Secondary build	ding units:
-----------------	-------------

Loop configuration of T-Atoms:	 T <sub>1-8</sub>

Isotypic framework	*Pau
structures:	ECR

Paulingite<sup>(1)</sup> CR-18<sup>(2)</sup>

4

### **References:**

- (1) Gordon, E.K., Samson, S. and Kamb, W.K. Science, 154, 1004-1007 (1966)
- (2) Vaughan, D.E.W. and Strohmaier, G. U.S. Patent 4,661,332 (1987)

Paulingite

## **Type Material**

# PAU

Crystal chemical data:

 $\label{eq:constraint} \begin{array}{l} |(Ca^{2+},K^{+}_{2},Na^{+}_{2})_{76}~(H_{2}O)_{700}|~[Al_{152}Si_{520}~O_{1344}]\text{-PAU} \\ \text{cubic, Im}~\overline{3}\text{m, a} = 35.093 \text{\AA}^{(1)} \end{array}$ 

15.5 T/1000Å<sup>3</sup> Framework density:

Channels:

<100> **8** 3.6x3.6\*\*\* | <100> **8** 3.6 x 3.6\*\*\*



8-ring viewed along <100>



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 9.9$ Å, $b = 14.1$ Å, $c = 14.0$ Å	
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
Secondary building units:	8 or 4	
Loop configuration of T-Atoms:	T <sub>1,2</sub>	
Isotypic framework structures:	*Phillipsite <sup><math>(1,2)</math></sup> [Al-Co-P-O]- <b>PHI</b> <sup><math>(3)</math></sup> Harmotome <sup><math>(2,4)</math></sup> ZK-19 <sup><math>(6)</math></sup>	

Alternate designation:

- (1) Steinfink, H. Acta Crystallogr., 15, 644-651 (1962)
- (2) Rinaldi, R., Pluth, J.J. and Smith, J.V. Acta Crystallogr., B30, 2426-2433 (1974)
- (3) Feng, P.Y., Bu, X.H. and Stucky, G.D. Nature, 388, 735-741 (1997)
- (4) Sadanaga, R., Marumo, F. and Yakéuchi, Y. Acta Crystallogr., 14, 1153-1163 (1961)

Wellsite<sup>(5)</sup> (discredited)

- (5) Cerny, P., Rinaldi, R. and Surdam, R.C. N. Jb. Miner. Abh., 128, 312-330 (1977)
- (6) Kuehl, G.H. Am. Mineral., 54, 1607-1612 (1969)

# **Type Material**

Crystal chemical data:	$\begin{split}  K_{2}^{+}(Ca^{2+},Na_{2}^{+})_{2} & (H_{2}O)_{12}  \left[Al_{6}Si_{10} O_{32}\right] \textbf{-PHI} \\ \text{monoclinic, P12}_{1}/m1 \\ a &= 9.865 \text{\AA, b} = 14.300 \text{\AA, c} = 8.668 \text{\AA, \beta} = 124.20^{\circ} \ ^{(2)} \\ (\text{Relationship to unit cell of Framework Type:} \\ a' &= a, b' &= c, c' = b/2 sin(\beta) \\ \text{or, as vectors, a'} &= a, b' &= c, c' = (b - a)/2) \end{split}$
Framework density:	15.8 T/1000Å <sup>3</sup>
Channels:	$[100] 8 3.8 \ge 3.8^* \leftrightarrow [010] 8 3.0 \ge 4.3^* \leftrightarrow [001] 8 3.2 \ge 3.3^*$



8-ring viewed along [100]



8-ring viewed along [010]



8-ring viewed along [001]



Idealized cell constants:	cubic, $\text{Im}\overline{3}\text{m}$ , a = 14.9Å								
Coordination sequences and vertex symbols:	$T_1(48,2)$ 4 9 17 28 42 60	81 105 132 162 4.4.4.6.8.8							
Secondary building units:	8-8 or 6-2 or 8 or 6 or 4								
Loop configuration of T-Atoms:									
Isotypic framework structures:	*Rho <sup>(1,2)</sup> [Be-As-O]- <b>RHO</b> <sup>(3)</sup> [Be-P-O]- <b>RHO</b> <sup>(4)</sup> [Co-Al-P-O]- <b>RHO</b> <sup>(5)</sup> [Mg-Al-P-O]- <b>RHO</b> <sup>(5)</sup>	[Mn-Al-P-O]- <b>RHO</b> <sup>(5)</sup> Deuterated Rho <sup>(6)</sup> Gallosilicate ECR-10 <sup>(7)</sup> LZ-214 <sup>(8)</sup> Pahasapaite <sup>(9.10)</sup>							

- (1) Robson, H.E., Shoemaker, D.P., Ogilvie, R.A. and Manor, P.C. Adv. Chem. Ser. , 121, 106-115 (1973)
- McCusker, L.B. and Baerlocher, Ch. In *Proc. 6th Int. Zeolite Conf.*, (eds. D.H. Olson and A. Bisio), pp. 812-822 (1984), Butterworths, Guildford, Surry
- (3) Gier, T.E. and Stucky, G.D. *Nature*, **349**, 508-510 (1991)
- (4) Harvey, G. and Meier, W.M. Stud. Surf. Sci. Catal., 49, 411-420 (1989)
- (5) Feng, P., Bu, X. and Stucky, G.D. Microporous and Mesoporous Materials, 23, 315-322 (1998)
- (6) Parise, J.B., Gier, T.E., Corbin, D.R. and Cox, D.E. J. Phys. Chem., 88, 1635-1640 (1984)
- (7) Newsam, J.M., Vaughan, D.E.W. and Strohmaier, K.G. J. Phys. Chem., 99, 9924-9932 (1995)
- (8) Breck, D.W. and Skeels, G.W. U.S. Patent 4,503,023, (1985)
- (9) Rouse, R.C., Peacor, D.R., Dunn, P.J., Campbell, T.J., Roberts, W.L., Wicks, F.J. and Newbury, D. N. Jb. Miner. Mh., 433-440 (1987)
- (10) Rouse, R.C., Peacor, D.R. and Merlino, S. Am. Mineral., 74, 1195-1202 (1989)

Crystal chemical data:

$$\begin{split} |(Na^{+},Cs^{+})_{12} \ (H_{2}O)_{44}| \ [Al_{12}Si_{36} \ O_{96}]\text{-}RHO \\ cubic, \ Im \ \overline{3}m, \ a = 15.031 \text{\AA}^{\ (2)} \end{split}$$

Framework density:

**Channels:** 

14.1 T/1000Å<sup>3</sup>

<100> **8** 3.6 x 3.6\*\*\* | <100> **8** 3.6 x 3.6\*\*\*



8-ring viewed along <100>

framework viewed along [001]

Idealized cell constants:	tetragonal, I4/mcm, $a = 18.1$ Å, $c = 9.0$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	combinations only
Loop configuration of T-Atoms:	$T_{1}$

Isotypic framework \*Roggianite<sup>(1)</sup>

The previously reported structure (the ROG type) was found to be incomplete and the code –ROG has been discredidted based on a decision by the IZA Structure commission.

#### **References:**

(1) Giuseppetti, G., Mazzi, F., Tadini, C. and Galli, E. N. Jb. Miner. Mh., 307-314 (1991)

Roggianite

Crystal chemical data:

$$\label{eq:ca2+} \begin{split} |Ca^{2+}{}_{16}\,(H_2O)_{19}| \,\, [Be_8Al_{16}Si_{32}\,O_{104}(OH)_{16}]\text{--}\textbf{RON} \\ tetragonal, \,I4/mcm, \,a = 18.33\text{\AA}, \,c = 9.16\text{\AA}^{(1)} \end{split}$$

Framework density: 18.2 T/1000Å<sup>3</sup>

Channels:

[001] **12** 4.3 x 4.3\*



12-ring viewed along [001]

structures:



framework viewed along [001]

Idealized cell constants:	monoclin	ic, C	C2/m	n, a =	= 7.2	Å, b	= 41	1.8Å	, c =	7.2Å	Α, γ= 90.0	0
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1  (8, 1) \\ T_2  (8, 1) \\ T_3  (8, 1) \\ T_4  (8, 1) \\ T_5  (4, 2) \end{array}$	4 4 4 4 4	9 10 9 11 8	19 21 21 21 21 20	39 37 42 40 44	59 58 57 61 55	78 91 82 89 80	117 117 119 116 118	155 144 151 145 152	189 194 188 191 204	235 241 239 239 228	$\begin{array}{c} 3{\cdot}4{\cdot}8_{3}{\cdot}9_{4}{\cdot}8_{3}{\cdot}9_{4}\\ 4{\cdot}4{\cdot}6_{2}{\cdot}8{\cdot}6_{2}{\cdot}8\\ 3{\cdot}4{\cdot}8_{2}{\cdot}9_{4}{\cdot}8_{2}{\cdot}9_{4}\\ 4{\cdot}5_{2}{\cdot}5{\cdot}8{\cdot}5{\cdot}8\\ 3{\cdot}3{\cdot}9_{4}{\cdot}9_{4}{\cdot}9_{4}{\cdot}9_{4}\end{array}$
Secondary building units:	combinati	ions	only	y								
Loop configuration of T-Atoms:		T <sub>1,3</sub>	[			T <sub>2</sub>			 	- 4		∠ T₅
Isotypic framework	*RUB-17	(1)										

## **RUB-17**

## **Type Material**

# **RSN**

Crystal chemical data:	$\begin{split}  K_{4}^{+}Na_{12}^{+}(H_{2}O)_{18}  \ [Zn_{8}Si_{28}O_{72}]\text{-}RSN \\ \text{monoclinic, }C1m1, \ a = 7.238\text{\AA}, \ b = 40.56\text{\AA}, \ c = 7.308\text{\AA}, \ \beta = 91.8^{\circ \ (1)} \end{split}$
Framework density:	16.8 T/1000Å <sup>3</sup>
Channels:	$[100] 9 3.3 \ge 4.4^* \leftrightarrow [001] 9 3.1 \ge 4.3^* \leftrightarrow [010] 8 3.4 \ge 4.1^*$
Stability:	Complete dehydration leads to destruction of the framework <sup>(1)</sup>



9-ring viewed along [100]



9-ring viewed along [001]

See Appendix A for 8-ring viewed along [010]

### **References:**

(1) Röhrig, C. and Gies, H. Angew. Chem., Int. Ed., 34, 63-65 (1995)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	monoclinic, C2/m, a = 14.1Å, b = 13.7Å, c = 7.4Å, $\beta$ = 102.4°	
Coordination sequences and vertex symbols:	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	4.5.4.6.5.6 4.4.5.8.6.6 4.5.5.6.6.8
Secondary building units:	5-3 or 4	
Loop configuration of T-Atoms:	$ \begin{array}{c c} \hline \\ T_1 \end{array} $ $ \begin{array}{c} \\ T_2 \end{array} $ $ \begin{array}{c} \\ T_3 \end{array} $	
Isotypic framework structures:	*RUB-3 <sup>(1,2)</sup>	

- (1) Marler, B., Grünewald-Lüke, A. and Gies, H. Zeolites, 15, 388-399 (1995)
- (2) Marler, B., Grünewald-Lüke, A. and Gies, H. Microporous and Mesoporous Materials, 26, 49-59 (1998)

Crystal chemical data:	$\begin{split}  (C_8H_{15}N)_2  & [Si_{24} O_{48}] \text{-RTE} \\ C_8H_{15}N &= \text{exo-2-aminobicyclo}[2.2.1.] \text{heptane} \\ & \text{monoclinic, C12/m1} \\ a &= 14.039\text{\AA, b} = 13.602\text{\AA, c} = 7.428\text{\AA, \beta} = 102.22^{\circ (1)} \end{split}$
Framework density:	17.3 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 3.7 x 4.4*



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 9.8Å, b = 20.5Å, c = 10.0Å, $\beta$ = 96.9°	
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 4{\cdot}6{\cdot}5{\cdot}6{\cdot}5{\cdot}8\\ 4{\cdot}4{\cdot}5{\cdot}8{\cdot}5{\cdot}8\\ 4{\cdot}5{\cdot}4{\cdot}6{\cdot}5{\cdot}5\\ 4{\cdot}5{\cdot}4{\cdot}8{\cdot}5{\cdot}5\end{array}$
Secondary building units:	4	
Loop configuration of T-Atoms:	$\begin{array}{c c} & & & \\ \hline \\ \hline \\ T_1 \end{array} \end{array} \begin{array}{c} T_2 \end{array} \begin{array}{c} \\ T_{3,4} \end{array}$	
Isotypic framework structures:	*RUB-13 <sup>(1)</sup>	

(1) Vortmann, S., Marler, B., Gies, H. and Daniels, P. Microporous Materials, 4, 111-121 (1995)

# **Type Material**

# RTH

Crystal chemical data:	$ (C_{10}H_{21}N^{+})_{2}  [B_{2}Si_{30}C_{10}H_{21}N^{+} = pentamonmonoclinic, C12/m$	$_{0}^{0}$ O <sub>64</sub> ]- <b>RTH</b> ethylpiperidinium 1, a = 9.659Å, b = 20.461Å, c = 9.831Å, $\beta$ = 96.58° <sup>(1)</sup>
Framework density:	16.6 T/1000Å <sup>3</sup>	
Channels:	[100] <b>8</b> 3.8 x 4.1* ↔	→ [001] <b>8</b> 2.5 x 5.6*



8-ring viewed along [100]



8-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	monoclinic, C2/m, a = 13.2Å, b = 13.3Å, c = 12.5Å, $\beta$ = 114.8°	
Coordination sequences and vertex symbols:	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	4·4·5·6·5·8 4·5·4·6·5·6 4·5·5·6·6·6 4·5·5·5·6·8 5·5·6·6·6·6
Secondary building units:	combinations only	
Loop configuration of T-Atoms:	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
Isotypic framework structures:	*RUB- $10^{(1)}$ [TMA-[[Si-O]-RUT <sup>(2)</sup> B-NU- $1^{(3)}$ Fe-NU- $1^{(3)}$ Ga-NU- $1^{(3)}$ NU- $1^{(4)}$	

- (1) Gies, H. and Rius, J. Z. Kristallogr., 210, 475-480 (1995)
- (2) Broach, R.W., McGuire, N.K., Chao, C.C. and Kirchner, R.M. J. Phys. Chem. Solids, 56, 1363-1368 (1995)
- (3) Bellussi, G., Millini, R., Carati, A., Maddinelli, G. and Gervasini, A. Zeolites, 10, 642-649 (1990)
- (4) Whittam, T.V. and Youll, B. U.S. Patent 4,060,590, (1977)

# **Type Material**

Crystal chemical data:	$\begin{split}  (C_4H_{12}N^+)_4  & [B_4Si_{32} O_{72}]\text{-}RUT \\ C_4H_{12}N^+ &= tetramethylamonium \\ monoclinic, & P12_1/a1 \\ a &= 13.112\text{\AA}, b = 12.903\text{\AA}, c = 12.407\text{\AA}, \beta = 113.50^{\circ (1)} \end{split}$
Framework density:	18.7 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



(1) Noble, G.W., Wright, P.A., Lightfoot, P., Morris, R.E., Hudson, K.J., Kvick, Å. and Graafsma, H. Angew. *Chem., Int. Ed.*, **36**, 81-83 (1997)

Crystal chemical data:	$\begin{split} & (C_{21}H_{40}N_2^{2+})_{2.6} (H_2O)_6  [Mg_5Al_{23}P_{28} O_{112}]\text{-}SAO \\ &C_{21}H_{40}N_2^{2+} = C_7H_{13}N - (CH_2)_7 - C_7H_{13}N \\ &C_7H_{13}N = \text{quinuclidine} \\ &\text{tetragonal, P4n2, a = 13.810Å, c = 21.969Å}^{(1)} \end{split}$
Framework density:	13.4 T/1000Å <sup>3</sup>
Channels:	<100> <b>12</b> 6.5 x 7.2** ↔ [001] <b>12</b> 7.0 x 7.0*



12-ring viewed along <100>



12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	tetragonal, I4/mmm, $a = 14.3$ Å, $c = 10.4$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4
Loop configuration of T-Atoms:	
Isotypic framework structures:	*STA-6 <sup>(1)</sup>

(1) Patinec, V., Wright, P.A., Lightfoot, P., Aitken, R.A. and Cox, P.A. J. Chem. Soc., Dalton Trans., 3909-3911 (1999)

8-ring viewed along [001]

4.2

Crystal chemical data:	$\begin{split}  (C_{14}H_{34}N_4^{\ 2^+})_{1.5}\ (H_2O)_{2.5} \ [Mg_3Al_{13}P_{16}\ O_{64}]\text{-}\mathbf{SAS}\\ C_{14}H_{32}N_4 &= 1,4,8,11\text{-}tetramethyl-1,4,8,11\text{-}tetraazatetradecane\\ tetragonal,\ P4/mnc,\ a &= 14.282\text{\AA},\ c &= 10.249\text{\AA}^{\ (1)} \end{split}$
Framework density:	15.3 T/1000Å <sup>3</sup>
Channels:	[001] <b>8</b> 4.2 x 4.2*
4.2	4.2

4.2



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , a = 12.9Å, c = 30.6Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6
Loop configuration of T-Atoms:	
Framework description:	ABBCBCCACAAB sequence of 6-rings
Isotypic framework structures:	*STA-2 <sup>(1)</sup>

(1) Noble, G.W., Wright, P.A. and Kvick, Å. J. Chem. Soc., Dalton Trans., 4485-4490 (1997)

Crystal chemical data:	$\begin{split}  (C_{18}H_{34}N_2^{2+})_3 & (H_2O)_{22.5}  \ [Mg_{5.4}Al_{30.6}P_{36} & O_{144}]\text{-SAT} \\ C_{18}H_{34}N_2^{2+} &= C_7H_{13}N - (CH_2)_4 - C_7H_{13}N \\ C_7H_{13}N &= quinuclidine \\ trigonal, R\overline{3}, a &= 12.726 \ \text{\AA}, c &= 30.939 \text{\AA}^{(1)} \end{split}$
Framework density:	16.6 T/1000Å <sup>3</sup>
Channels:	⊥ [001] 3.0 x 5.5***



8-ring viewed normal to [001]



framework viewed along [001]

Idealized cell constants:	tetragonal,	P4/	'nm	m (0	origi	n cho	oice 2	2), a	= 18	3.7Å	, c = 9.4Å	
Coordination sequences and vertex symbols:	$\begin{array}{l} T_1  (16, 1) \\ T_2  (16, 1) \\ T_3  (16, 1) \end{array}$	4 4 4	9 9 9	17 17 17	29 29 29	45 45 45	65 65 63	88 88 84	113 114 112	143 144 144	179 177 177	$\begin{array}{c} 4{\cdot}4{\cdot}4{\cdot}8{\cdot}6{\cdot}8\\ 4{\cdot}4{\cdot}4{\cdot}8{\cdot}6{\cdot}8\\ 4{\cdot}4{\cdot}4{\cdot}8{\cdot}6{\cdot}8\end{array}$
Secondary building units:	6-6 or 6 o	or 4	1									
Loop configuration of T-Atoms:		Γ <sub>1-3</sub>										
Isotypic framework structures:	*Mg-STA- Co-STA-7	-7 <sup>(1)</sup>										

Zn-STA-7<sup>(1)</sup>

### **References:**

(1) Wright, P.A., Maple, M.J., Slawin, A.M.Z., Patinec, V., Aitken, R.A., Welsh, S. and Cox, P.A. J. Chem. Soc., Dalton Trans., 1243-1248 (2000)

# **Type Material**

Crystal chemical data:	$\begin{split} & (C_{18}H_{42}N_6)_{1.96} \ (H_2O)_7  \ [Mg_{4.8}Al_{19.2}P_{24} \ O_{96}]\text{-}SAV \\ &C_{18}H_{42}N_6 = 1,4,7,10,13,16\text{-}hexamethyl-1,4,7,10,13,16\text{-}hexaazacyclooctadecane} \\ & \text{tetragonal, P4/n, a} = 18.773\text{\AA, c} = 9.454\text{\AA}^{(1)} \end{split}$
Framework density:	14.4 T/1000Å <sup>3</sup>
Channels:	<100> <b>8</b> 3.8 x 3.8** ↔ [001] <b>8</b> 3.9 x 3.9*



8-ring viewed along <100>



8-ring viewed along [001]



framework viewed along [100] (top left: projection down [100])

Idealized cell constants:	tetragonal, I4/mmm, $a = 18.5$ Å, $c = 27.1$ Å												
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1 \ (32, 1) \\ T_2 \ (32, 1) \\ T_3 \ (32, 1) \\ T_4 \ (32, 1) \end{array}$	4 4 4 4	9 9 9 9	17 17 17 17	27 28 27 27	38 41 39 40	55 57 56 59	78 77 77 79	102 101 100 99	129 130 126 126	157 162 157 158	$\begin{array}{c} 4.6.4.8\\ 4.4.4.6.\\ 4.4.4.8\\ 4.4.4.8\\ 4.4.4.8_{2}.1\end{array}$	
Secondary building units:	8-8 or 8	or 4	Ļ										
Loop configuration of T-Atoms:		$\Gamma_1$	E			T <sub>2-4</sub>							
Isotypic framework structures:	*UCSB-80 UCSB-8M UCSB-8M UCSB-8Z1	$ \begin{bmatrix} o^{(1)} \\ g^{(1)} \\ n^{(1)} \\ n^{(1)} \end{bmatrix} $											

(1) Bu, X.H., Feng, P.Y. and Stucky, G.D. Science, 278, 2080-2085 (1997)

## **Type Material**

Crystal chemical data:	$\begin{split}  (C_9H_{24}N_2^{2^+})_{16}  & [Al_{32}Co_{32}P_{64} O_{256}]\text{-}\textbf{SBE} \\ C_9H_{22}N_2 &= 1,9\text{-}diaminononane \\ tetragonal, P4/nnc, a &= 19.065\text{\AA}, c = 27.594 \text{\AA}^{(1)} \end{split}$
Framework density:	12.8 T/1000Å <sup>3</sup>

Channels:

 $<\!\!100\!\!> \mathbf{12} \ 7.2 \ge 7.4^{**} \leftrightarrow [001] \ \mathbf{8} \ 4.0 \ge 4.0^*$ 



12-ring viewed along <100>



8-ring viewed along [001] and



second 8-ring along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /mmc, a = 17.2Å, c = 27.3Å							
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$							
Secondary building units:	4							
Loop configuration of T-Atoms:	$ \begin{array}{c c} & & & \\ \hline & & \\ & & $							
Isotypic framework structures:	*UCSB-6GaCo <sup>(1)</sup> UCSB-6Co <sup>(1)</sup> UCSB-6GaMg <sup>(1)</sup> UCSB-6GaZn <sup>(1)</sup> UCSB-6Mg <sup>(1)</sup> UCSB-6Mn <sup>(1)</sup> UCSB-6Zn <sup>(1)</sup>							

(1) Bu, X.H., Feng, P.Y. and Stucky, G.D. Science, **278**, 2080-2085 (1997)

 _	_	 			

Crystal chemical data:	$\begin{split} & (C_9H_{24}N_2)^{2+}{}_{12}  \ [Ga_{24}Co_{24}P_{48} \ O_{192}]\text{-}\textbf{SBS} \\ &C_9H_{22}N_2=1,9\text{-}diaminononane} \\ & \text{trigonal, } P\overline{3}1c, \ a=17.836\text{\AA}, \ c=27.182\text{\AA}^{(1)} \end{split}$					
Framework density:	12.8 T/1000Å <sup>3</sup>					
Channels:	[001] <b>12</b> 6.8 x 6.8 <sup>*</sup> ↔ $\perp$ [001] <b>12</b> 6.9 x 7.0 <sup>**</sup>					



12-ring viewed along [001]



12-ring viewed normal to [001]

See Appendix A for 8-ring along [001]



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	trigonal, $R\overline{3}m$ , $a = 17.2$ Å, $c = 41.0$ Å					
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					
Secondary building units:	6 or 4-2					
Loop configuration of T-Atoms:	$ \begin{array}{c c} & & & \\ \hline & & \\ & & $					
Isotypic framework structures:	$*UCSB-10GaZn^{(1)}$ UCSB-10Co <sup>(1)</sup> UCSB-10Mg <sup>(1)</sup> UCSB-10Zn <sup>(1)</sup>					

(1) Bu, X.H., Feng, P.Y. and Stucky, G.D. Science, 278, 2080-2085 (1997)
## **Type Material**

$$\begin{split} |(C_{10}H_{26}N_2O_3^{\ 2^+})_{18}| & [Ga_{36}Zn_{36}P_{72} \ O_{288}]\text{-}\textbf{SBT} \\ C_{10}H_{24}N_2O_3 = 4,7,10\text{-}trioxa\text{-}1,13\text{-}tridecanediamine} \\ trigonal, R\overline{3}, a = 18.080\text{\AA}, c = 41.951\text{\AA}^{\ (1)} \end{split}$$

Framework density: 12.1 T/1000Å<sup>3</sup>

Channels:

 $[001] \ \textbf{12} \ \textbf{6.4} \ \textbf{x} \ \textbf{7.4}^{*} \leftrightarrow \bot [001] \ \textbf{12} \ \textbf{7.3} \ \textbf{x} \ \textbf{7.8}^{**}$ 



12-ring viewed along [001]



12-ring viewed normal to [001]

See Appendix A for 8-ring viewed along [102]



framework viewed normal to [010] (top left: projection down [010])

Idealized cell constants:	monoclini	c, P	121	l,a:	= 11	.4Å,	b = 5.1Å	, c =	: 13.9	βÅ, $β = 100.9°$	
<b>Coordination sequences</b>	T <sub>1</sub> (2, 1)	4	12	20	37	62	82 114	142	192	238	5.5.5.5.6.12
and vertex symbols:	$T_2(2, 1)$	4	10	19	35	58	86 108	144	183	233	$4{\cdot}5{\cdot}4{\cdot}5{\cdot}6{\cdot}12$
	$T_3(2, 1)$	4	10	20	35	57	83 116	141	181	230	$4 \cdot 5 \cdot 4 \cdot 5 \cdot 12 \cdot *$
	$T_4(2, 1)$	4	12	22	36	56	86 114	150	179	232	5.5.5.5.6.*
	$T_5(2, 1)$	4	12	22	37	55	83 120	149	177	227	5.6.6.6.6.6
	$T_6(2, 1)$	4	12	24	37	54	80 117	158	184	219	5.6.6.6.6.6
	T <sub>7</sub> (2, 1)	4	12	23	41	58	78 111	154	198	235	5.5.5.5.6.12
Secondary building units:	5-2										



Isotypic framework	*SSZ-48 <sup>(1)</sup>
structures:	

(1) Wagner, P., Terasaki, O., Ritsch, S., Nery, J.G., Zones, S.I., Davis, M.E. and Hiraga, K. J. Phys. Chem. B, 103, 8245-8250 (1999)

Crystal chemical data:	[Si <sub>14</sub> O <sub>28</sub> ]-SFE monoclinic, P12 <sub>1</sub> 1 $a = 11.153$ Å, $b = 5.002$ Å, $c = 13.667$ Å, $\beta = 100.63^{\circ}$ <sup>(1)</sup>
Framework density:	18.7 T/1000Å <sup>3</sup>
Channels:	[010] <b>12</b> 5.4 x 7.6*
	7.6

5.4



5.4



	T (4 1)						monoclinic, P2 <sub>1</sub> /m, a = 11.5Å, b = 21.7Å, c = 7.2Å, $\beta$ = 93.2°					
Coordination sequences	$I_1(4, 1)$	4	12	20	34	56	87	115	143	176	224	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
and vertex symbols:	$T_2(4, 1)$	4	12	20	34	56	88	115	142	177	225	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
r	$T_3(4, 1)$	4	11	22	38	57	80	111	148	189	228	4.5.5.6.5.10
,	$T_4(4, 1)$	4	11	22	39	54	84	110	145	189	234	4.5.5.6.5.10
,	$T_5(4, 1)$	4	11	23	37	57	82	113	150	184	228	4.5.5.6.5.10
,	$T_{6}(4, 1)$	4	11	20	31	58	86	115	142	174	225	$4 \cdot 6_2 \cdot 5 \cdot 5 \cdot 5 \cdot 5$
r.	$T_7(4, 1)$	4	11	19	36	55	82	113	148	181	220	4.6.5.5.5.5
r	$T_8(4, 1)$	4	11	23	36	59	79	114	147	183	229	4.5.5.6.5.10
Secondary building units:	5-3											
Loop configuration of T-Atoms:			_	_		Taa						
Isotypic framework structures:	*SSZ-44 <sup>(1)</sup>	1,2				1 <sub>3-8</sub>						

Z ∧

Х

(1) Wagner, P., Zones, S.I., Davis, M.E. and Medrud, R.C. Angew. Chem., Int. Ed., 38, 1269-1272 (1999)

Crystal chemical data:	[Si <sub>32</sub> O <sub>64</sub> ]-SFF monoclinic, P2 <sub>1</sub> /m, a = 11.485 Å, b = 21.946Å, c = 7.388Å, $\beta$ = 94.70° <sup>(1)</sup>
Framework density:	17.2 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 5.4 x 5.7*



10-ring viewed along [001]



framework viewed along [100] (top left: projection down [100])

Idealized cell constants:	tetragonal, I4 <sub>1</sub> /	amd	(origi	n cho	pice 2), a = 10.3Å, c = 34.4Å	
Coordination sequences and vertex symbols:	$\begin{array}{rrrr} T_1  (16,m) & 4 \\ T_2  (16,m) & 4 \\ T_3  (16,2) & 4 \\ T_4  (16,m) & 4 \end{array}$	11 2 11 2 11 2 12 2	22 37 21 37 23 38 24 42	62 63 62 61	89    120    155    202    257    4      86    121    152    196    258    4      92    113    159    210    244    4      87    128    168    205    250    5	6.5.5.5.5 6.5.5.5.5 6.5.5.5.5 .6.5.6.5.6
Secondary building units:	5-3					
Loop configuration of T-Atoms:	T <sub>1-3</sub>		+	 T <sub>4</sub>		
Isotypic framework	*Sigma-2 <sup>(1)</sup>					

structures:

(1) McCusker, L.B. J. Appl. Crystallogr., 21, 305-310 (1988)

Crystal chemical data:	$ (C_{10}H_{17}N)_4 $ [Si <sub>64</sub> O <sub>128</sub> ]-SGT C <sub>10</sub> H <sub>17</sub> N = 1-aminoadamantane tetragonal, I4 <sub>1</sub> /amd, a = 10.239Å, c = 34.383Å <sup>(1)</sup>
Framework density:	17.8 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only



framework viewed along [100]

Idealized cell constants:	cubic, $Im\overline{3}m$ , $a = 9.0$ Å	
Coordination sequences and vertex symbols:	$T_1 (12, \overline{4}2m)4 \ 10 \ 20 \ 34 \ 52 \ 74 \ 10$	00 130 164 202 4.4.6.6.6.6
Secondary building units:	6-2 or 6 or 4	
Loop configuration of T-Atoms:		
Framework description:	ABC sequence of 6-rings	
Isotypic framework structures:	*Sodalite <sup>(1,2)</sup> [Al-Co-P-O]-SOD <sup>(3)</sup> [Al-Ge-O]-SOD <sup>(4)</sup> [Be-As-O]-SOD <sup>(5)</sup> [Be-P-O]-SOD <sup>(5)</sup> [Be-Si-O]-SOD <sup>(6)</sup> [Co-Ga-P-O]-SOD <sup>(7)</sup> [Ga-Co-P-O]-SOD <sup>(3)</sup> [Ga-Ge-O]-SOD <sup>(4)</sup> [Ga-Si-O]-SOD <sup>(8)</sup> [Zn-As-O]-SOD <sup>(9)</sup> [Zn-Ga-As-O]-SOD <sup>(7)</sup> [Zn-Ga-P-O]-SOD <sup>(7)</sup> [Zn-P-O]-SOD <sup>(9)</sup> [Ca <sub>8</sub> (WO <sub>4</sub> ) <sub>2</sub> ][Al <sub>12</sub> O <sub>24</sub> ]-SOD <sup>(10)</sup>	AlPO-20 plus numerous compositional variants <sup>(11,12)</sup> Basic sodalite <sup>(13,14)</sup> Bicchulite <sup>(15)</sup> Danalite <sup>(16)</sup> $G^{(17)}$ Genthelvite <sup>(18)</sup> Hauyn <sup>(19)</sup> Helvin <sup>(20)</sup> Hydroxo sodalite <sup>(21)</sup> Nosean <sup>(22)</sup> Silica sodalite <sup>(23)</sup> TMA sodalite <sup>(24)</sup> Tugtupite <sup>(25,26)</sup>

Crystal chemical data:	$ Na_{8}^{+}Cl_{2}^{-} $ [Al <sub>6</sub> Si <sub>6</sub> O <sub>24</sub> ]-SOD cubic, P43n, a = 8.870Å <sup>(2)</sup>
Framework density:	17.2 T/1000Å <sup>3</sup>
Channels:	apertures formed by 6-rings only

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- (2) Loens, J. and Schulz, H. Acta Crystallogr., 23, 434-436 (1967)
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- (24) Baerlocher, Ch. and Meier, W.M. Helv. Chim. Acta, 52, 1853-1860 (1969)
- (25) Sorensen, H. Am. Mineral., 48, 1178 (1963)
- (26) Hassan, I. and Grundy, H.D. Can. Mineral., 29, 385-390 (1991)



framework viewed normal to [001] (top left: projection down [001])

Idealized cell constants:	monoclini	e, C	C2/m	n, a =	= 14.	1Å, 1	b =	18.27	Å, c =	= 7.5	Å, $\beta = 99.0^{\circ}$	
Coordination sequences	T <sub>1</sub> (8, 1)	4	12	20	34	56	88	114	143	173	224	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
and vertex symbols:	T <sub>2</sub> (8, 1)	4	11	22	39	55	82	111	149	188	223	4.5.5.6.5.10
-	$T_3(8, 1)$	4	11	23	36	59	80	113	147	183	227	4.5.5.6.5.10
	$T_4(4, m)$	4	11	19	36	54	84	110	146	179	226	4.6.5.5.5.5
	T <sub>5</sub> (4, m)	4	11	20	31	58	84	117	137	174	229	$4 \cdot 6_2 \cdot 5 \cdot 5 \cdot 5 \cdot 5$
Secondary building units:	5-3											

Loop configuration of T-Atoms:				
	Ĭ	<b>T</b> <sub>1</sub>	Ĭ	T <sub>2-5</sub>

Isotypic framework	*SSZ-35 <sup>(1)</sup>
structures:	ITQ-9 <sup>(2)</sup>

- (1) Wagner, P., Zones, S.I., Davis, M.E. and Medrud, R.C. Angew. Chem., Int. Ed., 38, 1269-1272 (1999)
- (2) Villaescusa, L.A., Barrett, P.A. and Camblor, M.A. Chem. Commun., 21, 2329-2330 (1998)

# **Type Material**

Crystal chemical data:	[Si <sub>16</sub> O <sub>32</sub> ]- <b>STF</b> triclinic, PĪ, a = 11.411Å, b = 11.527Å, c = 7.377Å $\alpha$ = 94.66°, $\beta$ = 96.21°, $\gamma$ = 104.89° <sup>(1)</sup> (Relationship to unit cell of Framework Type: V' = V/2)
Framework density:	17.3 T/1000Å <sup>3</sup>
Channels:	[001] <b>10</b> 5.4 x 5.7*



10-ring viewed along [001]



framework viewed along [100]

Idealized cell constants:	orthorhombic, Fmmm, $a = 13.5$ Å, $b = 17.8$ Å, $c = 17.9$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	4-4=1
Loop configuration of T-Atoms:	$\begin{array}{c c} & & & & & \\ \hline & & & \\ T_1 \end{array} \end{array} \begin{array}{c} & & & \\ T_2 \end{array} \end{array} \begin{array}{c} & & & \\ T_3 \end{array} \begin{array}{c} & & \\ T_4 \end{array}$
Isotypic framework structures:	*Stilbite <sup>(1-3)</sup> Barrerite <sup>(4)</sup> Stellerite <sup>(5)</sup> Synthetic barrerite <sup>(6)</sup> Synthetic stellerite <sup>(6)</sup> Synthetic stilbite <sup>(7)</sup>
Alternate designation:	Desmine (discredited) Epidesmin (obsolete)

- Galli, E. and Gottardi, G. *Miner. Petrogr. Acta*, **12**, 1-10 (1966)
  Slaughter, M. *Am. Mineral.*, **55**, 387-397 (1970)

## **Type Material**

Crystal chemical data:	$\begin{split} & \mathrm{Na}_{4}^{+}\mathrm{Ca}^{2+}{}_{8}^{2} (\mathrm{H}_{2}\mathrm{O})_{56}   [\mathrm{Al}_{20}\mathrm{Si}_{52}  \mathrm{O}_{144}]\text{-}\mathbf{STI} \\ & \text{monoclinic, C12/m1, a = 13.64Å, b = 18.24Å, c = 11.27Å, \beta = 128.0^{\circ}  ^{(3)} \\ & (\mathrm{Relationship \ to \ unit \ cell \ of \ Framework \ Type: \\ & \mathrm{a'} = \mathrm{a, \ b'} = \mathrm{b, \ c'} = \mathrm{c/2sin}(\beta) \\ & \mathrm{or, \ as \ vectors, \ a'} = \mathrm{a, \ b'} = \mathrm{b, \ c'} = (\mathrm{c} - \mathrm{a})/2) \end{split}$
Framework density:	16.3 T/1000Å <sup>3</sup>
Channels:	[100] <b>10</b> 4.7 x 5.0* $\leftrightarrow$ [001] <b>8</b> 2.7 x 5.6*



10-ring viewed along [100]



8-ring along [001]

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- (3) Galli, E. Acta Crystallogr., **B27**, 833-841 (1971)
- (4) Galli, E. and Alberti, A. Bull. Soc. fr. Minéral. Cristallogr., 98, 331-340 (1975)
- (5) Galli, E. and Alberti, A. Bull. Soc. fr. Minéral. Cristallogr., 98, 11-18 (1975)
- (6) Ghobarkar, H., Schaef, O. and Guth, U. J. Solid State Chem., 142, 451-454 (1999)
- (7) Ghobarkar, H. and Schaef, O. J. Phys. D: Appl. Phys., **31**, 3172-3176 (1998)



framework viewed normal to [100]

**Idealized cell constants:** monoclinic,  $P12_1/n1$ , a = 13.1Å, b = 21.9Å, c = 13.6Å,  $\beta = 102.9^{\circ}$ 

<b>Coordination sequences</b>	$T_1(4, 1)$	4	11	22	36	55	84 111	142	179	233	4.5.5.7.6.9
and vertex symbols:	$T_{2}(4, 1)$	4	10	23	37	57	78 108	146	187	225	4.4.5.9.6.7
·	$T_{3}(4, 1)$	4	11	20	35	54	84 108	142	178	225	4.6.5.6.5.7
	$T_4(4, 1)$	4	10	19	32	55	81 109	141	174	223	4.5.4.6.5.5
	$T_5(4, 1)$	4	9	21	38	57	78 104	144	195	220	4.4.4.9.5.7
	$T_{6}(4, 1)$	4	10	20	40	57	78 105	143	191	226	4.5.4.7.5.9
	$T_7(4, 1)$	4	10	20	35	57	77 108	139	184	230	4.6.4.6.5.7
	$T_8(4, 1)$	4	10	19	35	54	77 108	146	174	215	4.5.4.9.5.6
	$T_{9}(4, 1)$	4	11	19	34	53	81 115	140	173	219	4.6.5.5.5.5
	$T_{10}(4, 1)$	4	10	21	31	51	83 115	134	172	216	4.6.4.6.5.5
	$T_{11}(4, 1)$	4	12	20	31	50	88 117	137	167	221	$5 \cdot 5_2 \cdot 5 \cdot 6 \cdot 6 \cdot 6$
	$T_{12}(4, 1)$	4	10	18	35	59	77 107	150	179	221	4.5.4.9.5.5
	$T_{13}(4, 1)$	4	10	20	38	55	75 104	149	185	218	4.4.5.6.5.9
	$T_{14}(4, 1)$	4	12	21	33	58	86 112	141	174	226	5.5.5.6.5.7
	$T_{15}(4, 1)$	4	11	21	33	55	78 111	145	175	217	4.5.5.6.5.9
	$T_{16}(4, 1)$	4	11	20	32	54	89 115	138	172	221	4.6.5.5.5.5

### Secondary building units: 5-1





Crystal chemical data:	$\begin{split}  (C_{13}H_{24}N^{+})_{4.1} \ F_{3.3}(OH)^{-}_{0.8} [Si_{64} \ O_{128}]\text{-}STT\\ C_{13}H_{24}N^{+} &= N, N, N\text{-trimethyl-1-adamantammonium}\\ \text{monoclinic, } P12_{1}/n1\\ a &= 12.959\text{\AA, } b = 21.792\text{\AA, } c = 13.598\text{\AA, } \beta = 101.85^{\circ \ (1)} \end{split}$
Framework density:	17.0 T/1000Å <sup>3</sup>
Channels:	$[101] 9 3.7 x 5.3^* \leftrightarrow [001] 7 2.4 x 3.5^*$



9-ring viewed along [101]



7-ring viewed along [001]

(1) Camblor, M.A., Díaz-Cabañas, M.-J., Pérez-Pariente, J., Teat, S.J., Clegg, W., Shannon, I.J., Lightfoot, P., Wright, P.A. and Morris, R.E. *Angew. Chem., Int. Ed.*, **37**, 2122-2126 (1998)



framework viewed along [001]

Idealized cell constants:	orthorhom	bic	, Cn	ncm	, a =	9.8Å	Å, b	= 23	.6Å,	c = 2	20.2Å	L .
Coordination sequences	T <sub>1</sub> (16, 1)	4	11	19	35	57	83	113	137	184	231	$4 \cdot 5 \cdot 5 \cdot 6 \cdot 5 \cdot 6_2$
and vertex symbols:	T <sub>2</sub> (16, 1)	4	11	21	35	58	87	103	144	188	227	$4 \cdot 5 \cdot 5 \cdot 6_2 \cdot 5 \cdot 10_3$
	T <sub>3</sub> (8, m)	4	11	22	39	62	82	104	142	178	225	$4 \cdot 10_6 \cdot 5 \cdot 6_3 \cdot 5 \cdot 6_3$
	T <sub>4</sub> (8, m)	4	11	21	41	61	77	107	134	186	232	$4 \cdot 5_2 \cdot 5 \cdot 10_4 \cdot 5 \cdot 10_4$
	T <sub>5</sub> (8, m)	4	11	19	34	56	78	116	152	184	208	$4 \cdot 5_2 \cdot 5 \cdot 6 \cdot 5 \cdot 6$
	T <sub>6</sub> (8, m)	4	11	21	33	53	80	112	155	187	214	$4 \cdot 10_2 \cdot 5 \cdot 6_3 \cdot 5 \cdot 6_3$
	T <sub>7</sub> (8, m)	4	12	20	35	55	81	119	142	182	216	$5 \cdot 6 \cdot 5 \cdot 6 \cdot 5_2 \cdot 10_2$
	T <sub>8</sub> (8, m)	4	12	23	32	49	86	124	147	167	219	$5 \cdot 6_2 \cdot 5 \cdot 6_2 \cdot 10 \cdot 10_4$
Secondary building units:	2-6-2											
Loop configuration of T-Atoms:		г	_			<u>-</u> т						
	•	<b>1</b> -6				<b>1</b> 7,8						

Isotypic framework structures:

\*Terranovaite<sup>(1)</sup>

#### **References:**

(1) Galli, E., Quartieri, S., Vezzalini, G., Alberti, A. and Franzini, M. Am. Mineral., 82, 423-429 (1997)

Terranovaite

**Type Material** 

# TER

Crystal chemical data:	$\begin{split} & Na^{+}_{4.2}K^{+}_{0.2}Mg^{2+}_{0.2}Ca^{2+}_{3.7}~(H_{2}O)_{29} ~[Al_{12.3}Si_{67.7}~O_{160}]\text{-}\textbf{TER}\\ &\text{orthorhombic, Cmcm, }a=9.747\text{\AA, }b=23.880\text{\AA, }c=20.068\text{\AA}^{~(1)} \end{split}$
Framework density:	17.1 T/1000Å <sup>3</sup>
Channels:	$[100] \ 10 \ 5.0 \ \mathbf{x} \ 5.0^* \leftrightarrow [001] \ 10 \ 4.1 \ \mathbf{x} \ 7.0^*$



10-ring viewed along [100]



10-ring viewed along [001]



framework viewed normal to [001]

Idealized cell constants:	orthorhom	bic,	Pm	ıma,	a =	14.0	Å, b = 7	.0Å,	c = 6	5.5Å	
<b>Coordination sequences</b>	T <sub>1</sub> (4, m)	4	9	19	35	52	72 100	131	163	201	$4 \cdot 8_3 \cdot 4 \cdot 8_3 \cdot 4_2 \cdot 8_4$
and vertex symbols:	T <sub>2</sub> (4, m)	4	9	19	33	50	74 100	129	165	201	$4 \cdot 8_3 \cdot 4 \cdot 8_3 \cdot 4_2 \cdot 8_4$
	$T_3$ (2, mm2)	) 4	8	18	34	50	68 100	130	160	204	$4_2 \cdot 4_2 \cdot 8_4 \cdot 8_4 \cdot 8_4 \cdot 8_4$

Secondary building units: 4=1

Loop configuration of **T-Atoms:** 



Isotypic framework
structures:

\*Thomsonite<sup>(1-3)</sup>  $[Al-Co-P-O]-THO^{(4)}$ [Ga-Co-P-O]-**THO**<sup>(4)</sup> Na-V<sup>(5)</sup> Synthetic thomsonite<sup>(6)</sup>

- (1) Taylor, W.H., Meek, C.A. and Jackson, W.W. Z. Kristallogr., 84, 373-398 (1933)
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## Thomsonite

## **Type Material**

# Crystal chemical data: $|Na_{4}^{+}Ca_{8}^{2+}(H_{2}O)_{24}| [Al_{20}Si_{20}O_{80}]$ -THO<br/>orthorhombic, Pncn, a = 13.088Å, b = 13.052Å, c = 13.229Å <sup>(3)</sup><br/>(Relationship to unit cell of Framework Type: a' = a, b' = 2b, c' = 2c)Framework density:17.7 T/1000Å<sup>3</sup>Channels:[100] 8 2.3 x 3.9\* $\leftrightarrow$ [010] 8 2.2 x 4.0\* $\leftrightarrow$ [001]8 2.2 x 3.0\* (variable<br/>due to considerable flexibility of framework)





8-ring viewed along [100]



8-ring viewed along [010]



8-ring along [001] (variable)

# THO



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cmcm, $a = 14.1$ Å, $b = 17.8$ Å, $c = 5.3$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6 or 5-1
Loop configuration of T-Atoms:	
Isotypic framework structures:	*Theta- $1^{(1,2)}$ ISI- $1^{(3)}$ KZ- $2^{(4)}$ NU- $10^{(5)}$ ZSM- $22^{(6,7)}$

- (1) Barri, S.A.I., Smith, G.W., White, D. and Young, D. Nature, 312, 533-534 (1984)
- (2) Highcock, R.M., Smith, G.W. and Wood, D. Acta Crystallogr., C41, 1391-1394 (1985)
- (3) Kozo, T. and Noboru, K. E. Patent A-170,003 (1986)
- (4) Parker, L.M. and Bibby, D.M. Zeolites, 3, 8-11 (1983)
- (5) Araya, A. and Lowe, B.M. Zeolites, 4, 280-286 (1984)
- (6) Kokotailo, G.T., Schlenker, J.L., Dwyer, F.G. and Valyocsik, E.W. Zeolites, 5, 349-351 (1985)
- (7) Marler, B. Zeolites, 7, 393-397 (1987)

Theta-1

# **Type Material**

# TON

Crystal chemical data:	$ Na_{n}^{+}(H_{2}O)_{4} $ [Al <sub>n</sub> Si <sub>24-n</sub> O <sub>48</sub> ]- <b>TON</b> , n < 2
	orthorhombic, $\text{Cmc2}_1$ , a = 13.859Å, b = 17.420Å, c = 5.038Å <sup>(7)</sup>

Framework density: 19.7 T/1000Å<sup>3</sup>

Channels:

[001] **10** 4.6 x 5.7\*



10-ring viewed along [001]



part of framework viewed along [001]

Idealized cell constants:	cubic, $Fm\overline{3}m$ , $a = 30.7$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-6 or 6 or 4
Loop configuration of T-Atoms:	T <sub>1,2</sub>
Isotypic framework structures:	*Tschörtnerite <sup>(1)</sup>

(1) Effenberger, H., Giester, G., Krause, W. and Bernhardt, H.J. Am. Mineral., 83, 607-617 (1998)

Crystal chemical data:

$$\begin{split} |Ca^{2+}{}_{64}(K^{+}{}_{2},Ca^{2+},Sr^{2+},Ba^{2+}){}_{48}Cu^{2+}{}_{48}~(OH)^{-}{}_{128}~(H_{2}O){}_{x}|~[Al_{192}Si_{192}~O_{768}]\text{-}\mathbf{TSC}\\ cubic,~Fm\overline{3}m,~a=31.62\text{\AA}^{(1)} \end{split}$$

Framework density: 12.1 T/1000Å<sup>3</sup>

Channels:

 $<\!\!100\!\!> \! \mathbf{8} 4.2 \ge 4.2^{***} \leftrightarrow <\!\!110\!\!> \! \mathbf{8} 3.1 \ge 5.6^{***}$ 



8-ring viewed along <100>



8-ring viewed along <110>



framework viewed along [001] (bottom left: projection down [001])

Idealized cell constants:	tetragonal	, P4	, a =	= 13	.0Å,	c = 4	4.9Å						
Coordination sequences and vertex symbols:	$\begin{array}{c} T_1  (4,  1) \\ T_2  (4,  1) \\ T_3  (4,  1) \\ T_4  (4,  1) \\ T_5  (1,  \overline{4}) \end{array}$	4 4 4 4	12 12 12 12 12	24 26 24 23 28	39 41 41 43 38	61 65 65 68 60	93 94 95 94 98	133 130 128 125 152	179 169 169 172 182	209 218 218 226 200	246 269 270 269 246	5.5.5.6 <sub>2</sub> 5.5.5.6.7 5.6.5.6.5 5.6.5.6.5 5.6.5.6.5 5.5.5.5.8	5.7 $12_6$ $5.6_2$ $5_2.6$ $5_2.8_2$
Secondary building units:	combinati	ons	onl	y									
Loop configuration of T-Atoms:	<b>_</b>	Г <sub>1-6</sub>											
Isotypic framework structures:	*VPI-8 <sup>(1)</sup>												

VET

(1) Freyhardt, C.C., Lobo, R.F., Khodabandeh, S., Lewis, J.E., Tsapatsis, M., Yoshikawa, M., Camblor, M.A., Pan, M., Helmkamp, M.M., Zones, S.I. and Davis, M.E. J. Am. Chem. Soc., **118**, 7299-7310 (1996)

VPI-8

Crystal chemical data:	[Si <sub>17</sub> O <sub>34</sub> ]- <b>VET</b> tetragonal, P $\overline{4}$ , a = 13.045Å, c = 5.034Å <sup>(1)</sup>
Framework density:	19.8 T/1000Å <sup>3</sup>
Channels:	[001] <b>12</b> 5.9 x 5.9*



12-ring viewed along [001]



framework viewed along [001]

Idealized cell constants:	hexagonal, P6 <sub>3</sub> /mcm, a = 18.3Å, c = 8.6Å										
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$										
Secondary building units:	6										
Loop configuration of T-Atoms:	$- \begin{array}{c} \hline \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ $										
Isotypic framework structures:	*VPI-5 <sup>(1-3)</sup> AlPO-54 <sup>(4)</sup> H1 <sup>(5)</sup> MCM-9 <sup>(6)</sup>										

- (1) Davis, M.E., Saldarriaga, C., Montes, C., Garces, J. and Crowder, C. Nature, 331, 698-699 (1988)
- (2) Richardson Jr., J.W., Smith, J.V. and Pluth, J.J. J. Phys. Chem., 93, 8212-8219 (1989)
- (3) McCusker, L.B., Baerlocher, Ch., Jahn, E. and Bülow, M. Zeolites, 11, 308-313 (1991)
- (4) Richardson Jr., J.W., Smith, J.V. and Pluth, J.J. J. Phys. Chem., 93, 8212-8219 (1989)
- (5) d'Yvoire, F. Bull. Soc. Chim. France, 1762-1776 (1961)
- (6) Derouane, E.G., Maistreiau, L., Gabelica, Z., Tuel, A., Nagy, J.B. and von Ballmoos, R. *Appl. Catal.*, **51**, L13-L20 (1989)

Crystal chemical data:	$ (H_2O)_{42} $ [Al <sub>18</sub> P <sub>18</sub> O <sub>72</sub> ]-VFI hexagonal, P6 <sub>3</sub> , a = 18.975Å, c = 8.104Å <sup>(3)</sup>
Framework density:	14.2 T/1000Å <sup>3</sup>
Channels:	[001] <b>18</b> 12.7 x 12.7*

18-ring viewed along [001]



framework viewed along [110]

Idealized cell constants:	tetragonal,	P4	$n_2/nc$	m (o	origi	n cho	oice	2), a	= 10	0.0Å	$, c = 34.1 \text{\AA}$	
Coordination sequences	T <sub>1</sub> (16, 1)	4	11	23	39	63	93	126	170	210	255	$4 \cdot 8 \cdot 5 \cdot 8_2 \cdot 5_2 \cdot 8_2$
and vertex symbols:	T <sub>2</sub> (8, m)	4	11	19	39	59	89	130	166	207	274	$4.5_{2}.5.8.5.8$
	T <sub>3</sub> (8, m)	4	9	20	37	61	92	117	152	201	246	$3 \cdot 4 \cdot 8 \cdot 8_2 \cdot 8 \cdot 8_2$
	T <sub>4</sub> (8, m)	4	9	20	37	62	87	119	158	195	248	$3 \cdot 4 \cdot 8_2 \cdot 8_3 \cdot 8_2 \cdot 8_3$
	T <sub>5</sub> (8, m)	4	9	21	41	59	85	133	155	195	261	$3 \cdot 4 \cdot 8 \cdot 8_3 \cdot 8 \cdot 8_3$
	T <sub>6</sub> (8, m)	4	10	18	39	65	83	119	169	218	236	$3 \cdot 8_3 \cdot 5 \cdot 5_2 \cdot 5 \cdot 5_2$
	T <sub>7</sub> (4, 2mm)	4	10	18	36	64	82	118	176	202	264	$3 \cdot 8_2 \cdot 5 \cdot 5 \cdot 5 \cdot 5$

Secondary building units: combinations only



Isotypic framework \*VPI-9<sup>(1)</sup> structures:

#### **References:**

(1) McCusker, L.B., Grosse-Kunstleve, R.W., Baerlocher, Ch., Yoshikawa, M. and Davis, M.E. *Microporous Materials*, **6**, 295-309 (1996)

# **Type Material**

Crystal chemical data:

Framework density:

 $\begin{aligned} &|\text{Rb}_{44}^{+}\text{K}_{4}^{+}(\text{H}_{2}\text{O})_{48}| \text{ [Zn}_{24}\text{Si}_{96}\text{ O}_{240}\text{]-VNI} \\ &\text{tetragonal, P4}_{1}2_{1}2, \text{ a} = 9.884\text{ Å, c} = 73.650\text{ Å}^{(1)} \\ &\text{(Relationship to unit cell of Framework Type: a' = a, b' = b, c' = 2c)} \\ &16.7 \text{ T}/1000\text{ Å}^{3} \end{aligned}$ 

**Channels:** 

 $\{<110>8\ 3.1\ x\ 4.0 \leftrightarrow [001]\ 8\ 3.5\ x\ .3.6\}^{***}$ 



8-ring along <110>



8-ring viewed along [001]



2nd 8-ring along <110>



framework viewed along [100]

**Idealized cell constants:** tetragonal, I4<sub>1</sub>/amd, a = 7.2Å, c = 41.8Å

Coordination sequences	T <sub>1</sub> (16, m)	4	9	21	42	61	81 123	3 159	198	246	$3 \cdot 4 \cdot 8_2 \cdot 9_4 \cdot 8_2 \cdot 9_4$
and vertex symbols:	T <sub>2</sub> (16, m)	4	11	21	40	61	93 122	2 151	195	251	$4 \cdot 5_2 \cdot 5 \cdot 8 \cdot 5 \cdot 8$
	$T_3 (4, \overline{4}m2)$	4	8	20	48	56	84 120	) 160	212	240	$3 \cdot 3 \cdot 9_4 \cdot 9_4 \cdot 9_4 \cdot 9_4$

Secondary building units: combinations only

Loop configuration of T-Atoms:



Isotypic framework structures:  $VPI-7^{(1,2)}$ Gaultite<sup>(3)</sup> VSV-7#<sup>(4)</sup>

# **Type Material**

Crystal chemical data:	$\begin{split} & Na^{+}_{26}H^{+}_{6}(H_{2}O)_{44}   [Zn_{16}Si_{56}  O_{144}] \text{-VSV} \\ &\text{orthorhombic, Fdd2, } a = 39.88\text{\AA, } b = 10.326\text{\AA, } c = 10.219\text{\AA}^{\ (2)} \\ &(\text{Relationship to unit cell of Framework Type:} \\ &a' = c,  b = a  \text{sqrt}(2),  c' = b  \text{sqrt}(2) \\ &\text{or, as vectors, } a = c ,  b = b - a,  c = a + b) \end{split}$
Framework density:	17.1 T/1000Å <sup>3</sup>
Channels:	$[01\overline{1}] 9 3.3 \ge 4.3^* \leftrightarrow [011] 9 2.9 \ge 4.2^* \leftrightarrow [011] 8 2.1 \ge 2.7^*$



9-ring along [01<sup>-</sup>]



9-ring along [011]

See Appendix A for 8-ring along [011] and 8-ring viewed along [100]

- (1) Annen, M.J., Davis, M.E., Higgins, J.B. and Schlenker, J.L. Chem. Commun., 1175-1176 (1991)
- (2) Röhrig, C., Gies, H. and Marler, B. Zeolites, 14, 498-503 (1994)
- (3) Ercit, T.S. and van Velthuizen, J. Can. Mineral., 32, 855-863 (1994)
- (4) Röhrig, C., Dierdorf, I. and Gies, H. J. Phys. Chem. Solids, 56, 1369-1376 (1995)



framework viewed along [001]

Idealized cell constants:	orthorhombic, Cccm, $a = 11.8$ Å, $b = 10.3$ Å, $c = 10.0$ Å												
Coordination sequences and vertex symbols:	T <sub>1</sub> (16, 1) T <sub>2</sub> (4, 222)	4 4	9 8	18 18	32 32	51 52	74 70	98 98	126 132	163 152	199 200		3·4·6·8·8·10 3·3·6·6·10·10
Secondary building units:	spiro-5												
Loop configuration of T-Atoms:		1	7			T <sub>2</sub>							

Isotypic framework structures: \*Weinebeneite<sup>(1)</sup>

#### **References:**

(1) Walter, F. Eur. J. Mineral., 4, 1275-1283 (1992)

Weinebeneite

# **Type Material**

Crystal chemical data:

$$\begin{split} &|Ca^{2+}{}_4\ (H_2O)_{16}|\ [Be_{12}P_8\ O_{32}(OH)_8]\text{-}\textbf{WEI} \\ & \text{monoclinic, C1c1, } a = 11.897\text{\AA, } b = 9.707\text{\AA, } c = 9.633\text{\AA, } \beta = 95.76^{\circ\ (1)} \end{split}$$

Framework density:

18.1 T/1000Å<sup>3</sup>

Channels:

 $[001] \ \textbf{10} \ \textbf{3.1} \ \textbf{x} \ \textbf{5.4}^* \leftrightarrow [100] \ \textbf{8} \ \textbf{3.3} \ \textbf{x} \ \textbf{5.0}^*$ 



10-ring viewed along [001]



8-ring viewed along [100]



framework viewed along [001]

Idealized cell constants:	hexagonal, $P\overline{6}2m$ , a = 13.6Å, c = 7.6Å													
Coordination sequences and vertex symbols:	$\begin{array}{l} T_{1}(12,1)\\ T_{2}(6,m)\\ T_{3}(2,3) \end{array}$	4 4 3	9 9 9	16 19 21	27 34 36	46 49 53	73 67 69	102 94 90	129 125 119	157 157 156	191 195 201			
Secondary building units:	combinations only													
Loop configuration of T-Atoms:		$\Gamma_1$				T <sub>2</sub>	_		 Т	3				

Isotypic framework structures: \*Wenkite<sup>(1,2)</sup>

- Wenk, H.-R. Z. Kristallogr., 137, 113-126 (1973)
  Merlino, S. Acta Crystallogr., B30, 1262-1266 (1974)

Wenkite

# **Type Material**

# -WEN

Crystal chemical data:

$$\begin{split} &|Ba^{2+}_{\phantom{2}4}(Ca^{2+},Na^{+}_{\phantom{2}2})_3~(SO_4^{\phantom{2}2-})_3~H_2O|~[Al_8Si_{12}~O_{39}(OH)_2]\text{--WEN} \\ &hexagonal,~P\overline{6}2m,~a=13.511\text{\AA},~c=7.462\text{\AA}^{\phantom{2}(2)} \end{split}$$

Framework density:

17 T/1000Å<sup>3</sup>

Channels:

 $<\!\!100\!\!> \mathbf{10} \ 2.5 \ \mathrm{x} \ 4.8^{**} \leftrightarrow [001] \ \mathbf{8} \ 2.3 \ \mathrm{x} \ 2.7^{*}$ 



10-ring viewed along <100>



8-ring viewed along [001]



Loop configuration of T-Atoms:



Isotypic framework structures: \*Yugawaralite<sup>(1-3)</sup> Sr-Q<sup>(4,5)</sup>

- (1) Kerr, I.S. and Williams, D.J. Z. Kristallogr., 125, 220-225 (1967)
- (2) Kerr, I.S. and Williams, D.J. Acta Crystallogr., B25, 1183-1190 (1969)
- (3) Leimer, H.W. and Slaughter, M. Z. Kristallogr., 130, 88-111 (1969)
- (4) Hawkins, D.B. Mater. Res. Bull., 2, 951-958 (1967)
- (5) Kvick, Å., Artioli, G. and Smith, J.V. Z. Kristallogr., 174, 265-281 (1986)
Yugawaralite

# **Type Material**

# YUG

Crystal chemical data:	$ Ca^{2+}_{2} (H_{2}O)_{8} $ [Al <sub>4</sub> Si <sub>12</sub> O <sub>32</sub> ]-YUG monoclinic, Pc, a = 6.73Å, b = 13.95Å, c = 10.03Å, $\beta$ = 111.5° <sup>(2)</sup> (Relationship to unit cell of Framework Type: a' = c, b' = b, c' = a)
Framework density:	18.3 T/1000Å <sup>3</sup>
Channels:	$[100] 8 2.8 x 3.6^* \leftrightarrow [001] 8 3.1 x 5.0^*$



8-ring viewed along [100]



8-ring viewed along [001]



framework viewed along [100]

Idealized cell constants:	orthorhombic, Pbcm, $a = 6.9$ Å, $b = 14.9$ Å, $c = 17.2$ Å
Coordination sequences and vertex symbols:	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
Secondary building units:	6-2 or 4
Loop configuration of T-Atoms:	$ \begin{array}{c c} & & & \\ \hline & & \\ & & $
Isotypic framework structures:	*ZAPO-M1 <sup>(1)</sup> GaPO-DAB-2 <sup>(2)</sup> UiO- $7^{(3,4)}$

#### **References:**

- (1) Marler, B., Patarin, J. and Sierra, L. Microporous Materials, 5, 151-159 (1995)
- (2) Meden, A., Grosse-Kunstleve, R.W., Baerlocher, Ch. and McCusker, L.B. Z. Kristallogr., 212, 801-807 (1997)
- (3) Akporiaye, D.E., Fjellvåg, H., Halvorsen, E.N., Hustveit, J., Karlsson, A. and Lillerud, K.P. *Chem. Commun.*, 601-602 (1996)
- (4) Akporiaye, D.E., Fjellvåg, H., Halvorsen, E.N., Hustveit, J., Karlsson, A. and Lillerud, K.P. J. Phys. Chem., **100**, 16641-16646 (1996)

# **Type Material**

Crystal chemical data:	$\begin{split}  (C_4H_{12}N^+)_8  & [Zn_8Al_{24}P_{32} \ O_{128}]\text{-}\textbf{ZON} \\ C_4H_{12}N^+ = tetramethylammonium \\ orthorhombic, Pbca, a = 14.226\text{\AA}, b = 15.117\text{\AA}, c = 17.557\text{\AA}^{(1)} \\ (\text{Relationship to unit cell of Framework Type: a' = 2a, b' = b, c' = c)} \end{split}$
Framework density:	17 T/1000Å <sup>3</sup>

Channels:

 $[100] \; \textbf{8} \; 2.5 \; x \; 5.1^* \leftrightarrow [010] \; \textbf{8} \; 3.7 \; x \; 4.4^*$ 



8-ring viewed along [100]



8-ring viewed along [010]



8-ring viewed along [001]

# CON



10-ring viewed along [010]



2nd 12-ring viewed along [001]



10-ring viewed normal to [001]

GIS



8-ring viewed along [010]

# MER





#### MFI

#### Isotypic framework structures:

 $[As-Si-O]-MFI^{(4)} \\ [Fe-Si-O]-MFI^{(5)} \\ [Ga-Si-O]-MFI^{(6)} \\ AMS-1B^{(7)} \\ AZ-1^{(8)} \\ Bor-C^{(9)} \\ Boralite C^{(10)} \\ Encilite^{(11)} \\ FZ-1^{(12)} \\ LZ-105^{(13)} \\ Monoclinic H-ZSM-5^{(14)} \\ Mutinaite^{(15)} \\ \end{tabular}$ 

 $\begin{array}{c} \text{NU-4}^{(16)} \\ \text{NU-5}^{(17)} \\ \text{Silicalite}^{(18)} \\ \text{TS-1}^{(19)} \\ \text{TSZ}^{(20)} \\ \text{TSZ-III}^{(21)} \\ \text{TZ-01}^{(22)} \\ \text{USC-4}^{(23)} \\ \text{USI-108}^{(24)} \\ \text{ZBH}^{(25)} \\ \text{ZKQ-1B}^{(26)} \\ \text{ZMQ-TB}^{(27)} \end{array}$ 

#### **References:**

- (4) Bhaumik, A. and Kumar, R. Chem. Commun., 869-870 (1995)
- (5) Patarin, J., Kessler, H. and Guth, J.L. Zeolites, 10, 674-679 (1990)
- (6) Awate, S.V., Joshi, P.N., Shiralkar, V.P. and Kotasthane, A.N. J. Incl. Phenom., 13, 207-218 (1992)
- (7) Klotz, M.R. U.S. Patent 4,269,813 (1981)
- (8) Chono, M. and Ishida, H. E. Patent B-113,116 (1984)
- (9) Taramasso, M., Perego, G. and Notari, B. In *Proc. 5th Int. Zeolite Conf.*, (ed. L.V.C. Rees), pp. 40-48 (1980), Heyden, London
- (10) Taramasso, M., Manara, G., Fattore, V. and Notari, B. GB Patent 2,024,790 (1980)
- (11) Ratnasamy, P. and Borade, M.B. E. Patent A-160,136 (1985)
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- (13) Grose, R.W. and Flanigen, E.M. U.S. Patent 4,257,885 (1981)
- (14) van Koningsveld, H., Jansen, J.C. and van Bekkum, H. Zeolites, 10, 235-242 (1990)
- (15) Vezzalini, G., Quartieri, S., Galli, E., Alberti, A., Cruciani, G. and Kvick, A. Zeolites, 19, 323-325 (1997)
- (16) Whittam, T.V. E. Patent B-65,401 (1986)
- (17) Whittam, T.V. E. Patent B-54,386 (1982)
- (18) Flanigen, E.M., Bennett, J.M., Grose, R.W., Cohen, J.P., Patton, R.L., Kirchner, R.M. and Smith, J.V. *Nature*, **271**, 512-516 (1978)
- (19) Taramasso, M., Perego, G. and Notari, B. U.S. Patent 4,410,501 (1983)
- (20) Ashibe, K., Kobayashi, W., Maejima, T., Sakurada, S. and Tagaya, N. E. Patent A-101,232 (1984)
- (21) Sakurada, S., Tagaya, N., Miura, T., Maeshima, T. and Hashimoto, T. E. Patent A-170,751 (1986)
- (22) Iwayama, K., Kamano, T., Tada, K. and Inoue, T. E. Patent A-57,016 (1982)
- (23) Young, D.A. U.S. Patent 4,325,929 (1982)
- (24) Hinnenkamp, J.A. and Walatka, V.V. U.S. Patent 4,423,020 (1983)
- (25) Holderich, W., Mross, W.D. and Schwartzmann, M. E. Patent B-77,946 (1986)
- (26) Kee Kwee, L.S.L. E. Patent A-148,038 (1984)
- (27) Kee Kwee, L.S.L. E. Patent A-104, 107 (1983)



8-ring viewed along [010]

RSN



8-ring viewed along [010]

SBS



8-ring along [001]



8-ring viewed along [102]

VSV





8-ring viewed along [100]

.8

#### **APPENDIX B**

#### **Rules for Framework Type Assignment**

The following is a set of rules to be applied by the Structure Commission of the IZA in assigning a three-letter code to a new framework type. The materials of interest are generally defined as open 4-connected 3D nets which have the general (approximate) composition  $AB_2$ , where A is a tetrahedrally connected atom and B is any 2-connected atom, which may or may not be shared, between two neighboring A atoms. Inclusion of other microporous materials is left to the discretion of the IZA Structure Commission, depending on the interest of the molecular sieve science community at large.

#### RULES

- (i) The IZA Structure Commission is the only body that can coordinate the assignment of a code to such frameworks. The framework types are idealized, with no reference to actual materials, symmetry, composition, etc. and, therefore, ONLY refer to the connectivity.
- (ii) The code for a 4-connected 3D framework type shall consist of three capital letters. Other frameworks of interest shall be indicated by a (-) in front of the code.
- (iii) The three letters of the code shall be mnemonic and must refer to an actual material (i.e. the type material). These materials are chosen to be:
  - mineral names (rules of the International Mineralogical Association followed).
  - commonly accepted synthetic material types.
  - in the absence of the above, the workers who first determined the structure have priority in assigning the name.
- (iv) No mnemonic code can be assigned without the structure being determined with the following exception:

For "polytypic" materials, codes can be assigned as useful. Such codes shall be marked with an asterisk.

- (v) Codes of framework types which turn out to be in error are discredited. Later use of the code is not permitted.
- (vi) For all cases where a decision of the Structure Commission is required, a two thirds majority vote of the full commission shall be required. Such votes are taken verbally at a meeting of the Structure Commission or are done in writing on the initiative of the Chairperson and Co-chairperson. All evidence substantiating a new framework type must accompany the ballot. The members are obliged to respond to this request within one month and the Chairperson and Co-chairperson will make all possible effort to solicit replies from all members.

## **APPENDIX C**

### **Topological Densities**

Topological density values  $TD_{10}$  including all values of the coordination sequence from  $N_0$  to  $N_{10}$ . TD = exact density as defined in the Explanatory Notes.

Code	$TD_{10}$	TD	Code	$TD_1$	0 <b>TD</b>	Code	$TD_{10}$	TD
ABW	833	0.703704	DFO	664	0.576042	MTW	912	0.776004
ACO	787	0.666667	DFT	840	0.711111	MWW	851	0.752127
AEI	689	0.583081	DOH	1002	0.882191	NAT	834	0.740741
AEL	904	0.766975	DON	851	0.728920	NES	922	0.818688
AEN	956	0.857768	EAB	735	0.628571	NON	1038	0.915319
AET	824	0.697917	EDI	786	0.666667	OFF	739	0.628571
AFG	816	0.693333	EMT	584	0.493095	OSI	892	0.777778
AFI	828	0.700000	EPI	979	0.845059	OSO	747	0.645000
AFN	777	0.661111	ERI	738	0.628571	-PAR	773	0.664915
AFO	907	0.769676	ESV	875	0.754994	PAU	728	0.623377
AFR	687	0.579229	EUO	965	0.872973	PHI	751	0.635556
AFS	656	0.568750	FAU	579	0.476190	RHO	641	0.533333
AFT	685	0.585714	FER	1021	0.887635	-RON	771	0.688981
AFX	689	0.585714	FRA	802	0.683983	RSN	914	0.786947
AFY	585	0.488889	GIS	726	0.611111	RTE	844	0.715873
AHT	853	0.729167	GME	694	0.585714	RTH	817	0.695757
ANA	933	0.800000	GON	926	0.787372	RUT	902	0.767499
APC	814	0.696296	GOO	840	0.716755	SAO	632	0.545455
APD	888	0.759019	HEU	909	0.778254	SAS	701	0.586667
AST	742	0.625000	IFR	798	0.678236	SAT	763	0.644444
ASV	787	0.666667	ISV	772	0.694533	SAV	690	0.587302
ATN	833	0.703704	ITE	824	0.711802	SBE	619	0.514323
ATO	894	0.760000	JBW	890	0.753333	SBS	617	0.534092
ATS	752	0.640000	KFI	681	0.571429	SBT	617	0.522344
ATT	768	0.647619	LAU	782	0.658201	SFE	892	0.767358
ATV	960	0.816667	LEV	719	0.605714	SFF	880	0.765073
AWO	828	0.708843	LIO	816	0.693333	SGT	962	0.862901
AWW	772	0.656085	LOS	816	0.693333	SOD	791	0.666667
*BEA	805	0.704545	LOV	879	0.754446	STF	877	0.748986
BIK	1052	0.907407	LTA	641	0.533333	STI	852	0.720342
BOG	781	0.659922	LTL	746	0.619048	STT	859	0.760705
BPH	667	0.568750	LTN	779	0.698452	TER	872	0.739316
BRE	901	0.778031	MAZ	823	0.697032	ТНО	784	0.666667
CAN	817	0.693333	MEI	728	0.630682	TON	1006	0.867111
CAS	1042	0.895949	MEL	944	0.808638	TSC	590	0.482539
CFI	892	0.765153	MEP	1059	0.955379	VET	1023	0.913737
CGF	819	0.695238	MER	738	0.622222	VFI	669	0.562500
CGS	718	0.613333	MFI	960	0.825819	VNI	971	0.896603
CHA	677	0.566667	MFS	995	0.866320	VSV	948	0.818000
-CHI	913	0.833441	MON	1033	0.885802	WEI	773	0.655864
-CLO	456	0.443290	MOR	938	0.802340	-WEN	755	0.640693
CON	784	0.670229	MSO	822	0.694444	YUG	935	0.797884
CZP	885	0.800000	MTF	1083	0.942112	ZON	798	0.679089
DDR	968	0.850801	MTN	1049	0.927590			
DAC	977	0.841190	MTT	1015	0.883181			

## **APPENDIX D**

### **Origin of 3-Letter Codes and Material Names**

Code	Abbreviated Name	Full Name
ABW		Li-A (Barrer and White)
ACO	ACP-1 (one)	Aluminium Cobalt Phosphate - one
AEI	$A1PO_4$ -18 (eighteen)	Aluminophosphate-eighteen
AEL	$AlPO_4$ -11 (eleven)	Aluminophosphate-eleven
AEN	Alpo-EN3	Aluminophosphate ethylenediamine (en) - three
AET	$AlPO_4$ -8 (eight)	Aluminophosphate-eight
AFI	$AlPO_4$ -5 (five)	Aluminophosphate-five
AFN	$AlPO_4$ -14 (forteen)	Aluminophosphate-forteen
AFO	$AlPO_4$ -41 (forty-one)	Aluminophosphate-forty-one
AFR	SAPO-40 (forty)	Silico-Aluminophosphate-forty
AFS	MAPSO-46 (forty-six)	$MgAl(P,Si)O_4-46$
AFT	$AlPO_4$ -52 (fifty-two)	
AFX	SAPO-56 (fifty-six)	Silico-Aluminophosphate-fifty-six
AFY	CoAPO-50 (fifty)	
AHT	$AlPO_4$ -H2 (two)	
APC	AlPO <sub>4</sub> -C	
APD	AlPO <sub>4</sub> -D	
AST	$AlPO_4$ -16 (sixteen)	
ASV	ASU-7 (seven)	Arizona State University - seven
ATN	MAPO-39 (thirty-nine)	MgAlPO <sub>4</sub> - thirty-nine
ATO	$AlPO_4$ -31 (thirty-one)	
ATS	MAPO-36 (thirty-six)	
ATT	$AlPO_4$ -12 (twelve)-TAMU	AlPO <sub>4</sub> -12-Texas A&M University
ATV	$AlPO_4$ -25 (twenty-five)	
AWO	$AlPO_4$ -21 (twenty-one)	
AWW	AlPO <sub>4</sub> -22 (twenty-two)	
*BEA	Zeolite Beta	
BPH	Beryllophosphate-H	Beryllophosphate-Harvey (or hexagonal)
CAS	Currier Currie	
CFI	$C_{11-5}$ (five)	California Institute of Technology - five
CGF	CoGaPO-5 (five)	Cobalt-Gallium-Phosphate-five
CGS	CoGaPO-6 (Six)	Cobalt-Gallium-Phosphate-six
-CLU	CIOVERITE CIT 1 (cm c)	Four-leafed clover shaped pore opening
CON	C11-1 (one)	Chinel Zinger handlate
	Deep dedeessil 2D	Chiral Zincophosphate
DDK	DAE 1 (ana)	Deca- & dodecanedra, S layers, monitoinedral
DFU	DAF - 1 (011c)	Davy Faraday Research Laboratory - two
рен рон	DAT-2 (1WO)	Dadogahadra 1 layar hayaganally stacked
DON	LITD 1 (one)	University of Texas at Dallas one
EAR		$TMA_{\mathbf{F}}$ (A jello and Barrer)
EMT	EMC-2 (two)	Flf (or Ecole Supérieure) Mulhouse Chimie two
ESV	$ERS_7$ (seven)	Eniricerche-molecular-sieve-seven
EUO	FIL-1 (one)	Edinburgh University - one
<b>E</b> 00		Eamourgh University - One

Code	Abbreviated Name	Full Name
GON	GUS-1 (one)	Gifu University Molecular Sieve - one
IFR	ITQ-4 (four)	Instituto de Tecnologia Quimica Valencia - four
ISV	ITO-7 (seven)	Instituto de Tecnologia Química Valencia - seven
ITE	ITO-3 (three)	Instituto de Tecnologia Química Valencia - three
JBW		Na-J (Barrer and White)
KFI	Z <b>K</b> -5 ( <b>fi</b> ve)	Zeolite Kerr - five
LOS	Losod	Low sodium aluminosilicate
LTA	Linde Type A	Zeolite A (Linde Division, Union Carbide)
LTL	Linde Type L	Zeolite L (Linde Division, Union Carbide)
LTN	Linde Type N	Zeolite N (Linde Division, Union Carbide)
MEI	ZSM-18 (eighteen)	Zeolite Socony Mobil - eighteen
MEL	ZSM-11 (eleven)	Zeolite Socony Mobil - eleven
MFI	ZSM-5 (five)	Zeolite Socony Mobil - five
MFS	ZSM-57 (fifty-seven)	Zeolite Socony Mobil - fifty-seven
MSO	MCM-61 (sixty-one)	Mobil Composition of Matter - sixty-one
MTF	MCM-35 (thirty-five)	Mobil Composition of Matter - thirty-five
MTN	ZSM-39 (thirty-nine)	Zeolite Socony Mobil - thirty-nine
MTT	ZSM-23 (twenty-three)	Zeolite Socony Mobil - twenty-three
MTW	ZSM-12 (twelve)	Zeolite Socony Mobil - twelve
MWW	MCM-22 (twenty-two)	Mobil Composition of Matter-twenty-two
NES	NU-87 (eighty-seven)	New (ICI) - eighty-seven
NON	Nonasil	Nonahedra, all silica composition
OSI	Ui <b>O</b> -6 ( <b>si</b> x)	University of Oslo-six
OSO	OSB-1 (one)	Universities of Oslo and Calif., Santa Barbara – one
-RON	Roggianite	
RSN	<b>R</b> UB-17 (seventeen)	Ruhr University Bochum - seventeen
RTE	<b>R</b> UB-3 (three)	Ruhr University Bochum - three
RTH	<b>R</b> UB-13 (thirteen)	Ruhr University Bochum - thirteen
RUT	<b>RU</b> B-10 (ten)	Ruhr University Bochum - ten
SAO	<b>STA-1</b> (one)	University of Saint Andrews - one
SAS	<b>STA-6</b> ( <b>si</b> x)	University of Saint Andrews - six
SAT	STA-2 (two)	University of Saint Andrews - two
SAV	Mg-STA-7 (seven)	University of Saint Andrews - seven
SBE	UCSB-8 (eight)	University of California, Santa Barbara - eight
SBS	UC <b>SB</b> -6 (six)	University of California, Santa Barbara - six
SBT	UC <b>SB</b> -10 (ten)	University of California, Santa Barbara - ten
SFE	SSZ-48 (forty-eight)	Standard Oil Synthetic Zeolite - fourty-eight
SFF	SSZ-44 (forty-four)	Standard Oil Synthetic Zeolite - fourty-four
SGT	Sigma-2 (two)	
STF	SSZ-35 (thirty-five)	Standard Oil Synthetic Zeolite - thirty-five
STT	SSZ-23 (twenty-three)	Standard Oil Synthetic Zeolite - twenty-three
TON	Theta-1 (one)	
VET	VPI-8 (eight)	Virgina Polytechnic Institute - eight
VFI	VPI-5 (five)	Virgina Polytechnic Institute - five
VNI	<b>V</b> PI-9 ( <b>ni</b> ne)	Virgina Polytechnic Institute - nine
VSV	VPI-7 (seven)	Virgina Polytechnic Institute - seven
ZON	ZAPO-M1 (one)	$(\mathbf{Zn},\mathbf{Al})\mathbf{PO}_4$ - <b>M</b> ulhouse - one

### ISOTYPIC MATERIAL INDEX

\* Type materials are marked with an asterisk

*ACP-1	ACO	Bor-C	MFI
ACP-3	DFT	Bor-D ( <b>MFI/MEL</b> intergrowth)	MEL
*Afghanite	AFG	Boralite C	MFI
Alpha	LTA	Boralite D	MEL
AlPO <sub>4</sub> -pollucite	ANA	*Brewsterite	BRE
*AlPO-5	AFI	Bystrite	LOS
*AlPO-8	AET	Ca-D	ANA
*AlPO-11	AEL	Ca-Q	MOR
*AlPO-12-TAMU	ATT	*Cancrinite	CAN
*AlPO-14	AFN	Cancrinite hydrate	CAN
*AlPO-16	AST	*Cesium Aluminosilicate	CAS
AlPO-17	ERI	CF-3	NON
*AlPO-18	AEI	CF-4	MTN
AlPO-20	SOD	CFSAPO-1A	AEN
*AlPO-21	AWO	*Chabazite	CHA
*AlPO-22	AWW	*Chiavennite	-CHI
AlPO-24	ANA	*Chiral Zincophosphate	CZP
*AlPO-25	ATV	*CIT-1	CON
*AlPO-31	АТО	CIT-4	BRE
AlPO-33	ATT	*CIT-5	CFI
AlPO-34	СНА	CIT-6	*BEA
AlPO-35	LEV	Clinoptilolite	HEU
AlPO-40	AFR	*Cloverite	-CLO
*AlPO-41	AFO	*Co-Ga-Phosphate-5	CGF
*AlPO-52	AFT	*Co-Ga-Phosphate-6	CGS
AlPO-53(A)	AEN	Co-STA-7	SAV
AlPO-53(B)	AEN	CoAPO-5	AFI
AlPO-54	VFI	CoAPO-44	СНА
*AlPO-C	APC	CoAPO-47	СНА
*AlPO-D	APD	*CoAPO-50	AFY
*AIPO-EN3	AEN	CoAPSO-40	AFR
*AlPO-H2	AHT	CoDAF-4	LEV
AlPO-H3	APC	CrAPO-5	AFI
Amicite	GIS	Cs beryllosilicate pollucite	ANA
Ammonioleucite	ANA	Cs,Fe silicate pollucite	ANA
AMS-1B	MFI	(Cs,K)-ZK-5	KFI
*Analcime	ANA	CSZ-1	EMT/FAU
*ASU-7	ASV	CZH-5	MTW
AZ-1	MFI	*Dachiardite	DAC
B-NU-1	RUT	*DAF-1	DFO
Ba-dominant brewsterite	BRE	*DAF-2	DFT
Barrerite	STI	Danalite	SOD
Basic cancrinite	CAN	Davyne	CAN
Basic sodalite	SOD	*Deca-dodecasil 3R	DDR
Bellbergite	EAB	Dehydrated Ca,NH <sub>4</sub> -Heulandite	HEU
Beryllophosphate X	FAU	Dehydrated Linde Type A	LTA
*Beryllophosphate-H	BPH	Dehydrated Na-Chabazite	СНА
*Beta	*BEA	Dehydrated Na-X	FAU
Bicchulite	SOD	Dehydrated US-Y	FAU
*Bikitaite	BIK	Deuterated Rho	RHO
*Boggsite	BOG	*Dodecasil 1H	DOH

Dodecasil-3C	MTN	K-exchanged Heulandite	HEU
ECR-5	CAN	K-F	EDI
ECR-18	PAU	K-M	MER
ECR-30	EMT/FAU	K-rich gmelinite	GME
*Edingtonite	EDI	Kehoeite	ANA
*EMC-2	ЕМТ	KZ-1	MTT
Encilite	MFI	KZ-2	TON
*Enistilbite	EPI	Large port mordenite	MOR
FRB-1	MWW	*I aumontite	LAU
*Frionite	FRI	Leonhardite	
*FRS_7	FSV	Leucite	
*EU 1		*Louwno	IFV
EU-1 FU 13	MTT	*Li A (Barrer and White)	ARW
*Equipoito		Linda D	СНА
		Linde D	
re-nu-i		Linde F	EDI DDU
*Femente	FER	Linde Q	БРН
FU-9	FER		
FZ-1			ERI/OFF
G	SOD	*Linde Type A	
Ga-NU-I	RUT	*Linde Type L	LTL
Gallosilicate ECR-10	RHO	*Linde Type N	LTN
Gallosilicate L	LTL	Linde W	MER
GaPO-14	AFN	Linde X	FAU
GaPO-34	СНА	Linde Y	FAU
GaPO-DAB-2	ZON	*Liottite	LIO
Garronite	GIS	*Losod	LOS
Gaultite	VSV	*Lovdarite	LOV
Genthelvite	SOD	Low-silica Na-P (MAP)	GIS
*Gismondine	GIS	LZ-105	MFI
*Gmelinite	GME	LZ-132	LEV
Gobbinsite	GIS	LZ-202	MAZ
Gonnardite	NAT	LZ-210	FAU
*Goosecreekite	GOO	LZ-211	MOR
Gottardiite	NES	LZ-212	LTL
*GUS-1	GON	LZ-214	RHO
H1	VFI	LZ-215	LTA
Harmotome	PHI	LZ-217	OFF
Hauvn	SOD	LZ-218	CHA
Helvin	SOD	LZ-219	HEU
*Heulandite	HEU	LZ-220	ERI
High natrolite	NAT	MAP	GIS
High-silica Na-P	GIS	*MAPO-36	ATS
Holdstite	MTN	*MAPO-39	ATN
Hsianghualite	ANA	MAPO-43	GIS
Hydroxo sodalite	SOD	*MAPSO 46	AFS
ISI 1	TON	Mariconaita	MOD
	I UN MTT	*Mozzito	MAZ
		MCM 0	VEI
ISI-0		NICNI-9 *MCM 22	
11 - U- I *ITO 2		· IVICIVI-22 *MCM 25	IVI VV VV MTE
*ITQ-3		· IVICIVI-33	
*11Q-4 *1TO 7	IF K	MCM-57	AET
*IIQ-/		MCM-58	IFK
IIQ-9	51f	*MCM-61	MSU
JDF-2	AEN	MeAPO-47	CHA
(K,Ba)-G,L	LTL	MeAPSO-47	CHA
K-Chabazite, Iran	CHA	*Melanophlogite	MEP

*Merlinoite	MER	SAPO-34	СНА
Mesolite	NAT	SAPO-35	LEV
Metanatrolite	NAT	SAPO-37	FAU
*Mg-STA-7	SAV	*SAPO-40	AFR
MgAPO-50	AFY	SAPO-42	LTA
Microsommite	CAN	SAPO-43	GIS
MnAPO-11	AEL	SAPO-47	CHA
Monoclinic ferrierite	FER	*SAPO-56	AFX
Monoclinic H-ZSM-5	MFI	Scolecite	NAT
*Montesommaite	MON	Si-CHA	CHA
*Mordenite	MOR	Sigma-1	DDR
MSC-1	AEN	*Sigma-2	SGT
Mutinaite	MFI	Silica sodalite	SOD
N-A	LTA	Silicalite	MFI
Na-B	ANA	Silicalite 2	MEL
Na-D	MOR	Siliceous Na-Y	FAU
Na-P1	GIS	*Sodalite	SOD
Na-P2	GIS	Sr-D	FER
Na-V	ТНО	Sr-Q	YUG
*Na-J (Barrer and White)	JBW	SSZ-16	AFX
*Natrolite	NAT	*SSZ-23	STT
NaZ-21	LTN	SSZ-24	AFI
Nepheline hydrate	JBW	SSZ-25	MWW
*Nonasil	NON	SSZ-26	CON
Nosean	SOD	SSZ-33	CON
NU-1	RUT	*SSZ-35	STF
NU-3	LEV	SSZ-42	IFR
NU-4	MFI	*SSZ-44	SFF
NU-5	MFI	SSZ-46	MEL
NU-10	TON	*SSZ-48	SFE
NU-13	MTW	*STA-1	SAO
NU-23	FER	*STA-2	SAT
*NU-87	NES	STA-5	BPH
Octadecasil	AST	*STA-6	SAS
*Offretite	OFF	Stellerite	STI
Omega	MAZ	*Stilbite	STI
*OSB-1	OSO	Svetlozarite (disordered variant)	DAC
P	KFI	Synthetic amicite	GIS
Pahasapaite	RHO	Synthetic analcime	ANA
*Partheite	-PAR	Synthetic  Na- [Al-Si-O]-JBW	JBW
*Paulingite	PAU	Synthetic barrerite	STI
Perhalite		Synthetic brewsterite	BRE
Phi	CHA	Synthetic Ca-garronite	GIS
*Phillipsite	PHI	Synthetic cancrinite	CAN
Pollucite	ANA	Synthetic edingtonite	EDI
PSH-3	MWW	Synthetic epistilbite	EPI
Q	KF1 DUG	Synthetic fault-free gmelinite	GME
*Rho	RHO	Synthetic garronite	GIS
*Roggianite	-RON	Synthetic gobbinsite	GIS
*KUB-3	KIE	Synthetic gonnardite	NAT
*KUB-10	KUT	Synthetic hsinghualite	
*KUB-13	KIH	Synthetic laumontite	
*KUB-1/	KSN	Synthetic lovdarite	
SAPO-5	AFI	Synthetic melanophlogite	MEP
SAPO 21	ALL	Synthetic merlinoite	NER
SAPU-31	AIU	symmetic mesonite	INAI

Synthetic natrolite	NAT	UiO-20	DFT
Synthetic offretite	OFF	USC-4	MFI
Synthetic scolecite	NAT	USI-108	MFI
Synthetic stellerite	STI	UTD-1	DON
Synthetic stilbite	STI	*UTD-1F	DON
Synthetic thomsonite	ТНО	UTM-1	MTF
Synthetic wairakite	ANA	Vishnevite	CAN
*Terranovaite	TER	*VPI-5	VFI
Tetragonal edingtonite	EDI	*VPI-7	VSV
*Theta-1	TON	*VPI-8	VET
Theta-3	MTW	*VPI-9	VNI
*Thomsonite	ТНО	VS-12	MTW
Tiptopite	CAN	VSV-7#	VSV
TMA sodalite	SOD	Wairakite	ANA
*TMA-E	EAB	*Weinebeneite	WEI
TMA-gismondine	GIS	Wellsite	PHI
TMA-O	OFF	*Wenkite	-WEN
TNU-1	CGS	Willhendersonite	СНА
TPAF AIPO-5	AFI	*Yugawaralite	YUG
TPZ-3	EUO	*ZAPO-M1	ZON
TPZ-12	MTW	ZBH	MFI
Triclinic bikitaite	BIK	Zeolite N	EDI
TS-1	MFI	Zeolite W	MER
TS-2	MEL	Zincophosphate X	FAU
*Tschörtnerite	TSC	ZK-4	LTA
Tschernichite	*BEA	*ZK-5	KFI
TsG-1	CGS	ZK-14	СНА
TSZ	MFI	ZK-19	PHI
TSZ-III	MFI	ZK-20	LEV
Tugtupite	SOD	ZK-21	LTA
TZ-01	MFI	ZK-22	LTA
UCSB-3GaGe	DFT	ZKQ-1B	MFI
UCSB-3ZnAs	DFT	ZMQ-TB	MFI
UCSB-6Co	SBS	Zn-STA-7	SAV
*UCSB-6GaCo	SBS	ZnAPSO-40	AFR
UCSB-6GaMg	SBS	ZSM-3	EMT/FAU
UCSB-6GaZn	SBS	ZSM-4	MAZ
UCSB-6Mg	SBS	*ZSM-5	MFI
UCSB-6Mn	SBS	*ZSM-11	MEL
UCSB-6Zn	SBS	*ZSM-12	MTW
*UCSB-8Co	SBE	*ZSM-18	MEI
UCSB-8Mg	SBE	ZSM-20	EMT/FAU
UCSB-8Mn	SBE	ZSM-22	TON
UCSB-8Zn	SBE	*ZSM-23	MTT
UCSB-10Co	SBT	ZSM-35	FER
*UCSB-10GaZn	SBT	*ZSM-39	MTN
UCSB-10Mg	SBT	ZSM-50	EUO
UCSB-10Zn	SBT	ZSM-51	NON
*UiO-6	OSI	*ZSM-57	MFS
UiO-7	ZON	ZSM-58	DDR
UiO-12-as	AEN	ZYT-6	CHA
UiO-12-500	AEN		