Subject and Author index

Numbers refer to the page where a definition or explanation of, and/or a *figure* or a **table** for, a given subject is found. Author names are given with the number of the first page of the paper in which they are involved.

2D tilings, anion topologies, 41 3D tilings, 44

A

Ab initio structure solution, 165
Aenigmatite, nodal representations, 36
Altomare, A., 79
Amplitude contrast, electron crystallography, 143
Anion packings, topology, 41
Anion-centred, octahedron, 17, polyhedral, 13
Antiperovskite units in the crystal structures of minerals, 17
Aperiodic mineral structures, 213, naturally occurring, 227, occurrences of, 225
Astrophyllite, nodal representations, 36
Atomic packing, 2

B

Background, 87 Bafertisite, crystal structure of, 9 Bartonite, frameworks separated into layers of cubes. 28 Bastisite, octahedral-tetrahedral framework in the structures of the scherbakovite-bastisite series. 34 Benitoite, octahedral-tetrahedral framework in the structure of, 34 Beraunite, crystal structure of, 21 Bindi, L., 213 Bond-valence table, 48 Boulangerite, crystal structure of, 54 Bragg peak, 84 Branchedness, 8 Butterfly-shaped cluster (FBB), consisting of four octahedral, 26

С

Calaverite, gnomonic projection of the crystal forms of, 215, incommensurately moderated structures, 228, reinterpretation, 216 Cancrinite-sodalite supergroup minerals, poly-

hedra building units present in the frameworks of the, 30 Cation packings and cation array, 3 Cation-centred polyhedra, 6 CBED pattern of α-quartz, 164 Chain borate minerals, FBBs in the crystal structures of. 23 Chain periodicity, 8 Chapuis, G., 213 Charoite, compositional hierarchy scheme for the crystal structure of, 52, EDT on finely intergrown polytypes, 169 Classification of minerals based on octahedraltetrahedral frameworks, 11 Classification parameters, 8 Coesite, zone axis pattern, 163 Complexity, 57, classification of minerals according to, 63 Composite modulated structures, naturally occurring, 235 Compositional hierarchy scheme, 48, 51, of an inorganic crystal structure, 50 Connectedness, 8 Convergent beam electron diffraction (CBED), 149.150 Coordination polyhedra, 6 Corner-sharing (OHg₄) tetrahedra, 16 Cosalite, crystal structure of, 54 Crystal structures in mineralogy, 1 Crystal symmetry, determination of, 161 Crystal system, expression of Q(hkl) depending on, 102 Crystal, redefinition, 217 Crystallography, methods of, 79 Cu oxysalt minerals, of fumarolic origin, 15 Cuocci, C., 79 Cupropearceite, 241, 242 Cylindrite-type minerals, 239

D

Debye cones and rings, 82 Decomposable system, crystal structure as a nearly, 46 Deerite, nodal representations, 36 Difference Fourier map, calculated from the

©Copyright 2017 the European Mineralogical Union and the Mineralogical Society of Great Britain & Ireland DOI: 10.1180/EMU-notes.19.index

dynamical refinement of the Hypso phase, 175 Diffraction contrast imaging, 144 Diffraction data, effects of size and structural disorder on, 185, resolution of modulated structures from, 222 Diffraction integrated intensities, 106 Dimensionality, 8 Direct space methods, 109 Djerfisherite, frameworks separated into layers of cubes, 28 Dolerophanite, crystal structure of, 14 Dolomite, STEM investigation of exsolution lamellae in. 145 Dual-phase modelling, 205 Dufrenite, crystal structure of, 21 Dynamical structure refinement, 172

Е

EDT on nanocrystalline minerals, vaterite, 166, 167 Elastic behaviour of crystalline materials, highpressure, 116 Electron crystallography, 139, scope and applications, 140 Electron diffraction, techniques, 147, tomography, 154 Electron energy-filtered TEM, 158, 159 Electron energy-loss spectroscopy, 158, 159 Energy-dispersive X-ray spectroscopy, 157 Environmental mineralogical importance, 183, 191 Equations of state, P-V and P-V-T, 117 Experimental techniques, electron crystallography, 141 Exsolution lamellae, STEM investigation of, in Carich dolomite, 145 Extinction symbol, determination of, 161, 162, ranked according to the calculated probability

value, **106** Extreme conditions, *in situ* experiments, 121

F

Feldspar, tetrahedral frameworks in, 29
Ferrihydrite, unit-cell approach to fitting the PDF, 198
Framework aluminosilicates of the cancrinite –sodalite supergroup, 31
Fresnoite, 236, incommensurately moderated structures, 232, structural variations observed for the different polyhedral, 237
Fumarolic origin, Cu oxysalt minerals, 15
Fundamental building blocks (FBBs), 22

G

Galena, crystal structure of, 53
Gatta, G.D., 79
Gemmi, M., 139
Geometrical isomers, 37
Gittinsite, 3D nets, 36
Gnomonic projection of the crystal forms of calaverite, 215
Graphical isomers, 37
Gustavite, crystal structure of, 56

H

HAPY phase, EDT in experimental petrology, 167, 168 Harmotome, tetrahedral frameworks in, 29 Hematite, HRTEM images of, 146 Heteropolyhedral chains, from uranophane topology, 42 Hierarchy, 45, and complexity, 50 High-pressure elastic behaviour of crystalline materials, 116 High-temperature elastic behaviour of crystalline materials, 114 Hilairite, octahedral-tetrahedral framework in the structure of. 35 History of crystallography, 213 Homologous series, 54 Howieite, nodal representations, 36 HRTEM images of hematite, 146 Hybrid methods, 111

I

Icosahedrite, 241, electron diffraction patterns for, 247 Imaging techniques, electron crystallography, 143 Incommensurately moderated structures, 228 Indexing, 101 Isomerism of structural units in minerals, 37

K

Kinematical structure refinement, 171 Kleinite, crystal structure of, 16 Klementová, M., 139 Kombatite, crystal structure of, 21 Krivovichev, S.K., 1

L

Labuntsovite-group minerals, octahedral-tetrahedral framework in the structures of, *33* Laue class, determination of, 161, 162 Laueite, octahedral-tetrahedral sheets in the structure of, *39* Lemoynite, nodal representations, 36

Levyclaudite, example of Q layer and H layer in, 244, 245

Linkedness, 8

Μ

Mackinawite, unit-cell approach to fitting the PDF, Manganese oxide, unit-cell approach to fitting the PDF. 200 Materials science, methods of crystallography, 79 Mellilite, 234, diffraction pattern in, 235, incommensurately moderated structures, 232. structural variations observed for the different polyhedra, 237 Metavauxite, octahedral-tetrahedral sheets in the structure of, 40 Methods of crystallography, 79 Michel, F.M., 183 Microblocks, as structure-forming units, 24, 25 Mixed anionic radicals (MARs), 9, classification of, 12 Modularity, 51 Modulated structures, resolution of, from diffraction data, 222 Moliterni, A., 79 Monte Carlo (Reverse), and whole nanoparticle simulation, 204 Multiplicity, 8 Murataite-(Y), crystal structure of, 4 N

Nanodiffraction, 148 Natrite, incommensurately moderated structures, 228, modulation of interatomic distances in the structure of, *232*, structure of the hexagonal modification of, 231

Nepheline structure, diffraction pattern of, 104 Networks and graphs, 27

Neutron vs. X-ray diffraction under extreme conditions, 123

Non-harmonic joint probability density isosurface for silver in the pearceite structure, 239 Nordite, nodal representations, *36*

0

Octahedral-tetrahedral framework in the structures of labuntsovite-group minerals, 33, in the structures of the scherbakovite-bastisite series, 34

Octahedral-tetrahedral frameworks, classification

of minerals based on, 11

Oxide minerals, cation arrays and arrangements of atoms, **5**

Oxysalt minerals, cation arrays and arrangements of atoms, **5**

P

Pair distribution function analysis, 183, 189, truncation 193 Palatinus, L., 139 Paracelsian, tetrahedral frameworks in, 29 Paulingite, crystal structure of, 64 Peak attenuation, 193 Peak overlap, 86 Pearceite-polybasite group, minerals of, 235, 238, 240, 241, non-harmonic joint probability density isosurface for silver in the pearceite structure, 239 PED and SAED patterns of almandine, 152 PED pattern, almandine, 152 Pellvite, nodal representations, 36 Pentlandite, frameworks separated into layers of cubes. 28 Periodic models, real-space fitting with, 195 Pharmacology, methods of crystallography, 79 Pharmacosiderite-related frameworks, octahedraltetrahedral clusters in. 26 Phase and orientation mapping, 156 Phase contrast, 145 Phase identification, 158 Phosphuranylite anion topology, 42 Polyhedral building units present in the frameworks of the cancrinite-sodalite supergroup minerals, 30 Polyphite, 20 Powder diffraction at extreme conditions, 113 Powder rings, 82 Powder X-ray diffraction, 81, typical profile, 83 Precession electron diffraction (PED), 151, 152 Preferred orientation, 87 Pseudo-laueite, octahedral-tetrahedral sheets in the structure of, 40 P-V and P-V-T equations of state, 117

Q

Qualitative analysis, 89 *Qualx2.0*, quantitative analysis, 93 Quantitative analysis, 93 Quartz, unit-cell approach to fitting the PDF, 203 Quasicrystals, naturally occurring, 241

R

Rapidcreekite, crystal structure of, 55
Rational indices, 213, reinterpretation of the law of, 225
Real-space analysis, 201
Real-space fitting with periodic models, 195
Reciprocal space, analysis, 201, methods, 107, of widenmannite from PEDT data, *156*Reverse Monte Carlo and whole nanoparticle simulation, 204
Rietveld refinement, 112
Ring periodicity, **8**Rizzi, R., 79
Robinsonite, crystal structure of, *54*Rockbridgeite, crystal structure of, *21*

S

Sarrabustite, structure of, 170 Scherbakovite-bastisite series, octahedral-tetrahedral framework in the structures of, 34 Schlegel diagrams and their use in crystal chemistry, 19, 21 Schwertmannite, unit-cell approach to fitting the PDF, 201 Selected area electron diffraction, 147, almandine, 152 Semi-quantitative analysis by Qualx2.0, 97 Silver, non-harmonic joint probability density isosurface for, in the pearceite structure, 239 Single-crystal spots, 82 Single-phase modelling, 205 Size, effects of, on diffraction data, 185 Sodalite, polyhedral building units present in the frameworks of the cancrinite-sodalite supergroup minerals, 30, 32 Solid-state chemistry, methods of crystallography, 79 Space-group determination, 105, 163 Spectroscopic techniques, 157 STEM investigation of exsolution lamellae in Carich dolomite, 145 Stewartite, octahedral-tetrahedral sheets in the structure of, 39 Stibnite, crystal structure of, 54 Structural disorder, effects of, on diffraction data, 185 Structural mineralogy, 1

Structure descriptions in mineralogy, 2
Structure evolution at high pressure and high temperature, 119
Structure refinement, 170
Structure solution, 100, 107
Sulfohalite, anion-centred octahedron in the crystal structure of, 17
Superspace, displacive modulation in, 219, electron density sections, 226, introduction to, 217, main and satellite reflections in, 218, symmetry in, 220

Т

Tetrahedral frameworks in paracelsian, *29* Tilings, 39 Total scattering experiments, 183, methodology, 187 Transition metal sulfides, 27

U

Unit-cell parameters, evolution of, 125

V

Vaterite crystal structure, EDT on nanocrystalline minerals, 166, Vikingite, crystal structure of, Vlasovite, nodal representations,

W

Whole-nanoparticle RMC refinement, 206 Widenmannite, reciprocal space of, from PEDT data, 156

Х

X-ray diffraction, powder, 81, problems with, 86
X-ray vs. neutron diffraction under extreme conditions, 123
XRD intensities, sphalerite, 186

Z

Zeolite CaAlSiO₄, high-pressure, high-temperature behaviour of, 124, *125*Zincenite, crystal structure of, *54*ZnS nanoparticles, PDF peak positions, 193
Zone axis pattern of coesite, *163*