## **Contents**

## Editorial --- V

Barbar	a Latuente, R. T. Downs, H. Yang, and N. Stone
1	The power of databases: The RRUFF project —— 1
1.1	Introduction —— 1
1.2	A brief history of the RRUFF project —— 2
1.3	The RRUFF database —— 5
1.3.1	Sample collection and characterization —— 5
1.3.2	Reference library —— 13
1.3.3	Search and access to mineral records —— 14
1.3.4	Software design and server infrastructure —— 14
1.4	Experimental observations during collection of Raman spectra — 15
1.4.1	Thermal effects of laser power —— 15
1.4.2	Effects of the incident laser wavelength —— 16
1.4.3	Fluorescence —— 17
1.4.4	Presence of inversion center —— 19
1.4.5	Metamict minerals —— 20
1.5	Applications of the RRUFF project —— 21
1.5.1	Crystal-chemistry analysis of Mars samples —— 24
1.5.2	The Mineral Evolution database —— 24
1.6	Future directions —— 24
Sergey	v. Krivovichev
2	Structural complexity of minerals and mineral parageneses: Information
	and its evolution in the mineral world —— 31
2.1	Introduction —— 31
2.2	Measuring structural complexity 32
2.2.1	Parsimony and its indices —— 32
2.2.2	Information-based complexity measures —— 34
2.2.3	Algorithmic complexity —— 39
2.3	Information-based structural complexity of minerals: Statistics and
	basic trends —— 48
2.4	Structural complexity and scalar hierarchy — 50
2.5	Structural complexity and the 'ease of crystallization' — 53
2.5.1	General notes —— 53
2.5.2	Silica polymorphs —— 54
2.5.3	Feldspar compositions —— 55

2.5.4	Serpentine-group minerals — 56
2.5.5	Micas and clay minerals —— 57
2.5.6	Metastability and structural complexity —— 57
2.6	Microevolution of structural complexity in natural processes — 58
2.6.1	Information and chemical reactions: oxidation of pyrite and the cascade
	of iron sulfate hydrates —— 58
2.6.2	Information and temperature: Natural zeolites —— 61
2.7	Macroevolution of structural complexity of minerals: Preliminary
	musings — 65
2.8	Information storage and processing in minerals versus living
	matter —— <b>66</b>
2.9	Conclusions —— 67
Sergey	V. Churakov
3	Ab initio simulations of mineral surfaces: Recent advances in numerical
	methods and selected applications —— 75
3.1	Introduction —— 75
3.2	Theoretical background and simulation methods —— 76
3.2.1	Structural rearrangements and surface symmetry —— 76
3.2.2	Stability of surfaces of simple ionic solids 78
3.2.3	Influence of the surface on the electronic structure —— 79
3.2.4	Theory of atomistic simulations —— 80
3.2.5	Thermodynamics of mineral surfaces —— 87
3.2.6	Acid-base properties of surfaces —— 88
3.2.7	Simulation packages —— 90
3.3	Case studies —— 91
3.3.1	Diamond 91
3.3.2	Rutile 92
3.3.3	Pyrite —— 94
3.3.4	Magnetite —— 96
3.3.5	Phyllosilicates —— 98
3.4	Outlook 99
Luca B	indi and Paul J. Steinhardt
4	Natural quasicrystals: A new frontier in mineralogy and its impact on our
	understanding of matter and the origin of the solar system —— 109
4.1	Prelude to quasicrystals —— 109
4.2	Revolution in Crystallography: Quasicrystals (1984) —— 110
4.3	Revolution in Mineralogy: Natural Quasicrystals (2009) —— 112
4.3.1	Extraordinary evidence —— 116
4.3.2	Impact —— <b>120</b>
4.4	Outlook — 123

Fabrizio	Nestola
5	Ringwoodite: its importance in Earth Sciences —— 127
5.1	History of ringwoodite —— 127
5.2	Crystal structure and Mg/Fe substitution —— 129
5.3	The effect of water on the crystal structure of ringwoodite —— 132
5.4	Ringwoodite stability field — 134
5.5	Thermo-elastic properties of ringwoodite —— 135
5.5.1	Bulk modulus —— 135
5.5.2	The effect of water on the bulk modulus of ringwoodite —— 136
5.5.3	Thermal expansion of anhydrous and hydrous ringwoodite —— 139
5.5.4	Thermo-elastic properties of ringwoodite: implications for Earth
J.J.4	Sciences — 140
5.6	Ascent of diamond-bearing kimberlite magma —— 141
5.7	Ringwoodite and the Earth's storage water capacity —— 142
	<b>3</b> ,
	Mugnaioli
6	Investigation of bio-related minerals by electron-diffraction tomography:
	Vaterite, dental hydroxyapatite, and crystalline nanorods in sponge
	primmorphs —— 149
6.1	Introduction —— 149
6.2	Automated diffraction tomography (ADT) —— 151
6.3	Experimental —— <b>154</b>
6.3.1	Conventional TEM, ADT and structure analysis —— <b>154</b>
6.3.2	Sponge primmorphs sample preparation —— 154
6.3.3	Vaterite synthesis —— 154
6.3.4	Human hydroxyapatite extraction —— 155
6.4	Characterization of unknown biominerals inside tissues: Crystalline
	nanorods in sponge primmorphs —— 155
6.5	Ab-initio structure determination of complex bio-related nanocrystalline
	minerals: Vaterite —— 157
6.6	Structure investigation of human calcified tissues:
	Dental hydroxyapatite —— 159
6.7	Conclusions and perspectives —— <b>161</b>
Frank G	feller
7	Mayenite $Ca_{12}Al_{14}O_{32}[X^{2-}]$ : From minerals to the first stable electride
-	crystals — 169
7.1	The discovery and chemical composition of mayenite
	Ca <sub>12</sub> Al <sub>6</sub> Al <sub>8</sub> O <sub>32</sub> [O] — <b>169</b>
7.2	The crystal structure of mayenite and its relation to the garnet
,	structure —— 170

Extra framework anions and structure distortion —— 170

7.3

## X — Contents

7.3.1	Centre, off-centre or both? —— 173
7.3.2	Extraframework occupants in "dry" mayenite —— 175
7.3.3	Hydroxylated mayenite —— 176
7.4	Zeolite or anti-zeolite? —— 178
7.5	Applications of mayenite ceramics — 179
7.5. <b>1</b>	Mayenite the first thermally and chemically stable electride 179
7.5.2	Active oxygen O <sup>-</sup> , O <sub>2</sub> in mayenite as support of syngas
	catalysis —— 180
7.5.3	Cation and anion doping of mayenite —— 181
7.6	The mineral mayenite —— 181
7.6.1	The mayenite supergroup —— 182
7.6.2	Achtarandite 185
7.6.3	Silicates with mayenite-type structure —— 187
7.7	Synthesis and structure of wadalite-group members —— 187
7.8	Outlook —— <b>190</b>

Index —— 197