

Shumwayite, $[(\text{UO}_2)(\text{SO}_4)(\text{H}_2\text{O})_2]_2 \cdot \text{H}_2\text{O}$, a new uranyl sulfate mineral from Red Canyon, San Juan County, Utah, USA

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ABSTRACT

The new mineral shumwayite (IMA2015-058), $[(\text{UO}_2)(\text{SO}_4)(\text{H}_2\text{O})_2]_2 \cdot \text{H}_2\text{O}$, was found in the Green Lizard and Giveaway-Simplot mines, White Canyon district, San Juan County, Utah, USA, where it occurs as a secondary alteration phase. At the Green Lizard mine, it is found in association with calcite, gypsum, plášilite, pyrite, rozenite and sulfur; at the Giveaway-Simplot mine, shumwayite is associated with rhomboclase and römerite. The mineral occurs as pale greenish-yellow monoclinic prisms, elongated on [100], up to ~0.3 mm long and commonly in subparallel to random intergrowths. The mineral is transparent with a vitreous lustre and has a white streak. It fluoresces bright greenish white under both longwave and shortwave ultraviolet radiation. The Mohs hardness is ~2. Crystals are brittle with perfect {011} cleavage and irregular fracture. The mineral is slightly deliquescent and is easily soluble in room temperature H_2O . The calculated density is 3.844 g cm^{-3} . Optically, shumwayite is biaxial (+/-), with $\alpha = 1.581(1)$, $\beta = 1.588(1)$, $\gamma = 1.595(1)$ (measured in white light). The measured $2V_x$ based on extinction data collected on a spindle stage is $89.8(8)^\circ$; the calculated $2V_x$ is 89.6° . Dispersion is strong, but the sense is not defined because the optic sign is ambiguous. No pleochroism was observed. The optical orientation is $X = \mathbf{b}$, $Y \approx \mathbf{c}$, $Z \approx \mathbf{a}$. Energy-dispersive spectrometer analyses (with H_2O based on the crystal structure) yielded the empirical formula $\text{U}_{2.01}\text{S}_{1.99}\text{O}_{12.00} \cdot 5\text{H}_2\text{O}$. Shumwayite is monoclinic, $P2_1/c$, $a = 6.74747(15)$, $b = 12.5026(3)$, $c = 16.9032(12) \text{ \AA}$, $\beta = 90.919(6)^\circ$, $V = 1425.79(11) \text{ \AA}^3$ and $Z = 4$. The crystal structure ($R_1 = 1.88\%$ for $2936 F > 4\sigma F$) contains UO_7 pentagonal bipyramids and SO_4 tetrahedra that link by corner-sharing to form $[(\text{UO}_2)(\text{SO}_4)(\text{H}_2\text{O})_2]$ chains along [100]. The chains and isolated H_2O groups between them are linked together only by hydrogen bonds. The mineral is named in honour of the Shumway family, whose members account for the discovery and mining of hundreds of uranium deposits on the Colorado Plateau, including the Green Lizard mine.

KEYWORDS: shumwayite, new mineral, uranyl sulfate, crystal structure, infrared and Raman spectroscopy, Green Lizard mine, Giveaway-Simplot mine, Red Canyon, White Canyon district, Utah, USA.

Introduction

THERE are numerous uranium mines and prospects in the White Canyon mining district of south-eastern Utah, USA (Chenoweth, 1993). Mineralization in the district was first recognized

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in the 1880s when gold seekers noted copper-bearing rocks in the lower part of White Canyon. The uranium mineralization was observed in the summer of 1898 by John Wetherill, while leading an archaeological expedition into Red Canyon. He noted yellow stains around a petrified tree at a site in Red Canyon. At that spot, he built a rock monument, in which he placed a piece of paper to claim the minerals. Wetherill probably did not know that the yellow stains represented uranium mineralization and, in any event, there was no market for uranium at that time. He did not pursue his discovery and did not share knowledge of it until 1943 when he described the spot to Preston V. Redd of Blanding, Utah, who went to the site, found Wetherill's monument and claimed the area as the Blue Lizard claim (Shumway, 1970). In 1920, uranium associated with copper mineralization was identified in the district, but uranium production did not begin until 1949. The peak years for uranium mining in the district were 1955 to 1961 and there was a second boom period between 1971 and 1979, after which the collapse of the uranium market resulted in the closing of all mines in the district. The only recent uranium mining activity occurred in 2012 at the Daneros mine in the Red Canyon area of the district.

Our interest in the minerals of the White Canyon mining district began several years ago with the collecting of minerals occurring in efflorescent crusts on the surfaces of mine walls of the long-inactive Blue Lizard mine. This has led to the description of numerous new mineral species, most of which are uranyl sulfates (*cf.* Kampf *et al.*, 2015*b*). Our efforts have now expanded to include similar mineralized areas in surrounding mines in

the Red Canyon area of the district. The new mineral shumwayite, described herein, was found in both the Green Lizard mine and the Giveaway-Simplot mine, both of which are in the vicinity of the Blue Lizard mine.

Shumwayite (*'sh\^m wei att'*) is named in honour of the Shumway family. Members of the family were involved in prospecting for uranium properties beginning in the early days and later became active miners. Family members account for the discovery and mining of hundreds of uranium deposits on the Colorado Plateau. Arah E. Shumway (1891–1968) prospected Red Canyon during the 1920s and was one of the first to stake mining claims and mine for uranium. Dan Shumway (b. 1946) was one of the claim stakers for the Green Lizard mine at which shumwayite was first recognized. Dr. Gary L. Shumway (b. 1938), Professor Emeritus of history at the University of California, Fullerton, is well-known for his research and publications on uranium mining and exploration. Both Dan and Gary Shumway have given permission on behalf of the Shumway family for the mineral to be named in its honour.

The new mineral and its name was approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA2015-058, Kampf *et al.*, 2015*c*). The description is based on five cotype specimens. Four cotypes are deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue numbers 65589 and 65590 from the Green Lizard mine and 65591 and 65592 from the Giveaway-Simplot mine. One cotype specimen from the Green



FIG. 1. Shumwayite on asphaltum from the Giveaway-Simplot mine; field of view: 1 mm.

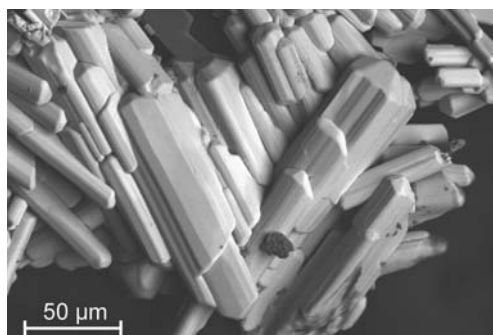


FIG. 2. Back-scatter SEM image of shumwayite from the Giveaway-Simplot mine.

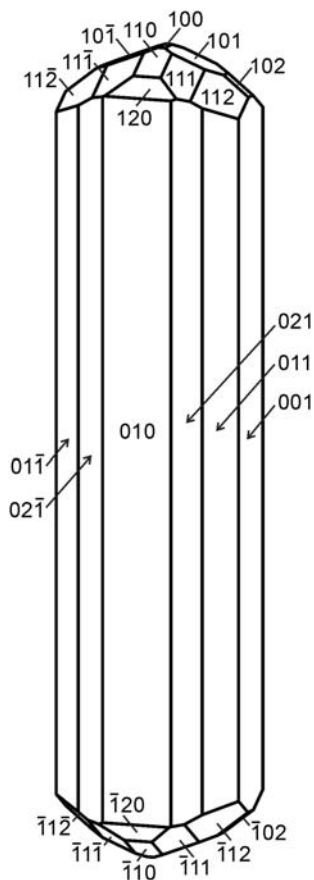


FIG. 3. Crystal drawing of shumwayite; clinographic projection in nonstandard orientation, a vertical.

Lizard mine is housed in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, registration number 4741/1.

Occurrence

Shumwayite was first discovered on specimens collected underground in the Green Lizard mine (37°34'37.10"N 110°17'52.80"W). Later it was identified on specimens collected underground in the Giveaway-Simplot mine (37°33'09.80"N 110°16'58.50"W), ~3 km SSE of the Green Lizard mine. These mines should both be considered type localities for the mineral. Both mines are in the White Canyon mining district, San Juan County, Utah, USA. The Green Lizard mine is near the head

of Low Canyon on the east side of Red Canyon, 2.1 km north of the Blue Lizard mine. The Giveaway-Simplot mine is on the east side of Red Canyon, 1.4 km SE of the Blue Lizard mine. The geology of these deposits is similar to that of the Blue Lizard mine (Kampf *et al.*, 2015b; Chenoweth, 1993).

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

Shumwayite is a relatively rare mineral in the secondary uranyl sulfate mineral assemblages at the Green Lizard and Giveaway-Simplot mines. At the Green Lizard mine, it is usually found on sandstone and is associated with calcite, gypsum, plášilite, pyrite, rozenite and sulfur. Other secondary minerals thus far found in the Green Lizard mine assemblage include beshtautite, boussingaultite, fermiite, johannite, natrozippeite, oppenheimerite, wetherillite and several other potentially new uranyl sulfate minerals, currently under study. At the Giveaway-Simplot mine, shumwayite is usually found on asphaltum and is associated with rietveldite (Kampf *et al.*, 2016), rhomboclase and römerite.

Uranyl sulfate minerals typically form by hydration–oxidation weathering of primary uranium minerals, mainly uraninite, by acidic solutions derived from the decomposition of associated sulfides (Finch and Murakami, 1999; Krivovichev and Plášil, 2013; Plášil, 2014). Shumwayite and other secondary minerals occurring in the efflorescent crusts of the Green Lizard and Giveaway-Simplot mines have formed by such a process. It is worth noting that the calcite found in association with shumwayite at the Green Lizard mine is embedded in the matrix and appears to be a remnant of earlier mineralization.

Physical and optical properties

Shumwayite forms pale greenish-yellow monoclinic prisms, often irregular and more or less rounded, up to ~0.3 mm long. Crystals commonly occur in subparallel to random intergrowths (Figs 1

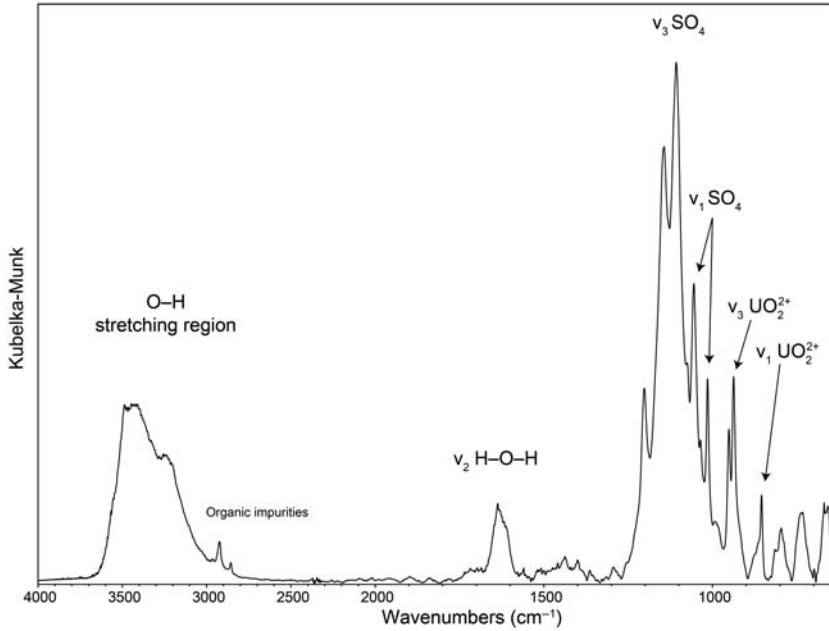


FIG. 4. Infrared (micro-DRIFTS) spectrum of shumwayite.

and 2). Prisms are elongated on [100]. The prism forms include {010}, {001}, {011}, {012} and {021}. The forms composing the complex

terminations could not be measured because of their small sizes; however, based upon scanning electron microscope (SEM) images (i.e. Fig. 2), the

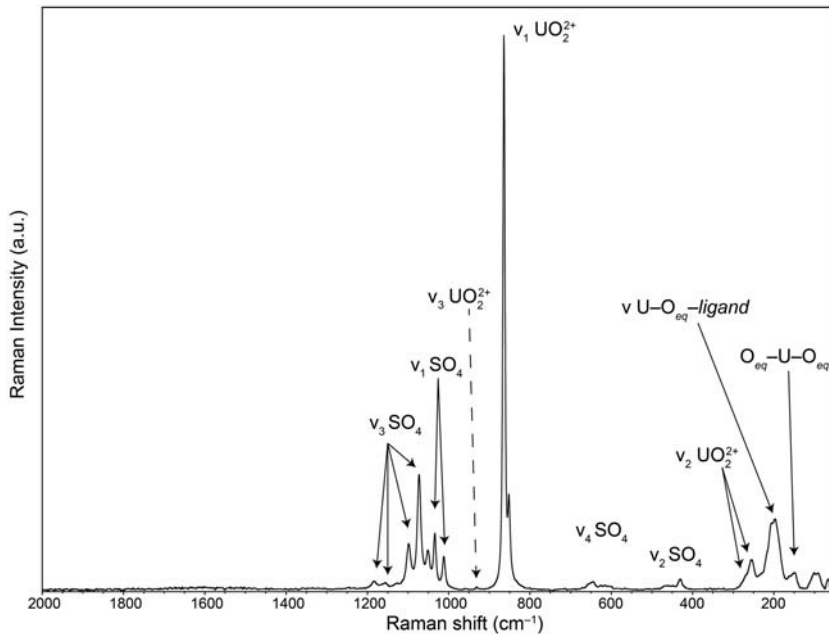


FIG. 5. Raman spectrum of shumwayite.

SHUMWAYITE, A NEW URANYL SULFATE FROM RED CANYON, UTAH, USA

TABLE I. Powder X-ray data (d in Å) for shumwayite. Only calculated lines with $I \geq 2$ are listed.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl
6	10.01	10.0513	4	0 1 1	23	2.602	2.6112	8	2 2 3	5	1.8664	1.8689	3	0 6 4
2	8.32	8.4505	3	0 0 2			2.5959	10	2 3 1			1.8591	2	3 3 3
39	6.97	7.0013	53	0 1 2			2.5861	9	2 3 1			1.8571	4	0 1 9
26	5.88	5.9373	21	1 1 0	30	2.528	2.5590	3	1 1 6	23	1.7944	1.8210	3	2 5 4
		5.8631	15	0 2 1			2.5401	20	1 4 3			1.8070	14	1 5 6
48	5.58	5.6266	27	1 1 1	7	2.438	2.5312	4	1 1 6	24	1.7332	1.8059	4	3 2 5
		5.5772	30	1 1 1			2.5264	17	1 4 3			1.7985	4	0 2 9
		5.3141	12	1 0 2			2.5131	4	2 3 2			1.7971	7	1 5 6
100	5.11	5.2317	8	1 0 2	10	2.347	2.4954	2	2 3 2	20	2.243	2.4736	4	0 5 1
		5.1363	100	0 1 3			2.4569	4	1 3 5			1.7816	3	3 2 5
44	4.86	5.0256	41	0 2 2	20	2.199	2.4453	3	2 2 4	19	1.6409	1.7728	2	2 6 0
		4.8262	27	1 1 2			2.4363	4	1 3 5			1.7647	3	2 6 1
38	4.40	4.4377	22	1 2 1	10	2.347	2.4119	3	1 2 6	24	1.7332	1.7616	2	2 6 1
		4.4133	29	1 2 1			2.3978	4	0 5 2			1.7600	2	2 1 8
5	4.18	4.1850	14	0 2 3	10	2.347	2.3886	4	1 2 6	24	1.7332	1.7475	3	0 7 2
47	4.04	4.0463	59	0 3 1			2.3447	21	1 5 0			1.7433	11	3 4 3
33	3.552	4.0120	10	1 2 2	20	2.243	2.2752	4	2 4 1	24	1.7332	1.7380	3	2 6 2
		3.7377	4	0 3 2			2.2686	7	2 4 1			1.7329	3	2 2 8
		3.6071	12	1 0 4			2.2477	14	1 1 7			1.7321	3	2 6 2
50	3.373	3.5755	4	1 2 3	20	2.199	2.2463	3	2 2 5	20	1.6796	1.7300	8	3 4 3
		3.5554	14	1 0 4			2.2256	7	1 1 7			1.7185	5	3 3 5
		3.5456	17	1 3 0			2.2189	2	2 4 2			1.7120	2	1 6 5
42	3.459	3.5375	4	1 2 3	22	2.141	2.2151	10	2 2 5	19	1.6409	1.7099	2	2 2 8
		3.5006	7	0 2 4			2.2067	2	2 4 2			1.6975	2	3 3 5
		3.4760	12	1 3 1			2.1991	4	3 1 1			1.6930	4	1 7 2
9	3.258	3.4657	34	1 1 4	17	2.0906	2.1965	3	1 3 6	14	1.6023	1.6903	4	1 7 2
		3.4198	19	1 1 4			2.1902	5	3 1 1			1.6867	7	4 0 0
		3.3733	47	2 0 0			2.1794	6	2 0 6			1.6798	2	3 2 6
25	3.066	3.3504	3	0 3 3	9	2.0566	2.1519	6	0 5 4	14	1.6023	1.6721	11	3 5 0
		3.2794	2	1 3 2			2.1495	5	3 1 2			1.6653	5	1 3 9
		3.2631	7	0 1 5			2.1453	9	2 0 6			1.6537	8	1 3 9
17	2.966	3.2597	3	1 3 2	9	2.0029	2.1329	7	3 1 2	11	1.5608	1.6457	4	1 0 10
		3.2568	2	2 1 0			2.1144	3	2 1 6			1.6445	4	3 1 7
		3.1504	3	2 0 2			2.1036	5	3 2 1			1.6397	2	2 6 4
38	2.809	3.1243	8	1 2 4	9	2.0029	2.0958	6	3 2 1	14	1.6023	1.6378	3	2 1 9
		3.0905	4	1 2 4			2.0892	2	0 3 7			1.6333	3	1 0 10
		3.0735	11	0 4 1			2.0844	6	2 3 5			1.6302	3	3 3 6
12	2.718	3.0549	9	2 1 2	21	1.9705	2.0831	6	0 1 8	4	1.5109	1.6295	2	1 6 6
		3.0233	10	2 1 2			2.0681	3	0 6 1			1.6222	2	1 6 6
		2.9734	10	0 2 5			2.0594	7	2 3 5			1.6189	4	3 1 7
9	2.809	2.9671	6	0 3 4	9	2.0029	2.0550	2	1 5 4	14	1.6023	1.6160	2	2 1 9
		2.9310	4	2 2 1			2.0455	4	3 2 2			1.6095	4	4 1 3
		2.9169	4	2 2 1			2.0232	7	0 6 2			1.6036	2	4 2 2
38	2.809	2.8387	15	2 1 3	9	2.0029	2.0060	2	2 4 4	14	1.6023	1.6006	3	1 7 4
		2.8168	13	0 0 6			2.0014	4	0 2 8			1.5972	2	2 2 9
		2.8133	6	2 2 2			1.9985	3	3 0 4			1.5956	6	4 1 3
12	2.718	2.8009	12	2 1 3	9	1.9096	1.9925	3	2 5 1	4	1.5109	1.5944	2	4 2 2
		2.7886	8	2 2 2			1.9816	2	1 1 8			1.5770	4	2 2 9
		2.7480	4	0 1 6			1.9791	7	3 3 0			1.5706	3	1 4 9
9	1.9096	2.7351	7	1 2 5	21	1.9705	1.9735	5	3 1 4	11	1.5608	1.5628	2	0 8 0
		2.7332	3	0 4 3			1.9721	6	3 0 4			1.5609	2	1 4 9
		2.7068	7	1 2 5			1.9480	3	3 1 4			1.5589	3	4 3 1
9	1.9096	2.6832	2	1 4 2	9	1.9096	1.9268	3	1 2 8	4	1.5109	1.5547	2	4 3 1
		2.6418	6	2 2 3			1.9210	2	3 3 2			1.5537	2	2 7 2
		2.6252	3	0 3 5			1.9108	9	0 4 7			1.5250	2	0 1 11
4	1.5109	2.6158	3	2 0 4	21	1.9705	1.8979	2	2 5 3	11	1.5608	1.5169	2	1 8 1
							1.8800	3	1 6 3			1.5084	2	0 7 6
							1.8744	2	1 6 3			1.5065	3	3 2 8

TABLE 2. Data collection and structure refinement details for shumwayite.*

Diffraction	Rigaku R-Axis Rapid II
X-ray radiation/power	MoK α ($\lambda = 0.71075$ Å)/50 kV, 40 mA
Temperature	293(2) K
Structural Formula	[(UO ₂)(SO ₄)(H ₂ O) ₂] ₂ ·H ₂ O
Space group	<i>P</i> 2 ₁ / <i>c</i>
Unit cell dimensions	<i>a</i> = 6.74747(15) Å <i>b</i> = 12.5026(3) Å <i>c</i> = 16.9032(12) Å β = 90.919(6)°
<i>V</i>	1425.79(11) Å ³
<i>Z</i>	4
Density (for above formula)	3.831 g cm ⁻³
Absorption coefficient	23.07 mm ⁻¹
<i>F</i> (000)	1448
Crystal size (µm)	60 × 50 × 20
θ range	3.02 to 27.48°
Index ranges	-7 ≤ <i>h</i> ≤ 8, -16 ≤ <i>k</i> ≤ 16, -21 ≤ <i>l</i> ≤ 21
Reflections collected/unique	13,166/3254; <i>R</i> _{int} = 0.032
Reflections with <i>F</i> > 4 σ (<i>F</i>)	2936
Completeness to $\theta = 27.48^\circ$	99.5%
Refinement method	Full-matrix least-squares on <i>F</i> ²
Parameter/restraints	220/15
Goof	1.058
Final <i>R</i> indices [<i>F</i> > 4 σ (<i>F</i>)]	<i>R</i> ₁ = 0.0188, <i>wR</i> ₂ = 0.0341
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0233, <i>wR</i> ₂ = 0.0352
Largest diff. peak/hole	+1.20/-0.68 e Å ⁻³

**R*_{int} = $\Sigma[F_o^2 - F_c^2(\text{mean})]/\Sigma[F_o^2]$. Goof = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. *R*₁ = $\Sigma|F_o| - |F_c|/\Sigma|F_o|$. *wR*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 *a* is 0.0100, *b* is 2.0476 and *P* is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.

forms include various combinations of the following: {100}, {110}, {120}, {101}, {10 $\bar{1}$ }, {102}, {10 $\bar{2}$ }, {111}, {11 $\bar{1}$ }, {112} and {11 $\bar{2}$ } (Fig. 3). No twinning was observed.

Crystals are transparent with a vitreous lustre. The mineral has a white streak. The mineral fluoresces bright greenish white under both long-wave and shortwave ultraviolet radiation. The Mohs hardness is ~2. Crystals are brittle with perfect {011} cleavage and irregular fracture. The mineral is slightly deliquescent and is easily soluble in room temperature H₂O. The density could not be measured because the mineral is soluble in Clerici

solution and there is insufficient material for physical measurement. The calculated density is 3.844 g cm⁻³ based on the empirical formula.

Optically, shumwayite is biaxial (+/-), with $\alpha = 1.581(1)$, $\beta = 1.588(1)$, $\gamma = 1.595(1)$ (measured in white light). The measured 2*V*_x based on extinction data collected on a spindle stage and analysed using *EXCALIBUR* (Gunter *et al.*, 2004) is 89.8(8)°; the calculated 2*V*_x is 89.6°. Dispersion is strong, but the sense is not defined because the optic sign is ambiguous. No pleochroism was observed. The optical orientation is *X* = **b**, *Y* ≈ **c**, *Z* ≈ **a**.

Infrared and Raman spectroscopy

A micro DRIFTS (diffuse reflectance Fourier-transform spectroscopy) of shumwayite was collected on a Nicolet Magna 760 FTIR spectrometer in the spectral range 4000–600 cm⁻¹, at a spectral resolution of 4 cm⁻¹, using an average of 128 scans and Happ–Genzel apodization. The spectrometer was connected to a Spectra Tech InspectIR micro-FTIR accessory. A small quantity of shumwayite crystals was powdered, mixed (diluted) with KBr, and analysed immediately to minimize dehydration effects. The KBr in the sample mixture was also used as a reference. The Raman spectrum was recorded with a Thermo-Scientific DXR Raman microscope interfaced to an Olympus microscope (50× objective) in the spectral region 50–2000 cm⁻¹ with a nominal resolution of ~5 cm⁻¹. The power of the frequency-stabilized single mode diode laser (780 nm) impinging on the sample ranged from 2 to 6 mW. The spectrometer was calibrated with a software-controlled calibration procedure (*Omnice8* software) using multiple neon emission lines (wavelength calibration), multiple polystyrene Raman bands (laser frequency calibration), and standardized white light sources (intensity calibration). Spectral manipulation, such as background correction, was done with *Omnice8* software.

Stretching and bending vibrations of H₂O

Infrared bands (Fig. 4) at 3500 (s), 3425 (s) and 3230 (sh) cm⁻¹ are assigned to the ν O–H stretching vibrations of the H₂O molecules. These wavenumbers are comparable to those observed for synthetic (UO₂)(SO₄)(H₂O)₂·2.5H₂O (3550–3220 cm⁻¹, Vlček *et al.*, 2009). According to the correlation given by Libowitzky (1999), the approximate O–H...O hydrogen bond lengths range between

TABLE 3. Atom coordinates and displacement parameters (\AA^2) for shumwayite.

	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>U_{eq}</i>	<i>U¹¹</i>	<i>U²²</i>	<i>U³³</i>	<i>U²³</i>	<i>U¹³</i>	<i>U¹²</i>
U1	0.25692(2)	0.17170(2)	0.02031(2)	0.01321(4)	0.01191(7)	0.01512(8)	0.01260(8)	-0.00110(6)	0.00009(6)	0.00039(6)
U2	0.75881(2)	0.44918(2)	0.17703(2)	0.01497(5)	0.01300(8)	0.01674(8)	0.01520(9)	-0.00158(6)	0.00103(6)	-0.00113(6)
S1	0.27376(14)	0.33455(8)	0.19398(7)	0.0161(2)	0.0114(4)	0.0174(5)	0.0194(6)	-0.0051(4)	0.0006(4)	-0.0014(4)
S2	0.77636(14)	0.17167(8)	0.10859(6)	0.0142(2)	0.0109(4)	0.0163(5)	0.0155(5)	-0.0021(4)	-0.0006(4)	0.0012(4)
O1	0.0892(5)	0.3943(3)	0.1929(3)	0.0458(11)	0.0147(16)	0.0326(19)	0.090(3)	-0.019(2)	-0.0006(18)	0.0084(14)
O2	0.3330(5)	0.3112(3)	0.2758(19)	0.0334(8)	0.051(2)	0.0347(19)	0.0144(17)	-0.0047(14)	-0.0038(16)	-0.0143(16)
O3	0.4240(4)	0.3992(2)	0.15407(19)	0.0249(7)	0.0191(15)	0.0295(17)	0.0259(19)	-0.0002(14)	-0.0010(13)	-0.0068(13)
O4	0.2452(4)	0.2326(2)	0.15131(18)	0.0206(7)	0.0216(15)	0.0209(15)	0.0194(17)	-0.0073(13)	0.0007(13)	-0.0029(12)
O5	0.8522(5)	0.0783(2)	0.1499(2)	0.0250(7)	0.0285(17)	0.0194(15)	0.0273(19)	0.0010(14)	0.0006(15)	0.0066(13)
O6	0.5834(4)	0.1493(3)	0.0710(2)	0.0270(7)	0.0161(15)	0.0390(19)	0.0259(19)	-0.0103(15)	-0.0038(13)	0.0002(13)
O7	0.7551(4)	0.2605(2)	0.16510(18)	0.0228(7)	0.0281(17)	0.0195(15)	0.0209(17)	-0.0053(13)	0.0051(14)	0.0004(12)
O8	0.9136(4)	0.2047(2)	0.04500(18)	0.0210(7)	0.0149(14)	0.0286(16)	0.0198(17)	0.0030(14)	0.0047(12)	0.0038(12)
O9	0.2854(5)	0.3040(2)	0.9882(2)	0.0256(7)	0.0303(17)	0.0216(16)	0.0251(18)	0.0031(14)	0.0057(14)	-0.0011(13)
O10	0.2198(4)	0.0365(2)	0.04663(19)	0.0208(7)	0.0203(15)	0.0202(15)	0.0218(17)	0.0000(13)	0.0016(13)	0.0005(12)
O11	0.7346(5)	0.4378(2)	0.27979(19)	0.0241(7)	0.0271(17)	0.0282(17)	0.0170(17)	-0.0005(14)	0.0001(13)	-0.0017(13)
O12	0.7898(5)	0.4631(3)	0.0744(2)	0.0306(8)	0.0367(19)	0.0307(18)	0.025(2)	-0.0013(15)	0.0055(15)	-0.0075(15)
OW1	0.0714(5)	0.1370(3)	0.89763(19)	0.0287(8)	0.0378(19)	0.0310(18)	0.0171(18)	-0.0040(15)	-0.0048(16)	-0.0066(16)
H1A	0.100(8)	0.161(3)	0.854(2)	0.034						
H1B	0.056(8)	0.074(2)	0.889(3)	0.034						
OW2	0.5494(5)	0.6070(3)	0.1806(2)	0.0342(9)	0.0283(19)	0.0228(17)	0.051(3)	-0.0060(17)	-0.0134(17)	0.0045(15)
H2A	0.469(7)	0.620(4)	0.147(3)	0.041						
H2B	0.591(7)	0.669(3)	0.193(3)	0.041						
OW3	0.4917(5)	0.1242(3)	0.9163(2)	0.0354(9)	0.036(2)	0.054(2)	0.0158(18)	0.0040(17)	0.0048(16)	0.0249(18)
H3A	0.584(6)	0.088(4)	0.923(3)	0.043						
H3B	0.465(8)	0.130(4)	0.8696(18)	0.043						
OW4	0.9632(4)	0.6064(3)	0.2015(2)	0.0247(7)	0.0220(17)	0.0259(17)	0.0261(19)	-0.0041(15)	-0.0021(14)	-0.0093(14)
H4A	1.037(6)	0.619(4)	0.166(2)	0.030						
H4B	1.025(7)	0.605(4)	0.2428(17)	0.030						
OW5	0.7747(6)	0.3578(3)	0.9181(2)	0.0384(9)	0.040(2)	0.050(2)	0.025(2)	0.0081(18)	-0.0033(17)	0.0002(19)
H5A	0.802(9)	0.405(3)	0.951(3)	0.046						
H5B	0.786(9)	0.303(3)	0.944(3)	0.046						

TABLE 4. Selected bond distances (Å) for shumwayite.

U1-O9	1.753(3)	U2-O11	1.753(3)	S1-O1	1.452(3)	Hydrogen bonds	D-H	H...A	D...A	<DHA
U1-O10	1.767(3)	U2-O12	1.760(3)	S1-O2	1.460(3)	D-H...A	0.82(2)	2.10(4)	2.812(5)	145(5)
U1-O4	2.344(3)	U2-O1	2.344(3)	S1-O3	1.469(3)	OW1-H1a...O2	0.81(3)	2.10(3)	2.858(4)	154(5)
U1-O6	2.368(3)	U2-O7	2.367(3)	S1-O4	1.476(3)	OW1-H1b...O5	0.80(3)	1.98(3)	2.765(5)	167(6)
U1-O8	2.396(3)	U2-O3	2.370(3)	<S1-O>	1.464	OW2-H2a...OW5	0.85(3)	1.92(3)	2.771(5)	176(6)
U1-OW1	2.444(3)	U2-OW2	2.428(3)	S2-O5	1.450(3)	OW2-H2b...O2	0.78(3)	2.10(3)	2.860(4)	165(6)
U1-OW3	2.458(3)	U2-OW4	2.432(3)	S2-O6	1.467(3)	OW3-H3a...O10	0.81(3)	1.95(3)	2.715(5)	157(5)
<U1-O _{ap} >	1.760	<U2-O _{ap} >	1.757	S2-O7	1.474(3)	OW3-H3b...O2	0.80(3)	2.01(3)	2.808(5)	170(5)
<U1-O _{eq} >	2.402	<U2-O _{eq} >	2.388	S2-O8	1.488(3)	OW4-H4a...OW5	0.81(3)	2.22(4)	2.951(5)	149(5)
				<S2-O>	1.470	OW4-H4b...O5	0.82(3)	2.26(4)	3.013(5)	153(5)
						OW5-H5a...O12				
						OW5-H5b...O8				

3.0 and 2.7 Å. Weak bands occurring in the infrared at 2925 and 2845 cm⁻¹ are probably due to organic impurities (C-H stretches).

Infrared bands at 1635 (w) and 1615 (w) cm⁻¹ are attributed to the ν₂ (δ) bending vibrations of structurally non-equivalent H₂O molecules. No corresponding bands are observed in the Raman spectrum, but this is not unusual as H₂O generally provides very weak Raman scattering.

There are weak infrared bands at 1435 and 1400 cm⁻¹, which might be attributable to splitting of the H₂O bending mode (Lane, 2007). Similar bands were observed by Vlček *et al.* (2009) for the synthetic phase. Weak infrared bands at 1365 and 1295 cm⁻¹ may be overtones and/or combination bands (cf., Bullock, 1969; Čejka, 1999).

Stretching and bending vibrations for UO₂²⁺ and SO₂²⁻

Raman bands (Fig. 5) at 1185 (w), 1155 (w), 1100 (ms), 1073 (s), 1050 (ms), and infrared bands at 1202, 1143, 1110 and 1055 cm⁻¹ are assigned to the split triply degenerate ν₃ antisymmetric stretching vibrations of the SO₄ tetrahedra. Raman bands at 1035 (ms) and 1015 (w) cm⁻¹ and an infrared band at 1015 (w) cm⁻¹ are assigned to the ν₁ symmetric stretching vibrations of SO₄ tetrahedra.

A very weak Raman band at 930 cm⁻¹ and infrared bands 951 (s) and 927 (s) cm⁻¹ are attributed to the ν₃ antisymmetric stretching vibration of the uranyl ion, UO₂²⁺. Strong Raman bands at 865 (vs) and 850 (s) cm⁻¹ are attributed to the ν₁ symmetric stretching vibration of the uranyl ion, as are weak infrared bands at 868 and 854 cm⁻¹. The inferred U-O bond lengths (after Bartlett and Cooney, 1989) for the uranyl ion of ~1.76 Å are within the range derived from the X-ray studies for shumwayite and its synthetic analogue ~1.77 Å (Van der Putten and Loopstra, 1974; Vlček *et al.*, 2009).

Weak infrared bands at 810, 795 and 730 cm⁻¹ may be associated with the libration modes of H₂O molecules. Weak Raman bands at 645 and 615 cm⁻¹ and medium-strong infrared bands at 670 and 655 cm⁻¹ are attributed to the ν₄ (δ) triply degenerate antisymmetric stretching vibrations of SO₄ tetrahedra. Weak Raman bands at 470 and 430 cm⁻¹ are related to the split ν₂ (δ) doubly degenerate bending vibrations of the SO₄ tetrahedra.

The assignment of vibrations in the low-energy part of the spectrum is difficult, generally. However, based on reported papers, it can be

inferred that the shoulder at 273 cm^{-1} and a medium-strong band at 255 cm^{-1} are due to $\nu_2(\delta)$ doubly degenerate bending vibrations of the UO_2^{2+} groups (*cf.*, Bullock and Parret, 1970; Ohwada, 1976, Brittain *et al.*, 1985; Plášil *et al.*, 2010). More intense splitting bands at 210 and 200 are assigned to the $\text{U-O}_{\text{eq}}\text{-ligand}$ stretching vibrations (Bullock and Parret, 1970; Plášil *et al.*, 2010). Weak Raman bands at 160 and 150 cm^{-1} are attributed to $-\text{O}_{\text{eq}}-\text{U-O}_{\text{eq}}-$ bending vibrations (Ohwada, 1976). Weak bands at the lowest energies can be assigned to unclassified lattice modes, most probably skeletal vibrations of the infinite chains of polyhedra.

Composition

The composition of shumwayite was determined using a CamScan4D SEM equipped with an Oxford Link ISIS energy-dispersive X-ray spectrometer. An operating voltage of 20 kV was used with a beam current of 3 nA and a $1\text{ }\mu\text{m}$ beam diameter. The energy-dispersive spectroscopy (EDS) mode on the SEM was chosen for the analyses instead of the wavelength-dispersive spectroscopy (WDS) mode on the electron microprobe (EMP) because of the instability of the phase under the electron beam. Attempts to use the WDS mode were unsuccessful because of significant decomposition after several seconds under the electron beam with the higher current necessary for this method. We have found the EDS mode with the stated analytical conditions, including the $1\text{ }\mu\text{m}$ beam diameter, to provide optimal results with similar phases. The standards used were synthetic UO_2 for U and synthetic BaSO_4 for S. The H_2O content was not determined directly because of the scarcity of pure material. Instead, the H_2O content was calculated by stoichiometry on the basis of 17 O apfu and confirmed by the crystal structure refinement. No other elements with atomic numbers higher than 8 were observed. Seven analyses on crystals from the Green Lizard mine gave the following results [average (range) (s.d.)]: UO_3 70.49 (70.06–70.73) (0.25), SO_3 19.45 (18.98–19.90) (0.31), H_2O 11.02 (crystal structure), total 100.96 wt%. The empirical formula (based on 17 O apfu) is $\text{U}_{2.01}\text{S}_{1.99}\text{O}_{12.00}\cdot 5\text{H}_2\text{O}$. The ideal structural formula is $[(\text{UO}_2)(\text{SO}_4)(\text{H}_2\text{O})_2]_2\cdot \text{H}_2\text{O}$, which requires UO_3 69.58, SO_3 19.47 and H_2O 10.95, total 100 wt%.

The Gladstone-Dale compatibility index $1 - (K_p/K_c)$ for the empirical formula is 0.004, in the range of superior compatibility (Mandarino,

2007). As noted by Kampf *et al.* (2015a), Gladstone-Dale calculations for uranyl sulfates should utilize $k(\text{UO}_3)=0.118$, as provided by Mandarino (1976).

X-ray crystallography and structure refinement

The powder X-ray study was carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatized $\text{MoK}\alpha$ radiation ($\lambda=0.71075\text{ \AA}$). A Gandolfi-like motion on the ϕ and ω axes was used to randomize the sample. Observed d -values and intensities were derived by profile fitting using *JADE 2010* software (Materials Data, Inc., California, USA). The powder data presented in Table 1 show good agreement with the pattern calculated from the crystal structure determination. Unit-cell parameters refined from the powder data using *JADE 2010* with whole pattern fitting are: $a=6.726(6)$, $b=12.493(7)$, $c=16.888(7)\text{ \AA}$, $\beta=91.01(4)^\circ$ and $V=1418.8(16)\text{ \AA}^3$.

The single-crystal reflection data for a crystal from the Green Lizard mine were collected using the same diffractometer and with the same radiation noted above. The *Rigaku CrystalClear* software package was used for processing the data, including the application of an empirical multi-scan absorption correction using *ABSCOR* (Higashi, 2001). The crystal structure was solved using *SIR2011* (Burla *et al.*, 2012) and found to be the same as that of synthetic $(\text{UO}_2)(\text{SO}_4)\cdot 2.5\text{H}_2\text{O}$ (Vlček *et al.*, 2009). *SHELXL-2013* (Sheldrick, 2008) was used for the refinement of the crystal structure. All non-hydrogen atoms were refined with anisotropic displacement parameters. Difference-Fourier maps allowed the location of all H-atom positions, which were then refined with soft restraints of $0.82(3)\text{ \AA}$ on the O–H distances and $1.30(3)\text{ \AA}$ on the H–H distances and with the U_{eq} of each H set to 1.2 times that of the donor O atom. Data collection and refinement details are given in Table 2, atom coordinates and displacement parameters in Table 3, selected bond distances in Table 4 and a bond-valence analysis in Table 5.

Description of the crystal structure

The crystal structure of shumwayite is shown in Fig. 6. The U site in the structure of shumwayite is surrounded by seven O atoms forming a squat UO_7 pentagonal bipyramid. This is the most typical

TABLE 5. Bond-valence analysis for shumwayite. Values are expressed in valence units.*

	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10	O11	O12	OW1	OW2	OW3	OW4	OW5	Σc
U1				0.57		0.54	0.54	0.51	1.78	1.73	1.78	1.75	0.47	0.48	0.46			6.06
U2	0.57		0.54													0.48		6.14
S1	1.59	1.56	1.52	1.49														6.16
S2					1.60	1.53	1.50	1.44										6.07
H1a		0.18											0.82					1.00
H1b					0.16								0.84				0.19	1.00
H2a													0.81					1.00
H2b		0.19											0.81					1.00
H3a								0.16							0.84			1.00
H3b		0.20												0.80				1.00
H4a															0.80	0.20		1.00
H4b															0.82			1.00
H5a												0.13						1.00
H5b																	0.87	1.00
Σa	2.16	2.13	2.06	2.06	1.94	2.07	2.04	2.06	1.78	1.89	1.78	1.88	2.13	2.10	2.10	2.10	2.16	1.00

* S^{6+} -O bond-valence parameters from Brown and Altermatt (1985); U^{6+} -O bond-valence parameters from Burns *et al.* (1997); hydrogen-bond strengths based on O-O bond lengths from Brown and Altermatt (1985).

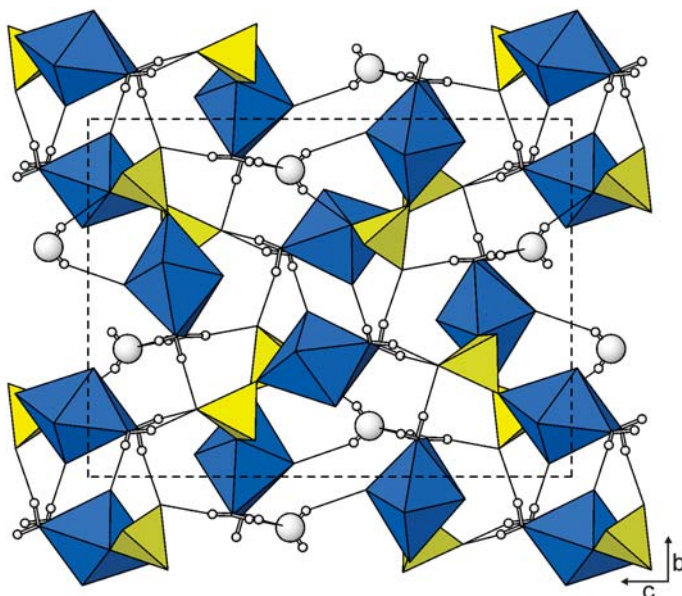


FIG. 6. The structure of shumwayite viewed down [100], the chain direction. UO_7 bipyramids are dark blue, SO_4 tetrahedra are yellow, O atoms of isolated H_2O groups are large white spheres and H atoms are small white spheres. Hydrogen bonds are shown as solid lines. The unit cell is shown by dashed lines.

coordination for U^{6+} , particularly in uranyl sulfates, where the two short apical bonds of the bipyramid constitute the uranyl group. Three of the five equatorial O atoms of the UO_7 bipyramid participate in SO_4 tetrahedra; the other two are H_2O groups. The linkages of pentagonal bipyramids and tetrahedra form an infinite neutral $[(\text{UO}_2)(\text{SO}_4)(\text{H}_2\text{O})_2]$ chain along [100] (Fig. 7). There is one isolated H_2O group between the chains. The chains and isolated H_2O groups are linked together by hydrogen bonds.

No other mineral structure contains chains like those in shumwayite; however, Burns (2005) lists

eight uranyl sulfates, chromates and selenates, including synthetic $(\text{UO}_2)(\text{SO}_4)\cdot 2.5\text{H}_2\text{O}$ (Van der Putten and Loopstra, 1974; Vlček *et al.*, 2009) with topologically identical chains. One of these phases, $(\text{UO}_2)(\text{SO}_4)\cdot 3.5\text{H}_2\text{O}$ (Brandenburg and Loopstra, 1973; space group: $C2/c$) has a dimorph (Zalkin *et al.*, 1978; space group: $P2_1ca$), not listed by Burns (2005), but containing the same kind of chains. Zalkin *et al.* (1978) referred to the $P2_1ca$ dimorph as $\alpha\text{-}(\text{UO}_2)(\text{SO}_4)\cdot 3.5\text{H}_2\text{O}$ and the $C2/c$ dimorph as $\beta\text{-}(\text{UO}_2)(\text{SO}_4)\cdot 3.5\text{H}_2\text{O}$. We have confirmed the natural counterpart of $\alpha\text{-}(\text{UO}_2)(\text{SO}_4)\cdot 3.5\text{H}_2\text{O}$ to occur at both the Green Lizard

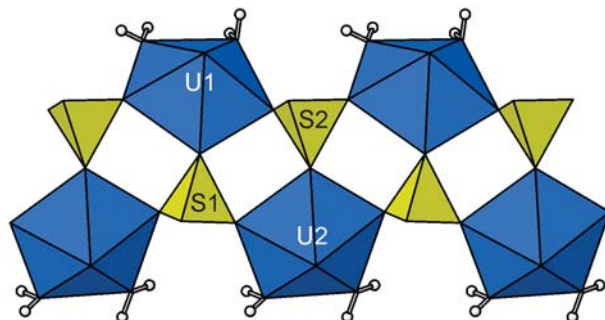


FIG. 7. The uranyl sulfate chain in shumwayite.

and Giveaway-Simplot mines, although this phase has not been found in crystals good enough for single crystal study.

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References

- Bartlett, J.R. and Cooney, R.P. (1989) On the determination of uranium-oxygen bond lengths in dioxo-uranium(VI) compounds by Raman spectroscopy. *Journal of Molecular Structure*, **193**, 295–300.
- Brandenburg, N.P. and Loopstra, B.O. (1973) Uranyl sulphate hydrate, $\text{UO}_2\text{SO}_4 \cdot 3\frac{1}{2}\text{H}_2\text{O}$. *Crystal Structure Communications*, **2**, 243–246.
- Brittain, H.G., Ansari, P., Toivonen, J., Niinisto, L., Tsao, L. and Perry, D.L. (1985) Photophysical studies of uranyl complexes. VIII. Luminescence spectra of $\text{UO}_2\text{SO}_4 \cdot 3\frac{1}{2}\text{H}_2\text{O}$ and two polymorphs of bis(urea) uranyl sulfate. *Journal of Solid State Chemistry*, **59**, 259–264.
- Brown, I.D. and Altermatt, D. (1985) Bond-valence parameters from a systematic analysis of the inorganic crystal structure database. *Acta Crystallographica*, **B41**, 244–247.
- Bullock, H. (1969) Raman and infrared spectroscopic studies of the uranyl ion: the symmetry stretching frequency, force constants, and bond lengths. *Journal of Chemical Society*, **A1969**, 781–784.
- Bullock, H. and Parret, F.W. (1970) The low frequency infrared and Raman spectroscopic studies of some uranyl complexes: the deformation frequency of the uranyl ion. *Canadian Journal of Chemistry*, **48**, 3095–3097.
- Burla, M.C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Mallamo, M., Mazzone, A., Polidori, G. and Spagna, R. (2012) *SIR2011*: a new package for crystal structure determination and refinement. *Journal of Applied Crystallography*, **45**, 357–361.
- Burns, P.C. (2005) U^{6+} minerals and inorganic compounds: insights into an expanded structural hierarchy of crystal structures. *The Canadian Mineralogist*, **43**, 1839–1894.
- Burns, P.C., Ewing, R.C. and Hawthorne, F.C. (1997) The crystal chemistry of hexavalent uranium: polyhedron geometries, bond-valence parameters, and polymerization of polyhedra. *The Canadian Mineralogist*, **35**, 1551–1570.
- Čejka, J. (1999) Infrared spectroscopy and thermal analysis of the uranyl minerals. Pp. 521–622. in: *Uranium: Mineralogy, Geochemistry and the Environment* (P.C. Burns and R.C. Finch, editors). Reviews in Mineralogy, **38**. Mineralogical Society of America, Washington, DC.
- Chenoweth, W.L. (1993) *The Geology and Production History of the Uranium Deposits in the White Canyon Mining District, San Juan County, Utah*. Miscellaneous Publication 93-3, Utah Geological Survey, USA.
- Finch, R.J. and Murakami, T. (1999) Systematics and paragenesis of uranium minerals. Pp. 91–179. in: *Uranium: Mineralogy, Geochemistry and the Environment* (P.C. Burns and R.C. Finch, editors). Reviews in Mineralogy, **38**. Mineralogical Society of America, Washington, DC.
- Gunter, M.E., Bandli, B.R., Bloss, F.D., Evans, S.H., Su, S.C. and Weaver, R. (2004) Results from a McCrone spindle stage short course, a new version of EXCALIBUR, and how to build a spindle stage. *The Microscope*, **52**, 23–39.
- Higashi, T. (2001) *ABSCOR*. Rigaku Corporation, Tokyo.
- Kampf, A.R., Kasatkin, A.V., Čejka, J. and Marty, J. (2015a) Plášilite, $\text{Na}(\text{UO}_2)(\text{SO}_4)(\text{OH}) \cdot 2\text{H}_2\text{O}$, a new uranyl sulfate mineral from the Blue Lizard mine, San Juan County, Utah, USA. *Journal of Geosciences*, **60**, 1–10.
- Kampf, A.R., Plášil, J., Kasatkin, A.V., Marty, J. and Čejka, J. (2015b) Fermitte, $\text{Na}_4(\text{UO}_2)(\text{SO}_4)_3 \cdot 3\text{H}_2\text{O}$, and oppenheimerite, $\text{Na}_2(\text{UO}_2)(\text{SO}_4)_2 \cdot 3\text{H}_2\text{O}$, two new uranyl sulfate minerals from the Blue Lizard mine, San Juan County, Utah, USA. *Mineralogical Magazine*, **79**, 1123–1142.
- Kampf, A.R., Plášil, J., Kasatkin, A.V., Marty, J., Čejka, J. and Lapčák, L. (2015c) Shumwayite, IMA 2015-058. CNMNC Newsletter No. 27, October 2015, page 1228; *Mineralogical Magazine*, **79**, 1229–1236.
- Kampf, A.R., Sejkora, J., Witzke, T., Plášil, J., Čejka, J., Nash, B.P. and Marty, J. (2016) Rietveldite, IMA 2016-081. CNMNC Newsletter No. 34, December 2016, page 1320; *Mineralogical Magazine*, **80**, 1315–1321.
- Krivovichev, S.V. and Plášil, J. (2013) Mineralogy and crystallography of uranium. Pp. 15–119 in: *Uranium: From Cradle to Grave* (P.C. Burns and G.E. Sigmon, editors). MAC Short Courses, **43**. Mineralogical Association of Canada, Winnipeg, Canada.
- Lane, M.D. (2007) Mid-infrared emission spectroscopy of sulfate and sulfate-bearing minerals. *American Mineralogist*, **92**, 1–18.

- Libowitzky, E. (1999) Correlation of O–H stretching frequencies and O–H···O hydrogen bond lengths in minerals. *Monatshefte für Chemie*, **130**, 1047–1059.
- Mandarino, J.A. (1976) The Gladstone–Dale relationship – Part 1: derivation of new constants. *The Canadian Mineralogist*, **14**, 498–502.
- Mandarino, J.A. (2007) The Gladstone–Dale compatibility of minerals and its use in selecting mineral species for further study. *The Canadian Mineralogist*, **45**, 1307–1324.
- Ohwada, K. (1976) Infrared Spectroscopic Studies of Some Uranyl Nitrate Complexes. *Journal of Coordination Chemistry*, **6**, 75–80.
- Plášil, J. (2014) Oxidation–hydration weathering of uraninite: the current state-of-knowledge. *Journal of Geoscience*, **59**, 99–114.
- Plášil, J., Buixaderas, E., Čejka, J., Sejkora, J., Jehlička, J. and Novák, M. (2010) Raman spectroscopic study of the uranyl sulphate mineral zippeite: low wavenumber and U–O stretching regions. *Analytical and Bioanalytical Chemistry*, **397**, 2703–2715.
- Shumway, G.L. (1970) *A History of the Uranium Industry on the Colorado Plateau*. University of Southern California, Los Angeles, unpublished PhD dissertation, 278 pp.
- Sheldrick, G.M. (2008) A short history of *SHELX*. *Acta Crystallographica*, **A64**, 112–122.
- Van der Putten and N., Loopstra, B.O. (1974) Uranyl sulphate $2.5\text{H}_2\text{O}$, $\text{UO}_2\text{SO}_4 \cdot 2.5\text{H}_2\text{O}$. *Crystal Structure Communications*, **3**, 377–380.
- Vlček, V., Čejka, J., Císařová, I., Goliáš, V. and Plášil, J. (2009) Crystal structure of $\text{UO}_2\text{SO}_4 \cdot 2.5\text{H}_2\text{O}$: Full anisotropic refinement and vibration characterization. *Journal of Molecular Structure*, **936**, 75–79.
- Zalkin, A., Ruben, H. and Templeton, D.H. (1978) Structure of a new uranyl sulfate hydrate, $\alpha\text{-}2\text{UO}_2\text{SO}_4 \cdot 7\text{H}_2\text{O}$. *Inorganic Chemistry*, **17**, 3701–3702.