

1 **Revision 1**

2

3 **Meyrowitzite, Ca(UO₂)(CO₃)₂·5H₂O, a new mineral with a novel uranyl-**
4 **carbonate sheet**

5

6 **ANTHONY R. KAMPF^{1§}, JAKUB PLÁŠIL², TRAVIS A. OLDS³, BARBARA P. NASH⁴, JOE**

7 **MARTY⁵ AND HARVEY E. BELKIN⁶**

8

9 ¹Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los
10 Angeles, CA 90007, USA

11 ²Institute of Physics ASCR, v.v.i., Na Slovance 1999/2, 18221 Prague 8, Czech Republic

12 ³Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre
13 Dame, IN 46556, USA

14 ⁴Department of Geology and Geophysics, University of Utah, Salt Lake City, Utah 84112, USA

15 ⁵5199 East Silver Oak Road, Salt Lake City, UT 84108, USA

16 ⁶United States Geological Survey (Ret.), Reston, VA 20190 USA

17

18 **ABSTRACT**

19 Meyrowitzite, Ca(UO₂)(CO₃)₂·5H₂O, is a new mineral species from the Markey mine, Red
20 Canyon, San Juan County, Utah, U.S.A. It is a secondary phase found on calcite-veined
21 asphaltum in association with gypsum, markeyite, and rozenite. Meyrowitzite occurs as
22 blades up to about 0.2 mm in length, elongate on [010], flattened on {100}, and exhibiting the
23 forms {100}, {001}, {101}, {110}, and {011}. The mineral is yellow and transparent with
24 vitreous luster and very pale yellow streak. Fluorescence is from weak greenish yellow to
25 moderate greenish blue. The Mohs hardness is *ca* 2, tenacity is brittle, fracture is irregular,

[§] Email: akampf@nhm.org

26 and there is one perfect cleavage, $\{-101\}$. The measured density is $2.70(2) \text{ g}\cdot\text{cm}^{-3}$. The
27 mineral is optically biaxial (+) with $\alpha = 1.520(2)$, $\beta = 1.528(2)$, and $\gamma = 1.561(2)$ (white light).
28 The $2V(\text{meas.}) = 53.0(6)^\circ$; weak dispersion, $r > v$; optical orientation: $Z = \mathbf{b}$, $Y \wedge \mathbf{a} \approx 19^\circ$ in
29 obtuse β ; pleochroism pale yellow, $X \approx Y < Z$. Electron microprobe analyses provided the
30 empirical formula $\text{Ca}_{0.94}(\text{U}_{1.00}\text{O}_2)(\text{CO}_3)_2 \cdot 5(\text{H}_{2.02}\text{O})$ on the basis of $\text{U} = 1$ and $\text{O} = 13 \text{ apfu}$, as
31 indicated by the crystal structure determination. Meyrowitzite is monoclinic, $P2_1/n$, $a =$
32 $12.376(3)$, $b = 16.0867(14)$, $c = 20.1340(17) \text{ \AA}$, $\beta = 107.679(13)^\circ$, $V = 3819.3(12) \text{ \AA}^3$, and $Z =$
33 12 . The structure ($R_1 = 0.055$ for $3559 I_o > 2\sigma I$) contains both UO_7 pentagonal bipyramids and
34 UO_8 hexagonal bipyramids, the later participating in uranyl tricarbonate clusters (UTC). The
35 two kinds of bipyramids and the carbonate groups link to form a novel corrugated
36 heteropolyhedral sheet. This is the first structural characterization of a uranyl-carbonate
37 mineral with a U:C ratio of 1:2. Meyrowitzite is apparently dimorphous with zellerite.

38

39 *Keywords:* meyrowitzite; new mineral species; uranyl tricarbonate; crystal structure; zellerite;
40 Markey mine, Red Canyon, Utah.

41

42 INTRODUCTION

43 Carbonate minerals containing U^{6+} are usually relatively soluble in aqueous solutions.
44 Aqueous uranyl-carbonate complexes are generally quite stable and are responsible for
45 uranium migration in the environment on a large scale (Langmuir, 1978; Clark *et al.*, 1995).
46 The most abundant complexes are uranyl monocarbonate, $[(\text{UO}_2)(\text{CO}_3)]^0$, uranyl dicarbonate,
47 $[(\text{UO}_2)(\text{CO}_3)_2]^{2-}$ and uranyl tricarbonate, $[(\text{UO}_2)(\text{CO}_3)_3]^{4-}$, with $\text{p}K_a$ values of 5.5, 7 and 9,
48 respectively (Langmuir, 1978). The most abundant uranyl carbonate minerals are those with a
49 U:C ratio of 1:3, which crystallize from solutions of relatively high pH, from neutral to
50 alkaline. However, very little data is available for minerals with a U:C ratio of 1:2; for

51 example, the mineral zellerite, $\text{Ca}[(\text{UO}_2)(\text{CO}_3)_2] \cdot 5\text{H}_2\text{O}$ (Coleman *et al.*, 1966), which occurs
52 commonly within the carbonate-rich alteration associations of supergene U minerals, has so
53 far eluded crystallographic characterization. Here, we present the description of the new
54 uranyl-carbonate mineral, meyrowitzite, $\text{Ca}(\text{UO}_2)(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$, a dimorph of zellerite, and the
55 first structural characterization of a uranyl-carbonate mineral with a U:C ratio of 1:2.

56 Meyrowitzite is named in honor of American analytical chemist Robert Meyrowitz
57 (1916-2013). Mr. Meyrowitz received his bachelor's degree in chemistry from the City
58 College of New York in 1936, after which he conducted research in microchemical analysis at
59 Brooklyn College (New York). During World War II, he served in the U.S. Army and,
60 because of his skills as a chemist, he was assigned to work on the Manhattan Project. After
61 the war, he joined the United States Geological Survey (USGS), from which he retired in
62 1973. In his years at the USGS, he was especially known for his knack for developing
63 innovative new methods for analyzing small and difficult to study mineralogical samples, and
64 is also well-known for his formulation of the high-index immersion liquids (1.74 to 2.00) that
65 are still in use for optical determinations (Meyrowitz and Larsen, 1951). He published
66 prolifically, often collaborating on the descriptions of new minerals (e.g. brockite, duttonite,
67 goldmanite, hendersonite, metazellerite, ningyoite, sahamalite, sherwoodite, simplotite,
68 weeksite and zellerite). Many of the new minerals species that he worked on were from the
69 uranium deposits of the western U.S. Among them was zellerite, the dimorph of the
70 meyrowitzite. Robert Meyrowitz' son Alan has approved of the naming of the mineral in his
71 father's honor.

72 The new mineral and name were approved by the Commission on New Minerals,
73 Nomenclature and Classification of the International Mineralogical Association (IMA 2018-
74 039). Two cotype specimens of meyrowitzite are deposited in the collections of the Natural
75 History Museum of Los Angeles County, Los Angeles, California, USA, catalogue numbers

76 66789 and 66790.

77

78

OCCURRENCE

79 Meyrowitzite was discovered on specimens collected underground in the Markey
80 mine, Red Canyon, White Canyon District, San Juan County, Utah, USA (37°32'57"N
81 110°18'08"W). The Markey mine is located about 1 km southwest of the Blue Lizard mine, on
82 the east-facing side of Red Canyon, about 72 km west of the town of Blanding, Utah, and
83 about 22 km southeast of Good Hope Bay on Lake Powell. The geology of the Markey mine
84 is quite similar to that of the Blue Lizard mine (Chenoweth, 1993; Kampf, *et al.*, 2015a),
85 although the secondary mineralogy of the Markey mine is notably richer in carbonate phases.
86 The information following is taken largely from Chenoweth (1993).

87 Jim Rigg of Grand Junction, Colorado began staking claims in Red Canyon in March
88 of 1949. The Markey group of claims, staked by Rigg and others, was purchased by the
89 Anaconda Copper Mining Company on June 1, 1951. After limited exploration and
90 production, the mine closed in 1955. The mine was subsequently acquired from Anaconda by
91 Calvin Black of Blanding, Utah under whose ownership the mine operated from 1960 to 1982
92 and was a leading producer in the district for nearly that entire period.

93 Mineralized channels are in the Shinarump member of the Chinle Formation. The
94 Shinarump member consists of medium- to coarse-grained sandstone, conglomeratic
95 sandstone beds and thick siltstone lenses. Ore minerals were deposited as replacements of
96 wood and other organic material and as disseminations in the enclosing sandstone. Since the
97 mine closed, oxidation of primary ores in the humid underground environment has produced a
98 variety of secondary minerals, mainly sulfates, as efflorescent crusts on the surfaces of mine
99 walls.

100 Meyrowitzite is a very rare mineral, found on calcite-veined asphaltum in association

101 with gypsum, markeyite (Kampf *et al.*, 2018) and rozenite. See Kampf *et al.* (2018) for a
102 more complete list of the secondary minerals identified from the Markey mine, including
103 several which are recently described new species.

104

105 **PHYSICAL AND OPTICAL PROPERTIES**

106 Crystals of meyrowitzite are blades up to about 0.2 mm in length, commonly in
107 irregular and radiating intergrowths (Fig. 1). Blades are elongate on [010], flattened on {100}
108 and exhibit the forms {100}, {001}, {101}, {110} and {011} (Fig. 2). No twinning was
109 observed. The mineral is yellow and transparent with vitreous luster and very pale-yellow
110 streak. Meyrowitzite exhibits variable fluorescence from weak greenish yellow to moderate
111 greenish blue under a 405 nm laser. It has a Mohs hardness of about 2, brittle tenacity,
112 irregular fracture, and one perfect cleavage on {-101}. The density measured by flotation in a
113 mixture of methylene iodide and toluene is 2.70(2) g·cm⁻³. The calculated density is 2.702
114 g·cm⁻³ using the empirical formula and 2.714 g·cm⁻³ using the ideal formula. The mineral is
115 easily soluble in H₂O at room temperature.

116 Meyrowitzite is optically biaxial (+) with $\alpha = 1.520(2)$, $\beta = 1.528(2)$, and $\gamma = 1.561(2)$
117 measured in white light. The $2V$ measured using extinction data analyzed with EXCALIBRW
118 (Gunter *et al.*, 2004) is 53.0(6)°; the calculated $2V$ is 53.3°. The dispersion is weak, $r > v$. The
119 optical orientation is $Z = \mathbf{b}$, $Y \wedge \mathbf{a} \approx 19^\circ$ in obtuse β . Crystals are weakly pleochroic in shades
120 of pale yellow, $X \approx Y < Z$. The Gladstone–Dale compatibility, $1 - (K_P/K_C)$, (Mandarino, 2007)
121 is -0.039 (excellent) using the empirical formula, and -0.035 (excellent) using the ideal
122 formula – where $k(\text{UO}_3) = 0.134$ as provided by Larsen (1921).

123

124 **RAMAN SPECTROSCOPY**

125 Raman spectroscopy was conducted on a Horiba XploRA PLUS. Because of

126 significant fluorescence using a 532 nm diode laser, the spectrum was recorded using a 785
127 nm diode laser. The spectrum from 1800 to 80 cm^{-1} is shown in Figure 3. In general, the
128 measured meyrowitzite spectrum is similar to the spectrum of zellerite (Frost *et al.*, 2008);
129 however, the spectrum of meyrowitzite contains larger number of bands (especially in the
130 region of UO_2^{2+} stretching vibrations), most probably due to lowering of the corresponding
131 site-symmetry: orthorhombic (zellerite) \rightarrow monoclinic (meyrowitzite).

132 A broad band composed of two overlapping bands at 1450 and 1380 cm^{-1} results from
133 the split doubly degenerate ν_3 $(\text{CO}_3)^{2-}$ antisymmetric stretching vibrations of the $(\text{CO}_3)^{2-}$
134 polyhedra. Medium to strong bands at 1100, 1095, 1080, and 1065 cm^{-1} are associated with
135 the ν_1 $(\text{CO}_3)^{2-}$ symmetric stretching vibrations. Splitting of these bands is consistent with the
136 presence of structurally non-equivalent carbonate units (Koglin *et al.*, 1979; Anderson *et al.*,
137 1980; Čejka, 1999 and 2005, and references therein); there are six independent C sites in the
138 structure of meyrowitzite (see below). A multi-component band of high intensity, composed
139 of overlapping bands at 850, 840, 835, and 825 cm^{-1} , is attributable to the ν_2 (δ) $(\text{CO}_3)^{2-}$
140 bending vibrations, and (in overlap) to the ν_1 $(\text{UO}_2)^{2+}$ symmetric stretching vibrations. Using
141 the empirical relation of Bartlett and Cooney (1989), we can infer the corresponding U–O
142 bond lengths from the above-mentioned wavenumbers (in the order as given above): 1.76,
143 1.77, 1.78, and 1.79 Å. The structure refinement provided U–O bond-lengths in the range of
144 1.75–1.80 Å; therefore, it is possible that all observed overlapping bands in the region 850–
145 825 cm^{-1} belong to the ν_1 $(\text{UO}_2)^{2+}$ symmetric stretching vibration. A strong component band,
146 composed of overlapping bands at 760 and 745 cm^{-1} , and a weak composite band at 687 cm^{-1}
147 are attributable to the ν_4 (δ) $(\text{CO}_3)^{2-}$ bending vibrations. Medium to strong bands at 270 and
148 240 cm^{-1} are attributable to split doubly degenerate ν_2 (δ) $(\text{UO}_2)^{2+}$ bending vibrations.
149 Medium-strong bands at 218, 145, and 125 cm^{-1} are attributable to the lattice modes (Koglin
150 *et al.*, 1979; Anderson *et al.*, 1980; Čejka, 1999 and 2005).

151

152

CHEMICAL ANALYSIS

153

154

155

156

157

158

159

160

161

162

163

164

165

166

167

168

X-RAY CRYSTALLOGRAPHY AND STRUCTURE DETERMINATION

169

170

171

172

173

174

Chemical analyses (3) were performed at the University of Utah on a Cameca SX-50 electron microprobe with four wavelength dispersive spectrometers and using Probe for EPMA software (Probe Software, Inc., Eugene, OR). Analytical conditions were 15 keV accelerating voltage, 10 nA beam current and a beam diameter of 5 μm . Raw X-ray intensities were corrected for matrix effects with a $\phi\rho(z)$ algorithm (Pouchou and Pichoir, 1991). Concentrations of total oxygen and carbon, calculated from the ideal formula, were used in the matrix correction.

It was impossible to obtain a good polish and crystal surfaces suffered further because of crystal dehydration; however, the beam produced no damage to the sample. Because insufficient material is available for direct determination of H_2O and CO_2 , they are calculated based upon the structure determination (2 C and 13 O *apfu*). Analytical data are given in Table 1. The empirical formula is $\text{Ca}_{0.94}(\text{U}_{1.00}\text{O}_2)(\text{CO}_3)_2 \cdot 5(\text{H}_{2.02}\text{O})$. The ideal formula is $\text{Ca}(\text{UO}_2)(\text{CO}_3)_2 \cdot 5\text{H}_2\text{O}$, which requires CaO 10.78, UO_3 54.98, CO_2 16.92, and H_2O 17.32, total 100 wt.%.

Both powder and single-crystal X-ray studies were carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer with monochromatized $\text{MoK}\alpha$ radiation. For the powder study, a Gandolfi-like motion on the ϕ and ω axes was used to randomize the sample, which consisted of several crystals. Observed d values and intensities were derived by profile fitting using JADE 2010 software (Materials Data, Inc. Livermore, CA). Data are given in Table 2. Unit cell parameters refined from the powder data using JADE 2010 with

175 whole pattern fitting are $a = 12.417(17)$, $b = 16.127(17)$, $c = 20.123(17)$ Å, $\beta = 107.53(4)^\circ$
176 and $V = 3842(7)$ Å³.

177 Crystals of meyrowitzite are of relatively poor quality for single-crystal study. The
178 best crystal fragment, which was used for the collection of structure data, exhibited significant
179 mosaicity, some spot streaking and some extra spots indicative of one or more satellite
180 crystals. This fragment, measuring only $80 \times 80 \times 30$ µm, provided usable data only to a
181 resolution of 0.88 Å. The Rigaku CrystalClear software package was used for processing the
182 structure data, including Lorentz and polarization corrections, and the application of an
183 empirical absorption correction using the multi-scan method with ABSCOR (Higashi, 2001).
184 The space group $P2_1/n$ was suggested by the Rigaku XPlain program, which readily led to a
185 structure solution using SIR2011 (Burla *et al.*, 2012). It should be noted that numerous
186 reflections violated the extinction conditions for space group $P2_1/n$, and particularly for the n
187 glide; however, efforts to obtain viable structure models in other space groups were
188 unsuccessful. We attribute the space-group violations to the imperfect nature of the crystal
189 fragment, as noted above, and this also led us to omit five poorly fitting reflections that did
190 not violate the extinction conditions. SHELXL-2013 (Sheldrick, 2015) was used for the
191 refinement of the structure. The limited data set allowed refinement with anisotropic
192 displacement parameters for all fully occupied sites, but not for four approximately half-
193 occupied H₂O sites (OW14, OW15, OW16 and OW17). It also did not allow the location of H
194 sites in difference Fourier maps. Data collection and refinement details are given in Table 3,
195 atom coordinates and displacement parameters in Table 4, selected bond distances in Table 5
196 and a bond valence analysis in Table 6.

197

198

DISCUSSION

199 There are three U sites in the structure of meyrowitzite. Two (U1 and U2) are
200 surrounded by eight O atoms forming a squat UO_8 hexagonal bipyramid; the other (U3) is
201 surrounded by seven O atoms forming a squat UO_7 pentagonal bipyramid. The two short
202 apical bonds of all three bipyramids constitute the UO_2^{2+} uranyl group. Of the six CO_3^{2-}
203 groups in the structure, three centered by C1, C2 and C3 share alternating equatorial edges of
204 the U1 hexagonal bipyramid, thereby forming the well-known uranyl tricarbonate (UTC) unit.
205 The other three, centered by C4, C5 and C6, share alternating equatorial edges of the U2
206 hexagonal bipyramid, forming a second UTC unit. The five equatorial corners of the U3
207 pentagonal bipyramid are shared with O atoms of the C1, C2, C3, C4 and C6 carbonate
208 groups. These linkages create a unique corrugated uranyl carbonate heteropolyhedral sheet
209 parallel to $\{10\cdot1\}$ (Figure 5). The U2 UTCs are oriented perpendicular to the plane of the
210 sheet (Figure 6) with the unshared corner of the C5 carbonate group pointing away from the
211 sheet. Three Ca atoms (Ca1, Ca2 and Ca3) are eight-coordinated to O atoms in the sheets and
212 to OW atoms, although Ca3 is effectively only seven-coordinated because two of its ligands
213 (OW15 and OW16) are only half-occupied. The Ca polyhedra do not link to one another;
214 instead, they share edges and corners with the polyhedra in the uranyl carbonate
215 heteropolyhedral sheets, thereby linking the sheets into a framework (Figure 7). The fully
216 occupied OW9 through OW13 sites and the half-occupied OW14 and OW17 sites are located
217 in the cavities in this framework.

218 Minerals with structures containing both UO_7 pentagonal bipyramid and UO_8
219 hexagonal bipyramid are rare. Other examples include ewingite,
220 $\text{Mg}_8\text{Ca}_8(\text{UO}_2)_{24}(\text{CO}_3)_{30}\text{O}_4(\text{OH})_{12}(\text{H}_2\text{O})_{138}$, (Olds *et al.*, 2017) and fontanite,
221 $\text{Ca}[(\text{UO}_2)_3(\text{CO}_3)_2\text{O}_2](\text{H}_2\text{O})_6$, (Hughes and Burns, 2003). The structure of ewingite is based on
222 a large and complex uranyl carbonate polyhedral cluster that bears no similarity to the
223 structure of meyrowitzite. Fontanite has uranyl carbonate sheets that are linked by CaO_8

224 polyhedra; however, the UO_7 and UO_8 polyhedra form edge-sharing chains within these
225 sheets and there are no UTC units, but rather uranyl dicarbonate units.

226 Meyrowitzite has a crystal structure based on a unique corrugated uranyl carbonate
227 heteropolyhedral sheet. Meyrowitzite is apparently dimorphous with zellerite (Coleman *et al.*,
228 1966); however, the structure of zellerite is not known. The PXRD patterns for meyrowitzite
229 and zellerite, compared graphically in Figure 4, are quite different. Although the strongest
230 peaks in the zellerite pattern are represented in the meyrowitzite pattern, the four strongest
231 lines in the meyrowitzite pattern are not in the zellerite pattern. Comparative data for
232 meyrowitzite and zellerite are provided in Table 7. In the Strunz system, meyrowitzite and
233 zellerite both belong in class 5.EB: uranyl carbonates with $\text{UO}_2:\text{CO}_3 > 1:1$ to $1:2$.

234

235

IMPLICATIONS

236 Numerous studies conducted over the past 50 years have led to a well-developed
237 understanding of the geochemistry of U- CO_3 systems (Langmuir, 1978; Chopin and Jensen,
238 2010; Maher *et al.*, 2013). All acknowledge that carbonate binds to uranium strongly and that
239 uranyl-carbonate complexes are among those most relevant to the environmental chemistry of
240 uranium. One of the most common species, the uranyl-tricarbonate complex (UTC), is
241 exceptionally stable in aqueous solutions and it is known to occur in 33 different uranyl-
242 carbonate minerals. Significant evidence suggests that additional polymeric UTC-hydrolyzed
243 U complexes are prevalent species in some systems (Müller *et al.*, 2008; Saini *et al.*, 1989;
244 Ciavatta *et al.*, 1980), and this combination is known in several exceptionally rare minerals,
245 including fontanite, $\text{Ca}[(\text{UO}_2)_3(\text{CO}_3)_2\text{O}_2](\text{H}_2\text{O})_6$ (Hughes and Burns, 2003), roubaultite,
246 $\text{Cu}_2(\text{UO}_2)_3(\text{CO}_3)_2\text{O}_2(\text{OH})_2(\text{H}_2\text{O})_4$ (Ginderow and Cesbron, 1985), wyartite,
247 $\text{Ca}(\text{CO}_3)[\text{U}^{5+}(\text{U}^{6+}\text{O}_2)_2\text{O}_4(\text{OH})](\text{H}_2\text{O})_7$ (Burns and Finch, 1999), bijvoetite-Y
248 $[\text{Y}_8(\text{H}_2\text{O})_{25}(\text{UO}_2)_{16}\text{O}_8(\text{OH})_8(\text{CO}_3)_{16}](\text{H}_2\text{O})_{14}$ (Li *et al.*, 2000), kamotoite-(Y),

249 $Y_2(UO_2)_4O_2(OH)_2(CO_3)_4(H_2O)_{12.54}$ (Plášil and Petříček, 2017), above-mentioned ewingite
250 (Olds *et al.*, 2017), and herein with the description of meyrowitzite. The structure of ewingite
251 suggests that relatively large polynuclear species containing hydrolyzed uranium and UTC
252 may have assembled in solution prior to crystal growth, or possibly at the crystal-solution
253 interface. Though we recognize the conditions required for their formation are very narrow,
254 these minerals reveal definite gaps in our understanding of uranyl-carbonate-hydroxide
255 equilibria that can be better determined through crystal-chemical studies of natural systems.
256 Crystallization of these minerals offers a diagnostic view into the conditions and speciation of
257 the solutions from which they crystallize. These missing data are necessary for producing
258 accurate models of contamination speciation in repositories for nuclear waste.

259 The fact that meyrowitzite contains a heretofore-unreported type of uranyl-carbonate
260 heteropolyhedral sheet makes its reported occurrence in a natural setting of significant
261 importance in expanding our understanding of uranyl-carbonate interactions in natural
262 systems. Furthermore, although based upon composition alone, meyrowitzite, with a U:C ratio
263 of 1:2, might have been expected to contain the uranyl-dicarbonate complex, $[(UO_2)(CO_3)_2]^{2-}$,
264 it is noteworthy that the determination of its structure shows it to contain instead a uranyl-
265 tricarboxylate complex. Based upon this, it is reasonable to conjecture that its dimorph zellerite
266 may also contain a uranyl-tricarboxylate complex, rather than a uranyl-dicarbonate complex.

267

268 ACKNOWLEDGEMENTS

269 Two anonymous reviewers and the Technical Editor are thanked for constructive
270 comments, which improved the manuscript. Associate Editor G. Diego Gatta is thanked for
271 shepherding the manuscript through the review process. Alan Meyrowitz is thanked for
272 providing background information about his father, Robert Meyrowitz. This study was

273 funded, in part, by the John Jago Trelawney Endowment to the Mineral Sciences Department
274 of the Natural History Museum of Los Angeles County.

275

276

REFERENCES

- 277 Anderson A., Chieh Ch., Irish D.E., and Tong J.P.K. (1980) An X-ray crystallographic,
278 Raman, and infrared spectral study of crystalline potassium uranyl carbonate,
279 $K_4UO_2(CO_3)_3$. *Canadian Journal of Chemistry*, **58**, 1651–1658.
- 280 Bartlett, J.R. and Cooney, R.P. (1989) On the determination of uranium-oxygen bond lengths
281 in dioxouranium(VI) compounds by Raman spectroscopy. *Journal of Molecular Structure*,
282 **193**, 295–300.
- 283 Burla, M. C., Caliendo, R., Camalli, M., Carrozzini, B., Cascarano, G.L., Giacovazzo, C.,
284 Mallamo, M., Mazzone, A., Polidori, G., and Spagna, R. (2012) *SIR2011*: a new package
285 for crystal structure determination and refinement. *Journal of Applied Crystallography*,
286 **45**, 357–361.
- 287 Burns, P.C. and Finch, R.J. (1999) Wyartite: crystallographic evidence for the first
288 pentavalent-uranium mineral. *American Mineralogist*, **84**, 1456–1460.
- 289 Čejka J. (1999) Infrared and thermal analysis of the uranyl minerals. *Reviews in Mineralogy*,
290 **38**, 521–622.
- 291 Čejka J. (2005) Vibrational spectroscopy of the uranyl minerals – infrared and Raman spectra
292 of the uranyl minerals. II. Uranyl carbonates. *Bulletin mineralogicko-petrologického*
293 *oddělení Národního muzea (Praha)*, **13**, 62–72 (in Czech).
- 294 Chenoweth, W.L. (1993) The Geology and Production History of the Uranium Deposits in the
295 White Canyon Mining District, San Juan County, Utah. *Utah Geological Survey*
296 *Miscellaneous Publication*, **93–3**.

- 297 Choppin, G. R. and Jensen, M. P. (2010) Actinides in Solution: Complexation and Kinetics.
298 In Morss, L. R., Edelstein, N. M. and Fuger, J. (eds) *The Chemistry of the Actinide and*
299 *Transactinide Elements*, 4th edition. Springer, Dordrecht, the Netherlands, pp. 2524–2621.
- 300 Ciavatta, L., Ferri, D., Grenthe, I., and Salvatore, F. (1981) The first acidification step of the
301 tris(carbonato)dioxouranate(VI) ion, $\text{UO}_2(\text{CO}_3)_3^{4-}$. *Inorganic Chemistry*, **20**, 463–467.
- 302 Coleman, R.G., Ross, D.R., and Meyrowitz, R. (1966) Zellerite and metazellerite, new uranyl
303 carbonates. *American Mineralogist*, **51**, 1567–1578.
- 304 Ferraris, G. and Ivaldi, G. (1988) Bond valence vs. bond length in O...O hydrogen bonds.
305 *Acta Crystallographica*, **B44**, 341–344.
- 306 Frost, R.L., Dickfos, M.J., and Čejka, J. (2008) Raman spectroscopic study of the uranyl
307 carbonate mineral zellerite. *Journal of Raman Spectroscopy*, **39**, 582–586.
- 308 Gagné, O.C. and Hawthorne, F.C (2015) Comprehensive derivation of bond-valence
309 parameters for ion pairs involving oxygen. *Acta Crystallographica*, **B71**, 562–578.
- 310 Ginderow, D. and Cesbron, F. (1985) The structure of roubaultite,
311 $\text{Cu}_2(\text{UO}_2)_3(\text{CO}_3)_2\text{O}_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$. *Acta Crystallographica*, **C41**, 654–657.
- 312 Gunter, M.E., Bandli, B.R., Bloss, F.D., Evans, S.H., Su, S.C., and Weaver, R. (2004) Results
313 from a McCrone spindle stage short course, a new version of EXCALIBUR, and how to
314 build a spindle stage. *The Microscope*, **52**, 23-39.
- 315 Higashi, T. (2001) *ABSCOR*. Rigaku Corporation, Tokyo.
- 316 Hughes, K.-A. and Burns, P.C. (2003) A new uranyl carbonate sheet in the crystal structure of
317 fontanite, $\text{Ca}[(\text{UO}_2)_3(\text{CO}_3)_2\text{O}_2](\text{H}_2\text{O})_6$. *American Mineralogist*, **88**, 962–966.
- 318 Kampf, A.R., Kasatkin, A.V., Čejka, J., and Marty, J. (2015) Plášilite,
319 $\text{Na}(\text{UO}_2)(\text{SO}_4)(\text{OH}) \cdot 2\text{H}_2\text{O}$, a new uranyl sulfate mineral from the Blue Lizard mine, San
320 Juan County, Utah, USA. *Journal of Geosciences*, **60**, 1–10.

- 321 Kampf, A.R., Plášil, J., Kasatkin, A.V., Marty, J., and Čejka, J. (2018) Markeyite, a new
322 calcium uranyl tricarbonate mineral from the Markey mine, San Juan County, Utah, USA.
323 *Mineralogical Magazine* **82**, (in press)
- 324 Koglin E., Schenk H.J., and Schwochau K. (1979) Vibrational and low temperature optical
325 spectra of the uranyl tricarbonate complex $[\text{UO}_2(\text{CO}_3)_3]^{4+}$. *Spectrochimica Acta*, **35A**,
326 641–647.
- 327 Langmuir, D. (1978) Uranium solution–mineral equilibria at low temperatures with
328 applications to sedimentary ore. *Geochimica et Cosmochimica Acta*, **42**, 547–569.
- 329 Larsen, E.S. (1921) The microscopic determination of the nonopaque minerals. U.S.
330 Geological Survey, Bulletin 679.
- 331 Li, Y., Burns, P.C., and Gault, R.A. (2000) A new rare earth-element uranyl carbonate sheet
332 in the structure of bijvoetite. *Canadian Mineralogist*, **38**, 153–162.
- 333 Maher, K., Bargar, J.R., and Brown, G.E., Jr. (2013) Environmental speciation of actinides.
334 *Inorganic Chemistry*, **52**, 3510–3532.
- 335 Mandarino, J.A. (2007) The Gladstone–Dale compatibility of minerals and its use in selecting
336 mineral species for further study. *Canadian Mineralogist*, **45**, 1307–1324.
- 337 Meyrowitz, R. and Larsen, E.S., Jr. (1951) Immersion liquids of high refractive index.
338 *American Mineralogist*, **36**, 746–750.
- 339 Müller, K., Brendler, V., and Foerstendorf, H. (2008) Aqueous uranium(VI) hydrolysis
340 species characterized by attenuated total reflection Fourier-transform infrared
341 spectroscopy. *Inorganic Chemistry*, **47**, 10127–10134.
- 342 Olds, T.A., Plášil, J., Kampf, A.R., Burns, P.C., Simonetti, A., and Sadergaski, L.R. (2017)
343 Ewingite: Earth’s most complex mineral. *Geology*, **45**, 1007–1010.
- 344 Olds, T., Sadergaski, L.R., Plášil, J., Kampf, A.R., Burns, P., Steele, I.M., Marty, J., Carlson,
345 S.M., and Mills, O.P. (2017) Leószilárdite, the first Na,Mg-containing uranyl carbonate

- 346 from the Markey Mine, San Juan County, Utah, USA. *Mineralogical Magazine* **81**, 743–
347 754.
- 348 Plášil, J. and Petříček, V. (2017) Crystal structure of the (*REE*)-uranyl carbonate mineral
349 kamotoite-(Y). *Mineralogical Magazine*, **81**, 653–660.
- 350 Pouchou, J.-L. and Pichoir, F. (1991) Quantitative analysis of homogeneous or stratified
351 microvolumes applying the model "PAP." In: Heinrich, K.F.J. and Newbury, D.E. (eds)
352 *Electron Probe Quantitation*. Plenum Press, New York, pp. 31–75.
- 353 Saini, R.D., Bhattacharyya, P.K., and Iyer, R.M. (1989) Photoluminescence studies of the
354 uranyl carbonate system. *Journal of Photochemistry and Photobiology, A: Chemistry*, **47**,
355 65–81.
- 356 Sheldrick, G.M. (2015) Crystal structure refinement with SHELXL. *Acta Crystallographica*,
357 **C71**, 3–8.
- 358

359

FIGURE CAPTIONS

360

Figure 1. Meyrowitzite on asphaltum. The field of view is 0.5 mm across.

361

Figure 2. Crystal drawing of meyrowitzite, clinographic projection in nonstandard

362

orientation, **b** vertical.

363

Figure 3. Raman spectrum of meyrowitzite recorded using a 785 nm diode laser.

364

Figure 4. Comparison of powder X-ray diffraction patterns for meyrowitzite and zellerite.

365

Figure 5. The uranyl carbonate sheet in the structure of meyrowitzite viewed down [10-1].

366

Figure 6. The structure of meyrowitzite viewed down [010]. The O atoms of isolated H₂O

367

groups are shown as white balls. The unit cell outline is shown by dashed lines.

368

Figure 7. The structure of meyrowitzite viewed down [100]. The O atoms of isolated H₂O

369

groups are shown as white balls. The unit cell outline is shown by dashed lines.

370

371

372 Table 1. Analytical results for meyrowitzite.

Constituent	Mean	Range	Stand. Dev.	Probe Standard	Normalized
CaO	12.67	12.51–12.93	0.22	diopside	10.18
UO ₃	68.77	68.14–69.86	0.95	syn. UO ₂	55.23
CO ₂ *					17.00
H ₂ O*					17.60
Total					100.01

373 * based on structure.

374

375 Table 2. Powder X-ray data (d in Å) for meyrowitzite. Only calculated lines with $I \geq 10$ are
 376 listed.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl		
100	12.11	{	53	12.3263	0 1 1	12	2.636	{	13	2.6529	-4 3 3
			47	11.7651	-1 0 1				26	2.6283	-4 2 5
48	9.52	{	24	9.5916	0 0 2	21	2.593	{	20	2.6044	4 0 2
			27	9.4964	-1 1 1				24	2.5940	0 2 7
59	8.19	{	54	8.2383	0 1 2	12	2.534	{	14	2.5328	3 2 4
20	7.74		26	7.7718	-1 1 2				15	2.5302	-2 4 6
68	5.96	{	17	6.0527	1 1 2	10	2.5070	{	10	2.5070	-2 3 7
			51	5.9603	-1 2 2				38	2.4791	-1 6 3
15	5.54	{	26	5.8826	-2 0 2	24	2.476	{	10	2.4745	4 3 1
			32	5.5357	2 1 0				23	2.4406	2 6 0
79	5.04	{	18	5.1643	0 3 1	9	2.380	{	16	2.3890	3 3 4
			19	5.0709	1 2 2				13	2.292	23
30	4.77	{	18	5.0604	-1 2 3	10	2.224	{	10	2.2630	5 2 0
			52	5.0186	1 0 3				12	2.2439	-5 3 2
45	4.359	{	34	4.7908	1 1 3	13	2.185	{	15	2.2187	-1 0 9
			12	4.5898	-1 3 2				12	2.1861	4 4 2
21	4.195	{	46	4.3721	2 2 1	6	2.143	{	12	2.1824	3 5 3
			22	4.3614	-2 2 3				15	2.1370	-5 0 7
32	4.057	{	12	4.2784	-2 1 4	12	2.0782	{	14	2.0884	-1 7 4
			22	4.2491	-1 2 4				12	2.0691	4 4 3
16	3.801	{	20	4.1448	1 3 2	16	2.0482	{	12	2.0544	0 6 6
			21	4.1033	-3 0 1				24	2.0500	-6 0 4
27	3.652	{	19	4.0524	-2 3 1	22	2.0006	{	20	2.0176	2 0 8
			24	4.0217	0 4 0				10	2.0129	-2 0 10
31	3.944	{	17	3.9760	-3 1 1	20	1.9662	{	29	1.9999	0 8 1
			20	3.9361	0 4 1				13	1.9827	-3 7 3
23	3.368	{	19	3.9217	-3 0 3	15	1.8847	{	10	1.9814	-4 6 4
			18	3.8101	-3 1 3				14	1.9790	1 1 9
19	3.294	{	15	3.8055	-1 4 1	27	1.8087	{	11	1.9587	-1 6 7
			16	3.6586	-1 3 4				10	1.8988	4 0 6
25	3.118	{	20	3.6528	-3 2 2	15	1.8847	{	14	1.8871	-5 4 7
			11	3.3721	-2 4 1				15	1.8862	-6 3 5
15	2.989	{	29	3.3604	1 0 5	26	1.7835	{	17	1.8264	-6 4 4
			17	3.3200	-2 4 2				20	1.8054	-3 8 2
26	2.852	{	10	3.3069	-3 2 4	11	1.6771	{	10	1.8034	2 4 8
			16	3.2894	1 1 5				26	1.8013	-5 6 1
10	2.763	{	15	3.2551	-2 0 6	13	1.6282	{	25	1.7998	1 8 4
			13	3.1383	1 4 3				10	1.7901	3 6 5
18	2.690	{	11	3.1202	0 3 5	18	1.7171	{	11	1.7848	-1 4 10
			13	3.0047	-3 3 4				12	1.7756	-2 8 5
			19	2.9711	0 2 6				12	1.7243	-7 0 1
			20	2.8710	-3 4 2				19	1.7175	3 8 2
			15	2.8486	1 4 4				13	1.7121	-7 2 2
			11	2.8452	-1 4 5				10	1.6868	-3 6 9
			14	2.8242	2 5 0				10	1.6833	-7 2 6
			16	2.7557	-2 4 5				13	1.6312	4 8 1
			26	2.6821	2 2 5				10	1.6276	-4 0 12

377 Table 3. Data collection and structure refinement details for meyrowitzite.
 378

379	Diffractometer	Rigaku R-Axis Rapid II
380	X-ray radiation/power	MoK α ($\lambda = 0.71075 \text{ \AA}$)/50 kV, 40 mA
381	Temperature	293(2) K
382	Structural Formula	Ca(UO ₂)(CO ₃) ₂ ·5H ₂ O
383	Space group	<i>P</i> 2 ₁ / <i>n</i>
384	Unit cell dimensions	<i>a</i> = 12.376(3) \AA
385		<i>b</i> = 16.0867(14) \AA
386		<i>c</i> = 20.1340(17) \AA
387		$\beta = 107.679(13)^\circ$
388	<i>V</i>	3819.3(12) \AA^3
389	<i>Z</i>	12
390	Density (for above formula)	2.714 g cm ⁻³
391	Absorption coefficient	13.207 mm ⁻¹
392	<i>F</i> (000)	2796
393	Crystal size	80 × 80 × 30 μm
394	θ range	3.07 to 22.44°
395	Index ranges	-13 ≤ <i>h</i> ≤ 13, -17 ≤ <i>k</i> ≤ 16, -21 ≤ <i>l</i> ≤ 21
396	Frames collected / exposure	36 / 25 min.
397	Reflections collected / unique	17068 / 4874; <i>R</i> _{int} = 0.085
398	Reflections with <i>I</i> > 2 σ <i>I</i>	3559
399	Completeness to $\theta = 27.48^\circ$	98.1%
400	Refinement method	Full-matrix least-squares on <i>F</i> ²
401	Parameter / restraints	459/0
402	GoF	1.052
403	Final <i>R</i> indices [<i>I</i> > 2 σ <i>I</i>]	<i>R</i> ₁ = 0.0553, <i>wR</i> ₂ = 0.1296
404	<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0818, <i>wR</i> ₂ = 0.1469
405	Largest diff. peak/hole	+2.05/-1.37 e \AA^{-3}
406	<i>R</i> _{int} = $\Sigma F_o^2 - F_c^2(\text{mean}) /\Sigma[F_o^2]$. GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. <i>R</i> ₁ = $\Sigma F_o - F_c /\Sigma F_o $.	
407	<i>wR</i> ₂ = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where <i>a</i> is 0.057, <i>b</i> is 98.855	
408	and <i>P</i> is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.	

409 Table 4. Atom coordinates and displacement parameters (\AA^2) for meyrowitzite.
 410

411		x/a	y/b	z/c	U_{eq}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
412	Ca1	0.7593(4)	0.3457(2)	0.7368(2)	0.0290(10)	0.036(3)	0.019(2)	0.030(2)	0.0017(18)	0.0074(19)	0.0002(18)
413	Ca2	0.6749(4)	0.5508(2)	0.4255(2)	0.0331(10)	0.046(3)	0.018(2)	0.039(2)	0.0028(19)	0.019(2)	0.0009(19)
414	Ca3	0.1484(5)	0.1091(3)	0.6308(3)	0.0581(14)	0.075(4)	0.030(3)	0.080(4)	-0.001(3)	0.040(3)	0.005(3)
415	U1	0.60111(7)	0.34393(4)	0.52659(4)	0.0276(2)	0.0375(5)	0.0153(4)	0.0270(4)	0.0009(3)	0.0054(4)	-0.0003(3)
416	U2	0.05568(7)	0.33897(5)	0.68741(5)	0.0377(3)	0.0420(6)	0.0198(4)	0.0570(6)	-0.0047(4)	0.0237(4)	-0.0035(4)
417	U3	0.76212(6)	0.59814(4)	0.74902(4)	0.0262(2)	0.0357(5)	0.0129(4)	0.0273(4)	-0.0021(3)	0.0056(3)	0.0001(3)
418	C1	0.5974(16)	0.1959(12)	0.6060(10)	0.028(5)	0.031(13)	0.025(12)	0.023(11)	0.015(10)	0.000(9)	-0.018(9)
419	C2	0.5142(19)	0.6277(15)	0.6177(11)	0.042(6)	0.044(15)	0.049(15)	0.027(13)	-0.015(12)	0.001(11)	-0.002(12)
420	C3	0.7143(18)	0.4874(12)	0.6019(11)	0.035(5)	0.037(14)	0.020(12)	0.034(13)	-0.008(11)	-0.012(10)	0.006(10)
421	C4	0.9818(18)	0.4932(12)	0.7280(10)	0.031(5)	0.033(14)	0.028(13)	0.032(12)	0.001(10)	0.008(10)	-0.012(10)
422	C5	0.253(2)	0.3137(14)	0.6425(13)	0.051(7)	0.058(18)	0.033(14)	0.068(17)	-0.010(12)	0.027(14)	-0.020(13)
423	C6	0.5804(19)	0.6933(13)	0.8124(12)	0.040(6)	0.033(15)	0.026(13)	0.059(15)	-0.006(11)	0.012(12)	0.006(11)
424	O1	0.8909(12)	0.6293(7)	0.8609(7)	0.039(4)	0.059(10)	0.008(7)	0.041(8)	-0.013(6)	0.003(7)	0.014(6)
425	O2	0.5428(13)	0.2016(8)	0.5410(7)	0.042(4)	0.066(11)	0.020(7)	0.035(9)	0.001(7)	0.009(8)	-0.014(7)
426	O3	0.6485(12)	0.2641(7)	0.6336(6)	0.036(4)	0.058(10)	0.016(7)	0.024(7)	0.016(6)	-0.004(7)	-0.005(7)
427	O4	0.5196(13)	0.6974(8)	0.5892(7)	0.040(4)	0.060(11)	0.025(8)	0.030(8)	0.003(7)	0.005(7)	-0.012(7)
428	O5	0.5694(10)	0.6083(8)	0.6814(7)	0.034(3)	0.016(7)	0.030(8)	0.047(9)	0.015(7)	-0.002(7)	-0.008(6)
429	O6	0.4405(12)	0.5750(8)	0.5799(6)	0.035(3)	0.043(9)	0.029(8)	0.028(8)	0.004(7)	0.003(7)	-0.008(7)
430	O7	0.7502(12)	0.5550(7)	0.6335(6)	0.034(3)	0.062(10)	0.009(7)	0.029(7)	-0.002(6)	0.013(7)	0.002(6)
431	O8	0.6969(12)	0.4220(8)	0.6329(6)	0.036(4)	0.068(11)	0.014(7)	0.020(7)	-0.006(6)	0.006(7)	-0.024(7)
432	O9	0.6874(12)	0.4815(8)	0.5351(6)	0.034(3)	0.054(10)	0.024(7)	0.022(8)	-0.010(6)	0.008(7)	-0.003(7)
433	O10	0.0716(13)	0.4899(8)	0.7085(8)	0.047(4)	0.051(11)	0.025(8)	0.069(11)	-0.009(7)	0.024(9)	-0.005(7)
434	O11	0.9489(12)	0.5639(8)	0.7482(8)	0.042(4)	0.044(10)	0.011(7)	0.070(11)	0.003(7)	0.014(8)	0.009(6)
435	O12	0.9290(12)	0.4250(8)	0.7304(8)	0.044(4)	0.045(10)	0.023(8)	0.071(11)	-0.009(8)	0.029(8)	0.005(7)
436	O13	1.3390(14)	0.3058(9)	0.6225(8)	0.052(4)	0.056(11)	0.035(9)	0.079(12)	0.018(8)	0.041(10)	0.010(8)
437	O14	0.1918(13)	0.2544(9)	0.6539(9)	0.052(4)	0.046(10)	0.033(9)	0.095(13)	-0.006(9)	0.048(10)	-0.003(8)
438	O15	0.2133(13)	0.3884(8)	0.6514(8)	0.045(4)	0.056(10)	0.014(7)	0.077(11)	-0.001(7)	0.039(9)	0.002(7)
439	O16	0.6442(12)	0.6321(8)	0.8209(7)	0.037(4)	0.039(9)	0.025(8)	0.051(9)	0.006(7)	0.022(7)	0.010(7)
440	O17	0.9005(12)	0.2643(8)	0.7108(8)	0.045(4)	0.043(10)	0.025(9)	0.074(11)	-0.015(8)	0.031(8)	-0.013(7)
441	O18	0.0126(13)	0.1893(8)	0.6706(9)	0.050(4)	0.036(10)	0.020(8)	0.104(13)	-0.010(8)	0.036(9)	-0.013(7)
442	O19	0.7239(12)	0.3057(8)	0.5103(7)	0.038(4)	0.040(9)	0.031(8)	0.041(8)	-0.015(7)	0.007(7)	-0.008(7)

443	O20	0.4758(12)	0.3843(9)	0.5419(7)	0.041(4)	0.047(10)	0.041(9)	0.034(8)	0.005(7)	0.014(7)	-0.001(7)
444	O21	0.1367(14)	0.3260(8)	0.7743(8)	0.052(4)	0.068(12)	0.017(8)	0.076(11)	-0.008(8)	0.032(9)	0.001(7)
445	O22	0.9722(14)	0.3546(9)	0.5997(8)	0.052(4)	0.063(12)	0.036(9)	0.057(10)	-0.007(8)	0.020(9)	-0.016(8)
446	O23	0.7814(12)	0.7007(7)	0.7220(7)	0.038(4)	0.056(10)	0.009(7)	0.047(9)	0.005(6)	0.011(8)	0.005(6)
447	O24	0.7443(11)	0.4941(7)	0.7771(6)	0.026(3)	0.039(9)	0.011(6)	0.021(7)	-0.002(5)	0.000(6)	0.001(6)
448	OW1	0.8697(14)	0.3414(8)	0.8553(7)	0.050(4)	0.077(12)	0.021(8)	0.044(9)	-0.005(7)	0.008(8)	0.014(8)
449	OW2	0.4310(12)	0.4793(9)	0.6980(7)	0.039(4)	0.034(9)	0.042(9)	0.043(9)	-0.003(7)	0.015(7)	-0.006(7)
450	OW3	0.5835(14)	0.3514(9)	0.7589(9)	0.060(5)	0.056(11)	0.037(9)	0.097(13)	0.013(9)	0.040(10)	0.004(8)
451	OW4	0.7873(15)	0.6445(10)	0.5215(9)	0.069(5)	0.065(13)	0.047(10)	0.076(12)	0.014(9)	-0.005(10)	-0.026(9)
452	OW5	0.2297(14)	0.0784(11)	0.7529(9)	0.071(5)	0.058(12)	0.073(13)	0.091(14)	0.030(11)	0.034(10)	0.017(10)
453	OW6	0.3441(18)	0.1329(14)	0.6280(13)	0.102(8)	0.089(17)	0.094(16)	0.15(2)	-0.015(15)	0.082(16)	0.000(13)
454	OW7	0.981(2)	0.0218(13)	0.6179(14)	0.116(9)	0.099(18)	0.075(14)	0.19(3)	-0.056(16)	0.074(17)	-0.031(13)
455	OW8	0.832(2)	0.4624(15)	0.4427(15)	0.130(9)	0.11(2)	0.100(18)	0.18(3)	-0.006(18)	0.032(18)	0.043(16)
456	OW9	0.225(3)	-0.0284(16)	0.6251(17)	0.162(12)	0.21(3)	0.082(18)	0.21(3)	-0.031(19)	0.08(3)	0.05(2)
457	OW10	0.455(3)	0.2152(16)	0.7872(19)	0.166(13)	0.15(3)	0.080(18)	0.29(4)	0.00(2)	0.10(3)	-0.014(18)
458	OW11	0.241(4)	0.1914(18)	0.8534(16)	0.193(16)	0.31(5)	0.10(2)	0.14(3)	0.027(19)	0.02(3)	0.08(3)
459	OW12	0.505(3)	0.0168(16)	0.4186(17)	0.199(18)	0.24(4)	0.086(19)	0.18(3)	0.00(2)	-0.07(3)	-0.05(2)
460	OW13	0.290(3)	0.1861(15)	0.4748(15)	0.141(11)	0.21(3)	0.079(17)	0.16(3)	-0.001(17)	0.10(2)	-0.019(18)
461	OW14*	0.966(5)	0.325(3)	0.465(3)	0.127(18)						
462	OW15*	0.011(7)	0.186(5)	0.517(4)	0.21(3)						
463	OW16*	0.101(5)	0.128(4)	0.514(3)	0.14(2)						
464	OW17*	0.046(7)	0.160(5)	0.374(4)	0.20(3)						

465 * 0.5 assigned occupancy.

466 Table 5. Selected bond distances (Å) for meyrowitzite.

467	Ca1–O8	2.345(13)	Ca2–OW8	2.35(2)	Ca3–OW16	2.27(5)
468	Ca1–OW3	2.351(16)	Ca2–O20	2.396(15)	Ca3–OW5	2.409(18)
469	Ca1–OW1	2.362(15)	Ca2–O9	2.435(13)	Ca3–O14	2.412(15)
470	Ca1–O17	2.365(15)	Ca2–O6	2.461(14)	Ca3–OW9	2.43(2)
471	Ca1–O3	2.489(13)	Ca2–OW2	2.482(14)	Ca3–O18	2.439(16)
472	Ca1–O12	2.494(15)	Ca2–O13	2.487(15)	Ca3–OW7	2.45(2)
473	Ca1–O24	2.546(12)	Ca2–OW4	2.512(17)	Ca3–OW6	2.47(2)
474	Ca1–O23	2.575(13)	Ca2–O15	2.565(14)	Ca3–OW15	2.81(8)
475	<Ca1–O>	2.441	<Ca2–O>	2.461	<Ca3–O>	2.461
476						
477	U1–O19	1.760(14)	U2–O21	1.745(17)	U3–O23	1.775(12)
478	U1–O20	1.792(14)	U2–O22	1.773(16)	U3–O24	1.801(11)
479	U1–O3	2.422(11)	U2–O15	2.412(14)	U3–O5	2.366(12)
480	U1–O6	2.428(12)	U2–O14	2.415(14)	U3–O11	2.382(14)
481	U1–O9	2.440(13)	U2–O17	2.430(13)	U3–O1	2.385(13)
482	U1–O2	2.444(13)	U2–O12	2.438(13)	U3–O7	2.388(12)
483	U1–O4	2.448(13)	U2–O10	2.463(13)	U3–O16	2.410(13)
484	U1–O8	2.454(11)	U2–O18	2.467(13)	<U3–O _{Ur} >	1.788
485	<U1–O _{Ur} >	1.776	<U2–O _{Ur} >	1.759	<U3–O _{eq} >	2.386
486	<U1–O _{eq} >	2.439	<U2–O _{eq} >	2.438		
487						
488	C1–O1	1.25(2)	C2–O4	1.27(3)	C3–O7	1.27(2)
489	C1–O2	1.28(2)	C2–O5	1.29(2)	C3–O8	1.27(2)
490	C1–O3	1.30(2)	C2–O6	1.31(2)	C3–O9	1.29(2)
491	<C1–O>	1.28	<C2–O>	1.29	<C3–O>	1.28
492						
493	C4–O12	1.29(2)	C5–O13	1.25(3)	C6–O16	1.24(2)
494	C4–O10	1.29(2)	C5–O14	1.28(3)	C6–O17	1.28(2)
495	C4–O11	1.31(2)	C5–O15	1.33(3)	C6–O18	1.30(3)
496	<C4–O>	1.30	<C5–O>	1.29	<C6–O>	1.27

497

498

499

500 Table 6. Bond-valence analysis for meyrowitzite. Values are expressed in valence units.*
 501

	Ca1	Ca2	Ca3	U1	U2	U3	C1	C2	C3	C4	C5	C6	H bonds	Σ
O1						0.53	1.46						0.18	2.17
O2				0.47			1.35						0.13	1.94
O3	0.23			0.49			1.28							1.99
O4				0.47				1.38					0.20	2.05
O5						0.55		1.31					0.19	2.05
O6		0.24		0.48				1.24						1.97
O7						0.52			1.38				0.17	2.08
O8	0.34			0.46					1.38					2.18
O9		0.26		0.47					1.31					2.05
O10					0.45					1.31			0.21	1.97
O11						0.53				1.31			0.16	1.99
O12	0.22				0.47					1.24				1.94
O13		0.23									1.46		0.19	1.88
O14			0.28		0.50						1.35			2.12
O15		0.18			0.50						1.18		0.13	1.99
O16						0.50						1.50		2.00
O17	0.32				0.48								1.35	2.15
O18			0.26		0.45								1.28	1.98
O19				1.75										1.75
O20		0.29		1.65										1.94
O21					1.80								0.20	2.00
O22					1.71								0.11	1.81
O23	0.18					1.70							0.15	2.03
O24	0.19					1.62							0.13	1.94
OW1	0.32													
OW2		0.23												
OW3	0.33													
OW4		0.21												
OW5			0.28											
OW6			0.24											
OW7			0.25											
OW8		0.33												
OW9			0.27											
OW15			0.05											
OW16			0.21											
Σ	2.13	1.98	1.84	6.24	6.36	5.94	4.08	3.93	4.08	3.86	3.98	4.12		

502 * Cation–O bond valence parameters are from Gagné and Hawthorne (2015). BVS to OW sites
 503 are not included, but hydrogen bond contributions to other O sites are included. Hydrogen-bond
 504 strengths based on O–O bond lengths from Ferraris and Ivaldi (1988). The isolated OW sites are
 505 not included.

506
 507

508 Table 7. Comparative data for meyrowitzite and zellerite.
 509

510		Meyrowitzite	Zellerite
511	Ideal formula	Ca(UO ₂)(CO ₃) ₂ ·5H ₂ O	Ca(UO ₂)(CO ₃) ₂ ·5H ₂ O
512	Space group	<i>P2₁/n</i>	<i>Pmn2₁</i> or <i>Pmnm</i> (probable)
513	<i>a</i> (Å)	12.376(3)	11.220(15)
514	<i>b</i> (Å)	16.0867(14)	19.252(16)
515	<i>c</i> (Å)	20.1340(17)	4.933(16)
516	β (°)	107.679(13)	
517	<i>V</i> (Å ³)	3819.3(12)	1065(2)
518	<i>Z</i>	12	4
519	Density _{meas.} (g·cm ⁻³)	2.70(2)	3.25(1)
520	Optical character	biaxial (+)	biaxial (+)
521	α	1.520(2)	1.536(5)
522	β	1.528(2)	1.559(5)
523	γ	1.561(2)	1.697(5)
524	<i>2V</i> (°)	53.0(6)	30–40
525	Reference	This study	Coleman <i>et al.</i> , 1966

Figure 1



Figure 2

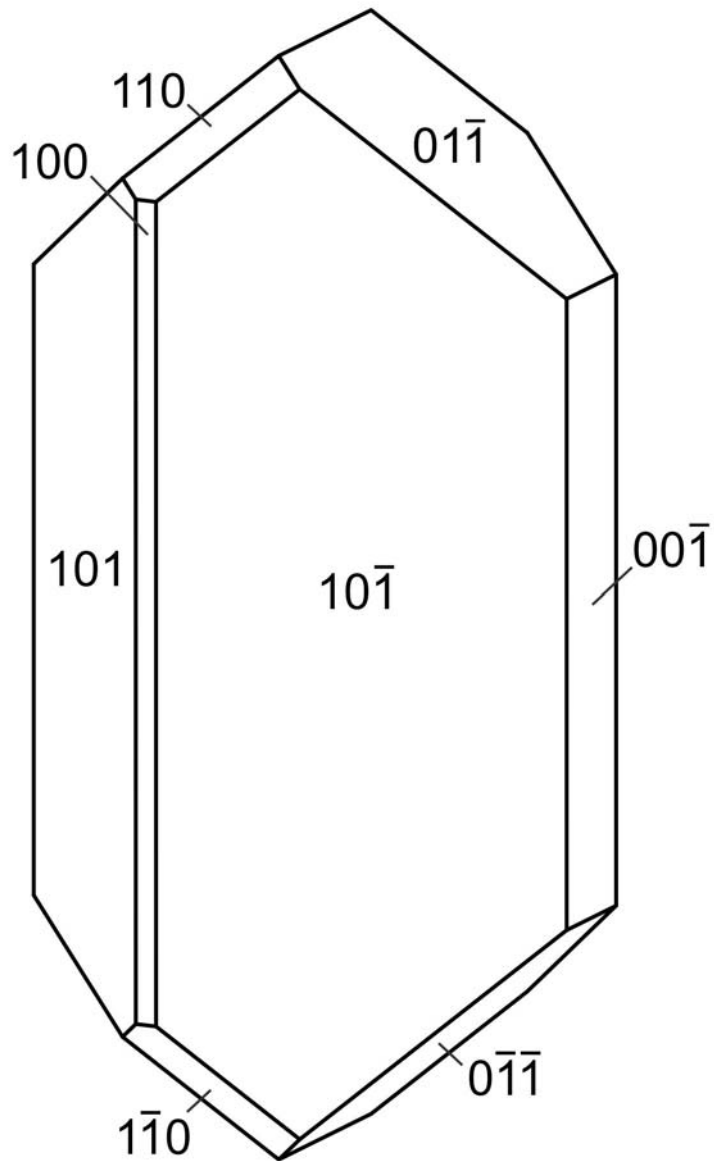


Figure 3

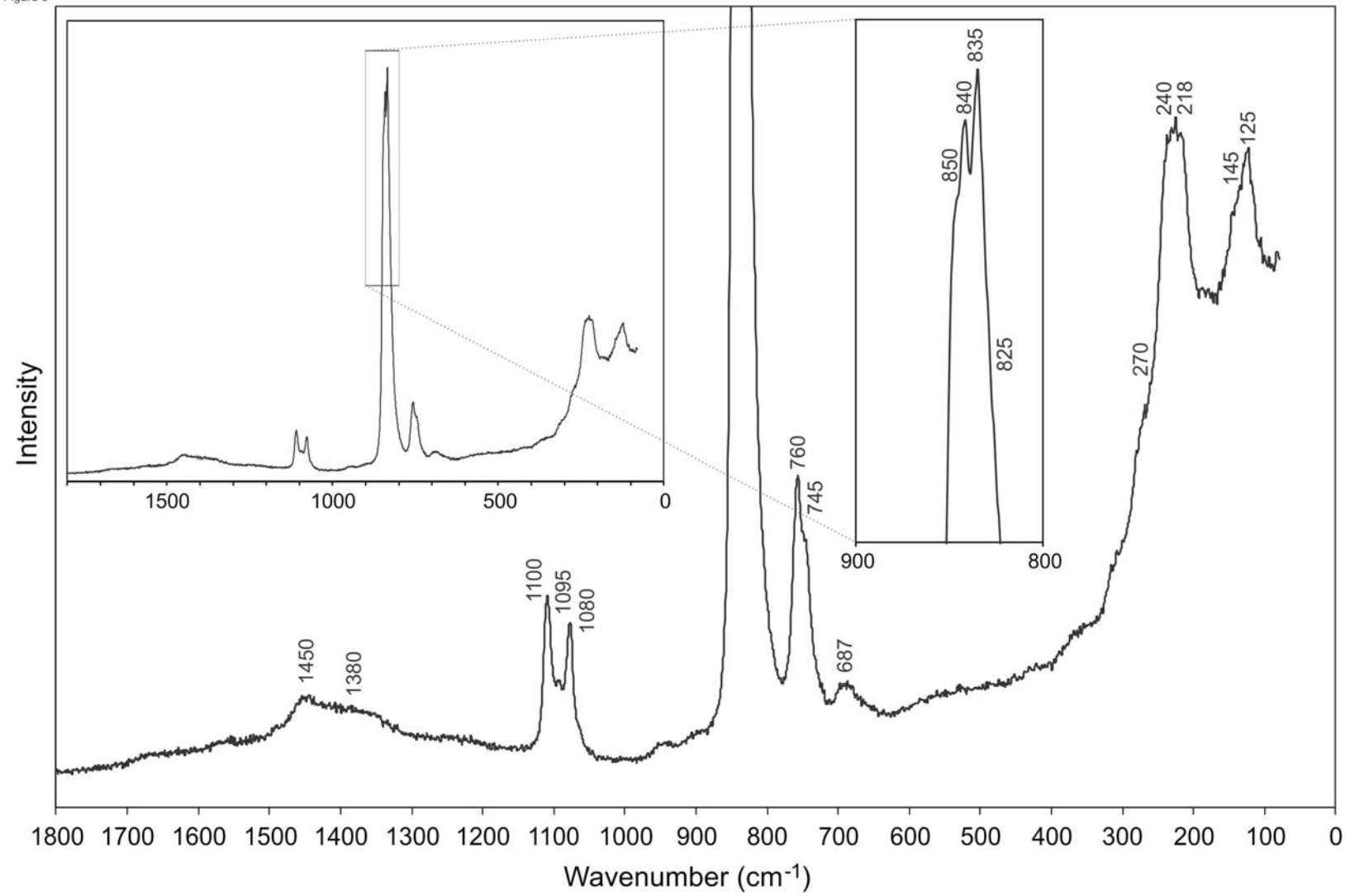


Figure 4

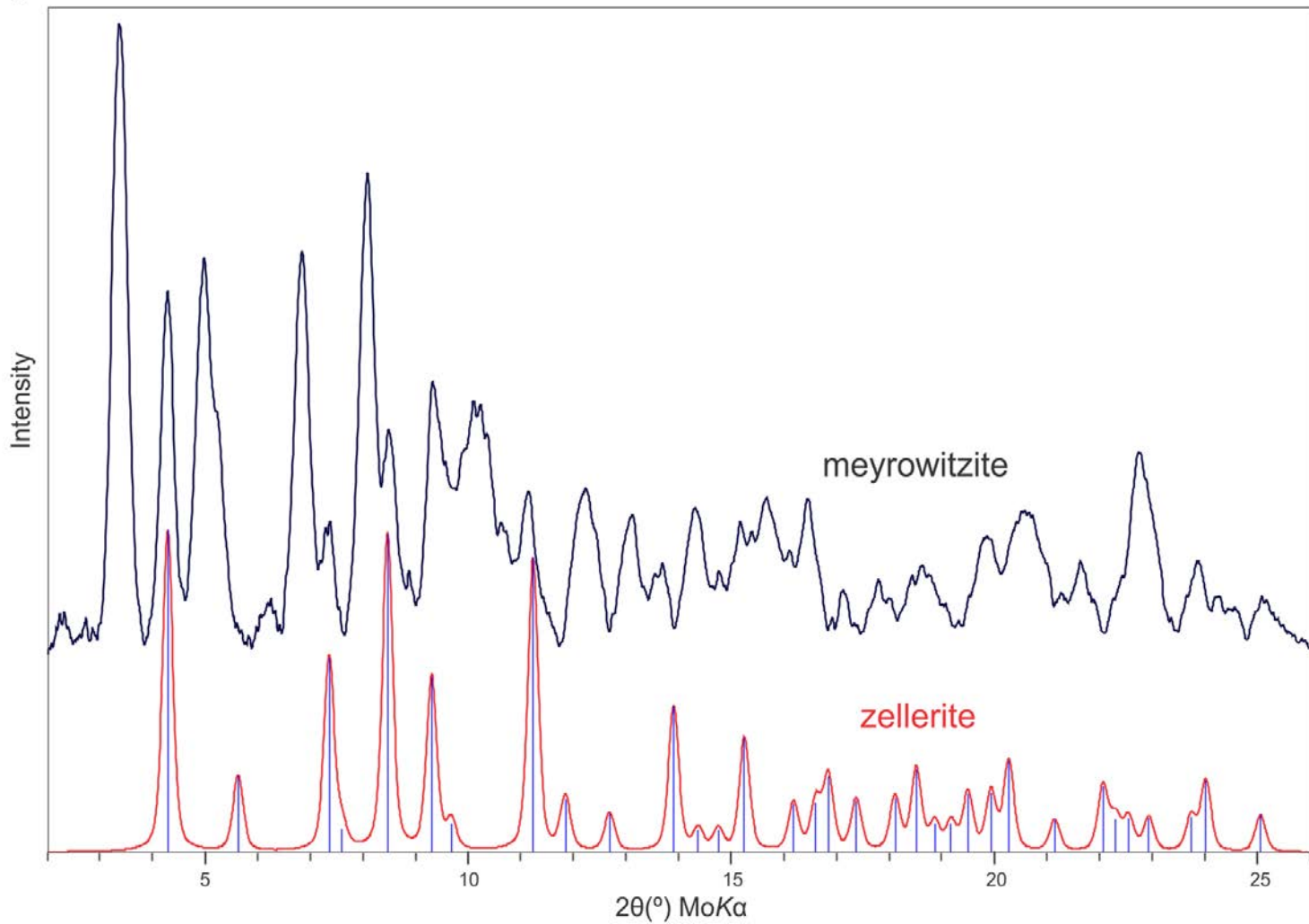


Figure 5

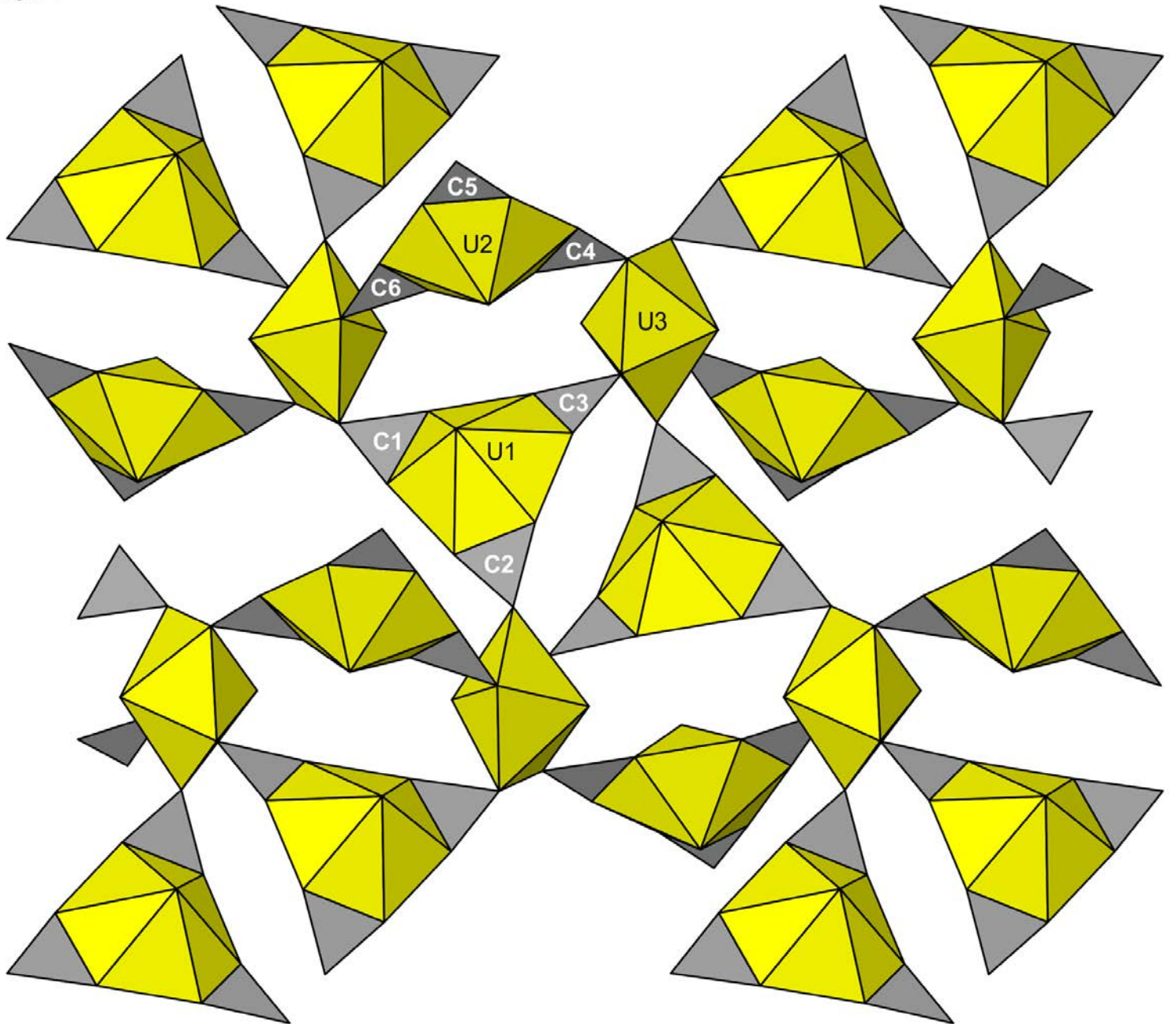


Figure 6

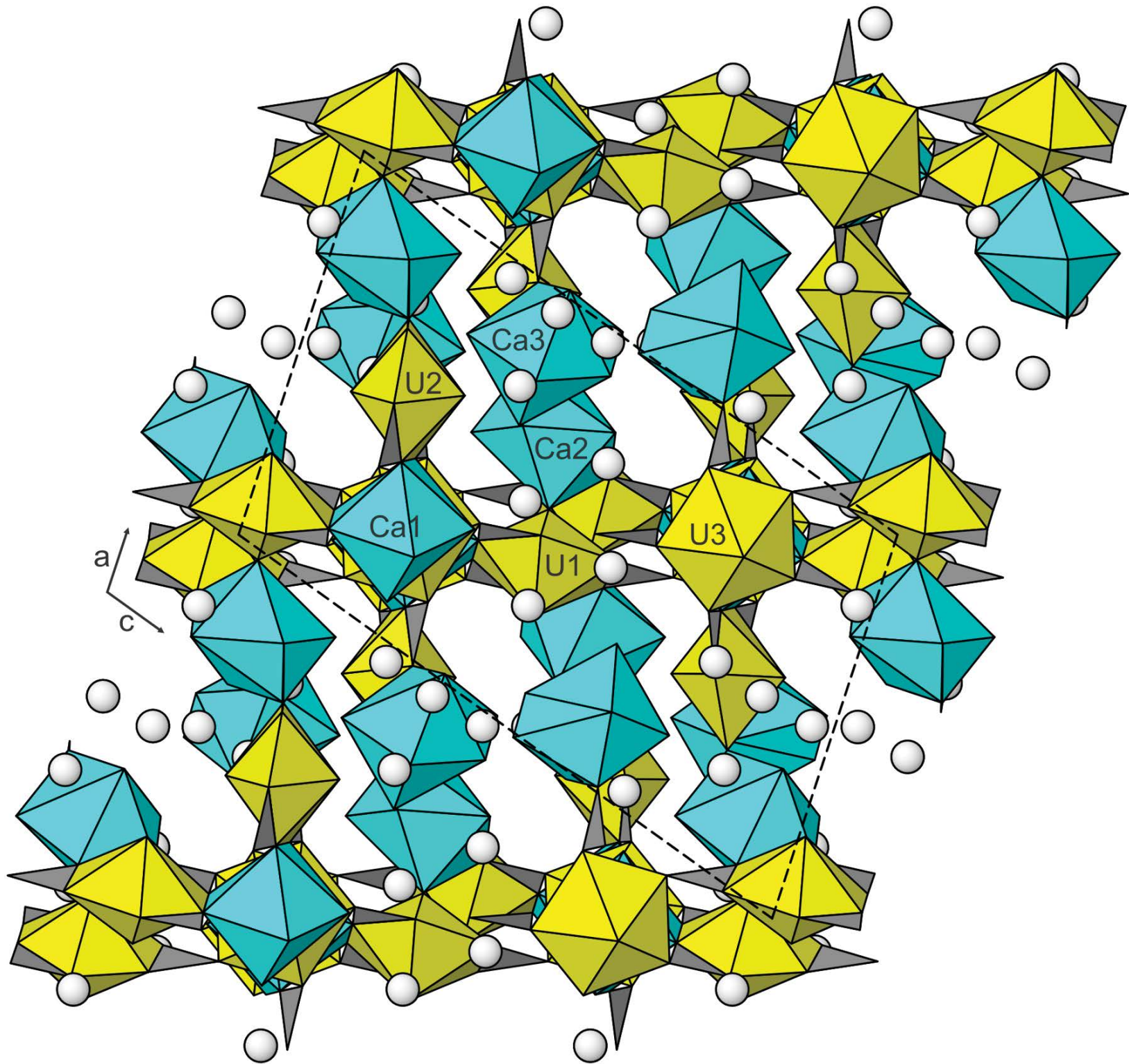


Figure 7

