Meisserite, $Na_5(UO_2)(SO_4)_3(SO_3OH)(H_2O)$, a new uranyl sulfate mineral from the Blue Lizard mine, San Juan County, Utah, USA

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ABSTRACT

Meisserite (IMA2013-039), $Na_5(UO_2)(SO_4)_3(SO_3OH)(H_2O)$, is a new uranyl sulfate mineral from the Blue Lizard mine, San Juan County, Utah (USA). It is named in honour of the prominent Swiss mineralogist Nicolas Meisser. The new mineral was found in a sandstone matrix and is associated with chalcanthite, copiapite, ferrinatrite, gypsum, johannite and another new Na-bearing uranyl sulfate, belakovskiite (IMA2013-075). Meisserite is a secondary mineral formed by the post-mining weathering of uraninite. The mineral is triclinic, $P\overline{1}$, a = 5.32317(10), b = 11.5105(2), c = 11.5105(2)13.5562(10) Å, $\alpha = 102.864(7)^{\circ}$, $\beta = 97.414(7)^{\circ}$, $\gamma = 91.461(6)^{\circ}$, V = 801.74(6) Å³, and Z = 2. Crystals are prisms elongated on [100], up to 0.3 mm long, exhibiting the forms {010} and {001}. Meisserite is pale green to yellowish green, translucent to transparent and has a very pale yellow streak. It is brittle, with fair cleavage on $\{100\}$ and $\{001\}$, and uneven fracture. The Mohs hardness is estimated at 2. Meisserite is somewhat hygroscopic and easily soluble in water. The calculated density based on the empirical formula is 3.208 g/cm³. Meisserite exhibits bright yellow green fluorescence under both long- and shortwave UV radiation. The mineral is optically biaxial (-), with $\alpha = 1.514(1)$, $\beta = 1.546(1)$, $\gamma = 1.557(1)$ (measured in white light). The measured 2V is 60(2)° and the calculated 2V is 60°. Dispersion is r > v, perceptible, and the optical orientation is $X \approx \mathbf{a}, Z \approx \mathbf{c}^*$. The mineral is pleochroic, with X (colourless) \leq Y (pale yellow) \approx Z (pale greenish yellow). The empirical formula of meisserite (based on 19 O a.p.f.u.) is Na_{5.05}(U_{0.94}O₂)(SO₄)₃[SO_{2.69}(OH)_{1.31}](H₂O). The Raman spectrum is dominated by the symmetric stretching vibrations of UO_2^{2+} , SO_4^{2-} and also weaker O–H stretching vibrations. The eight strongest powder X-ray diffraction lines are $[d_{obs}$ in Å (*hkl*) I_{rel}]: 13.15 (001) 81, 6.33 (012) 62, 5.64 (021,020) 52, 5.24 (100,012,101) 100, 4.67 (101) 68, 3.849 (121,102,022) 48, 3.614 $(0\bar{3}2,\bar{1}\bar{1}3)$ 41, and 3.293 ($\bar{1}13,004$) 43. The crystal structure of meisserite ($R_1 = 0.018$ for 3306 reflections with $I_{obs} > 3\sigma I$ is topologically unique among known structures of uranyl minerals and inorganic compounds. It contains uranyl pentagonal bipyramids linked by SO₄ groups to form chains. Na^+ cations bond to O atoms in the chains and to an SO₃OH group and an H₂O group between the chains, thereby forming a heteropolyhedral framework.

* E-mail: plasil@fzu.cz DOI: 10.1180/minmag.2013.077.7.07 **Keywords:** Meisserite, new mineral, uranyl sulfate, crystal structure, Raman spectroscopy, infrared spectroscopy, oxidation zone, acid-mine drainage, uranium, Blue Lizard mine, Utah.

Introduction

URANYL SULFATE minerals are widespread in most uranium deposits because uraninite is commonly associated with pyrite, marcasite and other sulfides. Oxidative alteration of sulfide minerals leads to the formation of solutions with low pH (Jambor et al., 2000). These acidic solutions are referred to as acid-mine drainage (AMD) when they have an anthropogenic origin, and they are responsible for leaching and transport of heavy elements on a large scale (Edwards et al., 2000; Evangelou and Zhang, 1995). Uraninite exposed to such conditions undergoes a hydration-oxidation weathering, followed by the release of U^{6+} , as the uranyl ion $[UO_2]^{2+}$, into solution. This very mobile form of U occurs in an array of hydrated oxo-hydroxo-sulfate complexes. Under appropriate natural conditions, solutions containing these complexes and various other cations and anions can form diverse suites of uranyl sulfate minerals. The observed occurrences of uranyl sulfates are related to underground alteration, where uraninite is exposed to the moist air in old mining adits or weathering in old mine dumps and mill-tailings (see e.g. Brugger et al., 2003; Plášil et al., 2012a,b; Schindler et al., 2012; Krivovichev and Plášil, 2013). Krivovichev and Plášil (2013) reviewed 20 known U⁶⁺ sulfate minerals that had been found in Nature. Since that report, four new uranyl sulfate minerals have been described (mathesiusite, IMA2013-046, Plášil et al., 2013); bluelizardite, IMA2013-062, Plášil et al., in prep.; belakovskiite, IMA2013-075, Kampf et al., in prep.) and meisserite, which is described here.

The new mineral honours the prominent Swiss mineralogist Nicolas Meisser (born 1964) who is Curator of Mineralogy and Petrography at the Musée Cantonal de géologie at Lausanne, Switzerland and has authored or co-authored 38 new-mineral descriptions or redeterminations. As meisserite is a new uranyl sulfate with unique structural topology, we are convinced that naming this mineral for Nicolas is an appropriate recognition for his important contributions to the mineralogy, crystallography and geochemistry of uranium. The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA2013-039). There are three cotype specimens of the new mineral, one stored in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia (registration number 4410/1), the second deposited in the collections of the Natural History Museum of Los Angeles County, Los Angeles, California, USA (catalogue number 64055) and the third deposited in the collections of the Musée cantonal de géologie, Lausanne, Switzerland under catalogue number MGL 92960.

Occurrence

Meisserite was found underground in the Blue Lizard mine, Red Canyon, White Canyon district, San Juan County, Utah, USA (37°33'26"N 110°17'44"W) by one of the authors (JM). The mineral is rare and occurs in association with other new uranyl sulfate minerals, which are currently under investigation. The Blue Lizard mine is located to the west of the town of Blanding on the north side of Red Canyon and close to the Markev mine. Underground workings in the Blue Lizard mine were first developed in the mid 1950s and yielded uranium ore with 0.20 - 0.50% U₃O₈ (Thaden *et al.*, 1964). Mineralized palaeostream 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 formed in a braided-stream environment during the Upper Triassic (Blakey and Gubitosa, 1984). Ore minerals were deposited as replacements of wood and other organic material and as disseminations in the enclosing sandstone. Since the mine closed in 1978, supergene 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.

Minerals found in direct spatial association with meisserite include chalcanthite, copiapite, ferrinatrite, gypsum, johannite and another new Na-containing uranyl sulfate (Fig. 1*a*) that has been submitted to the CNMNC for approval under the name belakovskiite (IMA2013-075). Primary minerals in the general assemblage include baryte, bornite, calcite, chalcopyrite, covellite,



FIG. 1. Meisserite from Blue Lizard mine, Utah, San Juan County, USA. (a) Meisserite (greenish yellow) in typical association with belakovskiite (IMA2013-075) (whitish fibrous) and blödite. FOV 2 mm. (b) Rarely developed prismatic crystals of meisserite. FOV 1.5 mm. Photo: J. Marty.

feldspar, pyrite, quartz and uraninite. Secondary, post-mining minerals in the general assemblage include atacamite, blödite, brochantite, chalcanthite, cobaltoblödite, copiapite, cyanotrichite, d'ansite, ferrinatrite, gypsum, halotrichite, johannite, kröhnkite, manganoblödite, metavoltine, natrochalcite, natrozippeite, pickeringite, pseudojohannite, rhomboclase, römerite, sideronatrite and tamarugite. The Blue Lizard mine is the type locality for the recently described new minerals manganoblödite and cobaltoblödite (Kasatkin *et al.*, 2013).

Physical and optical properties

Crystals of meisserite usually occur as intergrowths with other uranyl sulfates, and only rarely are found as isolated crystal aggregates. Crystals are prisms up to 0.3 mm long, elongated on [100] (Fig. 1b) with prism forms $\{010\}$ and $\{001\}$; terminations of the crystals probably consist of multiple forms, none of which could be measured because the crystals occur in intergrowths. Meisserite is pale green to vellowish green and has a very pale yellow streak. Crystals are translucent to transparent with a vitreous lustre. They are brittle, with fair cleavage on $\{100\}$ and {001}, and have uneven fracture. The Mohs hardness is estimated at 2. There is insufficient material for the direct determination of density. A density of 3.208 g/cm³ was calculated based on the unit-cell dimensions from single-crystal X-ray data and electron microprobe results. Meisserite is somewhat hygroscopic. It shows bright yellow green fluorescence under both long- and shortwave UV radiation. The mineral is optically biaxial negative, with $\alpha = 1.514(1)$, $\beta = 1.546(1)$, $\gamma = 1.557(1)$ (measured with white light). The measured 2V is 60(2)° and the calculated 2V (calc.) is 60°. Dispersion is r > v, perceptible, and the optical orientation is $X \approx a, Z \approx c^*$. The mineral is pleochroic, with X (colourless) < Y (pale yellow) $\approx Z$ (pale greenish yellow). The Gladstone-Dale compatibility, $1 - (K_p/K_c)$, is superior (0.018) for the empirical formula and the single-crystal cell.

Chemical composition

Quantitative chemical analyses of meisserite were obtained using a Cameca SX100 electron microprobe (WDS mode, 15 kV, 2 nA and 15 µm beam diameter) at the Institute of Geological Sciences, Masaryk University in Brno, Czech Republic. The following X-ray lines and standards were used: K_{α} lines: S (SrSO₄), Na (sanidine), M_{β} lines: U (rutherfordine). Other elements, such as K, Ca and Mg, were sought, but none was above the detection limits (~0.1 wt.% for the analytical conditions used). Peak counting times (CT) were 10-20 s and the counting time for background was 50% of the peak CT. The measured intensities were converted to element concentrations using the PAP program (Pouchou and Pichoir, 1985). Analytical results are given in Table 1. The H₂O content was calculated by stoichiometry based on the crystal-structure analysis (see below). Raman spectroscopy (see below) confirmed the presence of OH and H₂O and the absence of other anions, such as PO₄, AsO₄ and CO₃. The empirical formula (based on

	Mean $(n = 4)$	Range	Std. dev
Na ₂ O	20.42	19.76-20.86	0.46
SO ₃	34.98	34.23-36.57	0.61
UO ₃	61.46	58.29-63.77	1.10
H ₂ O	3.90*		
Total	101.16		
Calculated on	the basis of 19 O a.p.f.u		
Na	5.05		
S ⁶⁺	4.00		
U ⁶⁺	0.94		
H ₂ O	1.66		

TABLE 1. Results of WDS analyses (in wt.%) of meisserite.

19 O a.p.f.u.) is $Na_{5.05}(U_{0.94}O_2)(SO_4)_3$ [SO_{2.69}(OH)_{1.31}](H₂O). The simplified formula is $Na_5(UO_2)(SO_4)_3(SO_3OH)(H_2O)$, which requires Na_2O 19.66, UO₃ 36.32, SO₃ 40.59, H₂O 3.43, total 100.00 wt.%.

Raman spectroscopy

The Raman spectrum of meisserite (Fig. 2) was recorded on a Thermo Scientific DXR Raman Microscope interfaced to an Olympus microscope (objective $50 \times$) in the $50-3400 \text{ cm}^{-1}$ spectral region with ~2 cm⁻¹ spectral resolution. The power of the frequency-stabilized single mode

diode laser (532 nm) impinging on the sample was set to 3 mW (20 s exposure, accumulation of 40 scans). The spectrometer was calibrated by a software-controlled (*Omnic 8*) calibration procedure 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 and band-component analysis was done with *Omnic 8* software. The interpretation of the spectrum follows those by Baran *et al.* (1999), Haile *et al.* (1998), Vchirawongkwin *et al.* (2010), Periasamy *et al.* (2009) and Sieber (1966).



FIG. 2. Raman spectrum of meisserite.

The dominant feature in the Raman spectrum is a band at 847 cm⁻¹, attributable to the v₁ (UO₂) symmetric stretching mode. The antisymmetric v₃ $(UO_2)^{2^+}$ stretching mode is not observable in the spectrum. The doubly degenerate bending mode of $(UO_2)^{2^+}$ (v₂) is located at 241 cm⁻¹. The U–O bond length inferred from the $UO_2^{2^+}$ symmetric stretching frequency, following the empirical relation given by Bartlett and Cooney (1989), is 1.76 Å. Corresponding bond lengths obtained from the refined structure are 1.764(2) for U–O17 and 1.774(2) for U–O18 (see below).

Vibrations attributable to SO₄ and SO₃OH groups, respectively, may partly overlap, which can be inferred e.g. from Haile et al. (1998) or Periasamy et al. (2009). Bands at 1068, 1045, 1031, 1019, 990 and 975 cm⁻¹ are assigned to v_1 symmetric stretching modes of SO₄ and SO₃OH. Those at 1239, 1213, 1186, 1153, 1139, 1139 and 1102 cm⁻¹ are attributable to the triply degenerate v₃ SO₄ and SO₃OH antisymmetric stretching vibrations. Raman bands at 633, 606 and 589 cm⁻¹ are assigned to triply degenerate v_3 (δ) antisymmetric bending vibrations of the tetrahedral units and those at 464, 448 and 414 cm^{-1} to the doubly degenerate v_2 (\delta) symmetric bending mode of the tetrahedra. The stretching mode v (S-OH) is assigned to the vibration at 890 $\rm cm^{-1}$.

The O–H stretching vibrations are generally weak in Raman spectra; however, they are observable in the meisserite spectrum as bands of weak intensity at 3497 and 3366 cm⁻¹. The inferred O...O distances for the corresponding hydrogen bonds, calculated based on the empirical relation given by Libowitzky (1999), are ~2.9 Å and ~2.78 Å, respectively. The weak vibrations at 199, 171, 123, 96 and 61 cm⁻¹ are attributed to the lattice modes.

X-ray crystallography and structure determination

All powder and single-crystal X-ray diffraction data were obtained using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer utilizing monochromatized MoK α radiation. Observed powder d_{hkl} values and intensities were derived by profile fitting using *JADE 2010* software. Data (in Å) are given in Table 2. Unitcell parameters refined from the powder data using *JADE 2010* with whole-pattern fitting are: *a* = 5.319(3), *b* = 11.499(3), *c* = 13.531(3) Å, α = 102.84(1)°, β = 97.45(1)°, γ = 91.41(1)° and *V* = 798.9(5) Å³. The observed powder data fit well with those calculated from the structure, also using *JADE 2010*.

The Rigaku CrystalClear software package was used for processing the diffraction data, including the application of an empirical multi-scan absorption correction using ABSCOR (Higashi, 2001). The structure was solved independently by direct methods using Sir2004 (Burla et al., 2005) and the charge-flipping algorithm (Oszlányi and Sütő, 2004, 2008; Palatinus, 2013) implemented in the Superflip program (Palatinus and Chapuis, 2007). The crystal structure was refined by the full-matrix least-squares algorithm of the Jana2006 program (Petříček et al., 2006) based on F^2 . All non-hydrogen atoms were refined with anisotropic atomic displacement parameters (ADP). The H atoms were treated as having ADP equal to 1.2^*U_{eq} of the corresponding O atom to which the particular H atom is linked. The O-H bonds were treated with soft constraints on the bond-length of 0.90(8) Å. The final R values obtained from the refinement were $R_1 = 0.018$ and $wR_2 = 0.044$ with a GoF = 1.36 for 3306 reflections with $[I > 3\sigma(I)]$. The crystallographic details, data collection and refinement statistics are given in Table 3. The final atomic coordinates and displacement parameters are given in Table 4. Based on the interatomic distances (Tables 5 and 6), the bond-valence analysis for the structure (Table 7) was carried out following the approach of Brown (1981, 2002). The crystallographic information file (CIF) and the structure factors list has been deposited with the Principal Editor of Mineralogical Magazine and and is available from www.minersoc.org/pages/ e journals/dep mat mm.html).

Description of the crystal structure

There are one U, four S, six Na, nineteen O and three H atoms in the asymmetric unit of the meisserite structure (Table 4). The crystal structure consists of a heteropolyhedral framework, with fundamental blocks of infinite uranyl-sulfate chains extended along [010] (Fig. 3). The U atom is strongly bonded to two O atoms (O17, O18), at distances of ~1.76 and ~1.77 Å, forming the uranyl ion, $UO_{2^{2^+}}^{2^+}$. It is further coordinated by five O ligands arranged at the apices of a pentagonal bipyramid with uranyl O atoms at the two vertices. The observed uranyl bond-lengths and $U-O_{equatorial}$ bond-lengths (Table 5) match closely the most typical values for [7]-coordinated

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TABLE 2. X-ray powder diffraction data for meisserite from Blue Lizard.

Iobs	d _{obs}	d_{calc}	Icalc	h k l	Iobs	$d_{\rm obs}$	d_{calc}	Icalc	h k l	Iobs	$d_{\rm obs}$	d_{calc}	Icalc	h k l
81	13.15	13.066	100	$ \begin{array}{c} 0 & 0 & 1 \\ 0 & 1 & 0 \end{array} $		(2.966	33	$\bar{1} 0 4$			1.947	3	$0\bar{4}6$
3 12	0.70	0.654	4	0 1 0 $0 \overline{1} 1$	93	2.969	2.963	14	032			1.931	3	033
0	9.70	9.034	0	0 1 1			2.900	12	$1 \overline{2} 2$			1.927	4	123
0	/./0	6 5 2 2	14	0 1 1		(2.940	10	1 2 2	47	1 0 1 0	1.925	2	$\frac{1}{2} \frac{3}{4} \frac{1}{1}$
62	633	6 3 0 0	20	$0 \ \overline{0} \ \overline{2}$ $0 \ \overline{1} \ \overline{2}$		(2.940	15	1 2 2	4/	1.918	1.910	1	$\frac{241}{152}$
02	0.55	5.500	29	012 $0\bar{2}1$	19	2.883 {	2.880	10	$113 \\ 0\bar{4}1$			1 013	5	0 6 2
52	5.64	5 507	12	021		(2.074	10	$1 \overline{2}$			1.913	6	0 0 2
		(5.266	58	100		(2.034	17	1 2 + 1 2 = 1 2			1 800	4	0.2.6
1.00	5 24	5 1 5 5	5	0 1 2	46	2.813	2.013	10	133			1.871	4	232
100	5.24	5 1 3 7	25	$\bar{1}$ 0 1 2	18	2 702	2 709	14	132	17	1.874	1.867	7	1232 127
		4870	6	$\frac{1}{1}$ 1 0	10	2.702	2.709	3	132 $1\overline{3}3$			1.863	4	$\frac{1}{1}$ $\frac{2}{2}$ $\frac{7}{6}$
26	182	4 827	8	$0 \overline{2} 2$			2.001	6	$1 \overline{1} 4$			(1.846	4	$2\bar{3}4$
20	4.02	4 768	4	021	26	2 633	2.633	19	200	15	1.850	1 843	5	214
		4 733	9	$\overline{1}$ $\overline{1}$ $\overline{1}$ 1	20	2.000	2.635	6				1 829	4	053
68	4 67	4 665	47	101			2 589	4	$1\bar{2}4$	9	1 808	1.807	4	$1\bar{6}2$
00	1.07	4 607	6	$\frac{1}{1}$ $\frac{1}{1}$ $\frac{1}{1}$		(2.561	3	033	,	1.000	(1 777	3	146
		4.520	6	1 1 1	11	2.553 {	2.550	7	$\bar{1}$ $\bar{3}$ 4	25	1.779	1.776	5	056
20	4.48	4.412	8	0 1 3			2.526	3	115			(1.739	3	144
		4.261	3	112	10	2.515	2.514	7	2 0 1	19	1 733	1.735	4	233
7	4.130	4.120	7	1 1 1		(2.486	3	ī 4 2	1)	1.755	1.719	3	156
		3.960	7	<u>1</u> 12	11	2 483	2.482	5	Ī 0 5			(1.709	5	301
10	3.960 {	3.946	5	120		(2.478	4	1 4 2	20	1.706	{ 1.703	4	Ī45
		3.893	4	023		(2.435	3	$\bar{2} \ 2 \ 0$	20	11/00	1.702	3	313
		(3.853	8	ī ī 1	19	2.420 {	2.419	4	ī 3 3			(1.687	3	107
48	3.849	3.848	3	1 0 2			2.389	4	Ī Ī 1	15	1.678	1.684	3	313
		3.841	19	0 2 2	3	2.335	2.333	6	1 4 3			1.674	6	028
	((3.779	9	0 1 3	12	2.272	2.275	8	Ī <u>3</u> 5	1.5	1 (10	£ 1.656	3	Ī 2 8
16	3.739	3.731	9	030			2.260	3	222	15	1.649	1.649	4	156
		3.720	3	Ī 2 1		(2.226	3	2 1 2	15	1 500	∫ 1.599	3	255
41	2614	3.613	20	032	19	2.213	2.208	3	<u>2</u> 14	15	1.590	1.586	5	332
41	3.614	3.598	13	<u>1</u> <u>1</u> 3		(2.206	7	0 5 3			(1.559	2	2 6 2
6	2 470	3.465	6	122			2.178	3	006	12	1 5 5 1	1.556	2	046
0	5.470	3.458	4	1 1 2			2.153	3	$\bar{2}$ $\bar{3}$ 1	15	1.551	1.551	2	324
	1	3.390	16	031			2.151	3	$\frac{2}{1}$ $\frac{1}{3}$			1.540	3	128
33	3.379 {	3.374	4	121		(2.127	4	126	24	1 5 1 7	{ 1.527	2	075
		3.347	22	$\frac{0}{1}$ 1 4	20	2 1 2 6	2.124	4	125	24	1.317	1.524	3	174
12	2 202	3.295	19	1 1 3	30	2.120	2.120	3	$\frac{2}{2}$ 1 4			1.519	3	2 6 1
45	5.295	3.267	13	$0 \ 0 \ 4$		(2.119	7	106			1.514	2	313
8	3 220	3.218	6	033			2.082	4	232			1.512	2	171
0	5.220	3.200	3	$\frac{1}{1}$ 1 3	7	2.022	2.026	4	151			(1.481	3	3 4 1
23	3.127	3.127	19	$\frac{1}{4} \frac{3}{2} \frac{0}{4}$		(1.998	3	205	12	1.478	{ 1.480	2	$\frac{3}{1}$
		3.071	4	131	7	1 989	1.994	6	234			(1.470	3	167
		3.012	8	$\frac{1}{1}$ $\frac{3}{1}$ $\frac{2}{1}$,	1.707	1.980	3	224	-		(1.443	2	226
		3.000	6	114		l	1.967	4	241 522	8	1.433	1.437	2	334
					16	1.959 {	1.956	3	233	~	1 400	1.427	2	256
					,	(1.934	0	214	0	1.409	1.40/	3	084

For *d* values greater than 1.56 Å, calculated lines with intensities of 3 or greater are shown. For *d* values less than 1.56 Å, calculated lines with intensities of 2 or greater are shown when they correspond to observed lines.

Structural formula Unit-cell parameters	Na ₅ (UO ₂)(SO ₄) ₃ (SO ₃ OH)(H ₂ O) a = 5.32317(10) Å b = 11.5105(2) Å c = 13.5562(10) Å $\alpha = 102.864(7)^{\circ}$ $\beta = 97.414(7)^{\circ}$ $\gamma = 91.461(6)^{\circ}$
V (Å ³) Z Space group $D_{\text{calc.}}$ (g.cm ⁻³) Temperature Wavelength Crystal dimensions (mm) Limiting θ angles Limiting Miller indices No. of reflections No. of reflections No. of unique reflections (criterion) Absorption correction (mm ⁻¹), method T_{\min}/T_{\max} Coverage, R_{int} F_{000}	801.74(6) 2 $P\bar{1}$ 3.264 (applicable for the above given formula) 298(2) K MoK α , 0.71075 Å 0.13 × 0.06 × 0.04 mm 3.11-27.47° -6 $\leq h < 6$, -14 $\leq k \leq 14$, -17 $\leq l \leq 17$ 13998 3627 3306 [$I > 3\sigma(I)$] 10.883, analytical 0.332/0.670 0.99, 0.027 732
Refinement 1	by Jana2006 on F ²
Param. refined, constraints, restraints	274, 3, 3
R_1, wR_2 (obs)	0.0180, 0.0439
R_1, WR_2 (all)	0.0215, 0.0457
GoF (obs, all)	1.36, 1.34
Weighting scheme	$1/(\sigma^2(F) + 0.0004F^2)$
$\Delta \rho_{\min}, \Delta \rho_{\max} (e A^{-3})$	-0.78, 0.78

TABLE 3. Summary of data-collection conditions and refinement parameters for meisserite.

U atoms provided by Burns et al. (1997). The five equatorial O atoms of the pentagonal bipyramid link to SO_4 tetrahedra. Four of the five SO_4 tetrahedra participate in chain linkages. The fifth sulfate group points towards the interlayer between adjacent chains, linked by its free vertices to four distinct Na⁺ cations. The sequence of the tetrahedral units within the chain can be represented as ...udududu.... There remains one symmetrically distinct SO₄ tetrahedron (S4), which is located between the chains and is linked by the weaker bonds only to Na⁺. The S4 tetrahedron is oriented up or down with respect to the bc plane. The S4 tetrahedron contains a protonated O atom (OH16), with a corresponding OH16-H16...Ow19 hydrogen bond (Table 6). The Ow19 atom links only to one Na6 atom and the bond-valence analysis (Table 7) identifies it as an H₂O group. Hydrogen bonds from the Ow19 are accepted by O4 ($Ur\Phi$) and O6 (Na3 Φ) atoms (Tables 6 and 7). Hydrogen bonds provide additional linkage in the framework structure. All of the Na sites were found to be fully occupied. The structural formula of meisserite, obtained from the refinement and bond-valence analysis, is Na₅(UO₂)(SO₄)₃(SO₃OH)(H₂O), with Z = 2.

Discussion

The meisserite structural topology has not previously been found in any naturally occurring uranyl sulfate; however, there are several synthetic compounds with structural units based upon clusters or chains of uranyl and sulfate polyhedra similar to those in the structure of meisserite. A similar infinite uranyl-sulfate chain is found in the structure of $K_2[(UO_2)(SO_4)_2]$

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U_{23}	0.00154(5) 0.0022(3)	0.0022(3)	0.0046(3)	0.0018(4)	0.0017(14)	0.0047(7)	0.0197(11)	0.0157(8)	0.0084(7)	-0.0168(11)	0.0123(13)	-0.0019(13)	-0.0021(11)	-0.0014(10)	0.0064(11)	-0.0002(11)	0.0025(11)	-0.0008(10)	0.0233(15)	0.0042(11)	0.0041(12)	0.0095(11)	0.0051(14)	-0.0013(13)	0.0043(12)	0.0027(13)	0.0041(11)	0.0013(11)	-0.0026(15)			
U_{13}	0.00252(5) 0.0011(3)	0.0047(3)	0.0049(3)	0.0071(4)	0.0023(10)	-0.0009(7)	0.0077(10)	-0.0023(7)	0.0030(7)	-0.0092(9)	-0.0035(14)	0.0034(11) -	0.0053(11) -	0.0013(10) -	0.0081(12)	0.0014(11) -	0.0161(13)	0.0005(10) -	0.0023(12)	0.0089(11)	0.0100(14)	0.0028(11)	0.0175(14)	0.0083(15) -	0.0070(11)	0.0005(12)	0.0029(10)	0.0006(10)	0.0048(16) -			
U_{12}	0.00027(5) -0.0005(3)	-0.0007(3)	0.0027(3)	-0.0009(4)	-0.0051(14)	-0.0109(7)	0.0091(11)	-0.0044(7)	0.0001(7)	-0.0123(11)	0.0002(14)	-0.0115(13)	0.0065(11)	-0.0003(10)	-0.0031(12)	-0.0027(11)	0.0038(12)	0.0006(10)	0.0006(13)	0.0049(12)	0.0036(13)	0.0037(11)	-0.0049(14)	0.0001(13)	0.0003(12)	-0.0020(12)	-0.0013(11)	0.0005(11)	-0.0213(18)			
U_{33}	0.00852(7) 0.0087(4)	0.0093(4)	0.0112(4)	0.0186(5)	0.0132(13)	0.0183(9)	0.0257(13)	0.0282(10)	0.0272(9)	0.0243(11)	0.0183(16)	0.0158(15)	0.0181(14)	0.0094(13)	0.0117(14)	0.0159(14)	0.0215(15)	0.0114(13)	0.0348(18)	0.0108(13)	0.0241(16)	0.0142(13)	0.0274(17)	0.0344(19)	0.0202(15)	0.0239(17)	0.0158(14)	0.0160(14)	0.0202(17)			
U_{22}	0.00957(7) 0.0140(4)	0.0112(4)	0.0118(4)	0.0205(5)	0.104(3)	0.0272(9)	0.0495(16)	0.0324(9)	0.0243(9)	0.0974(19)	0.0266(16)	0.0418(18)	0.0206(14)	0.0185(13)	0.0259(15)	0.0280(15)	0.0113(13)	0.0130(12)	0.0428(19)	0.0246(15)	0.0105(14)	0.0180(13)	0.0350(18)	0.0191(15)	0.0278(16)	0.0333(17)	0.0279(15)	0.0245(15)	0.041(2)			
U_{11}	0.01315(8) 0.0132(4)	0.0183(5)	0.0164(4)	0.0195(5)	0.0171(13)	0.0366(10)	0.0179(12)	0.0208(8)	0.0249(9)	0.0341(11)	0.0464(19)	0.0188(15)	0.0208(14)	0.0169(13)	0.0313(16)	0.0168(14)	0.0363(17)	0.0166(13)	0.0168(15)	0.0252(15)	0.051(2)	0.0209(14)	0.0324(17)	0.0390(18)	0.0175(14)	0.0205(15)	0.0140(13)	0.0145(13)	0.054(2)			
U_{eq}	0.01041(5) 0.0121(3)	0.0128(3)	0.0125(3)	0.0196(3)	0.0466(11)	0.0281(6)	0.0287(9)	0.0263(6)	0.0251(6)	0.0566(9)	0.0301(11)	0.0269(10)	0.0205(9)	0.0157(8)	0.0223(9)	0.0212(9)	0.0221(9)	0.0143(8)	0.0293(11)	0.0195(9)	0.0281(10)	0.0167(8)	0.0308(11)	0.0317(11)	0.0216(9)	0.0268(10)	0.0322*	0.0193(9)	0.0190(9)	0.0403(12)	0.0483^{*}	0.0483^{*}
z/c	0.421436(10) 0.14996(7)	0.36262(7)	0.64320(7)	0.06747(8)	0	0.08994(12)	1/2	0.25123(13)	0.32254(13)	0.11352(15)	0.0909(2)	0.1505(2)	0.1105(2)	0.25806(19)	0.2774(2)	0.3616(2)	0.3597(2)	0.46037(19)	0.3309(2)	0.26893(19)	0.3980(2)	0.56277(19)	0.1416(2)	0.0879(2)	0.0487(2)	-0.0331(2)	-0.085(3)	0.3568(2)	0.4885(2)	0.1920(3)	0.251(3)	0.205(4)
y/b	0.726339(11) 0.61313(8)	1.02464(8)	0.60341(8)	0.17485(9)	1/2	0.32662(15)	0	0.49703(15)	0.21045(14)	0.9623(2)	0.7039(3)	0.5562(3)	0.5217(2)	0.6709(2)	1.0682(2)	1.0214(2)	0.9044(2)	1.1035(2)	0.3748(3)	0.3569(2)	0.5256(2)	0.6662(2)	0.1245(3)	0.3042(3)	0.1365(2)	0.1239(3)	0.132(4)	0.6982(2)	0.7599(2)	0.8665(3)	0.912(4)	0.799(3)
x/a	0.51553(2) 0.53696(16)	0.48968(17)	0.47165(17)	-0.96290(18)	0	-0.4716(3)	0	0.0011(3)	0.9482(3)	0.5866(4)	0.5202(6)	0.2901(5)	-0.2907(5)	0.6528(5)	0.5627(5)	0.2126(5)	0.5863(5)	0.6176(5)	0.2566(5)	-0.3360(5)	0.5954(6)	0.3715(5)	-1.0691(6)	-0.9695(6)	-0.7105(5)	-1.1472(5)	-1.079(8)	0.2030(5)	0.8268(5)	0.9502(7)	1.017(10)	0.922(10)
Atom	U S1	S2	S3	S4	Nal	Na2	Na3	Na4	Na5	Na6	01	02	03	04	05	90	07	08	60	010	011	012	013	014	015	OH16	H16	017	018	Ow19	H19a	H19b

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* Refined isotropically.

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TABLE 5. Selected interatomic distances (in Å) for the structure of meisserite.

U-017 U-018 U-04 U-07 U-08 ⁱ	1.764(2) 1.774(2) 2.380(3) 2.419(3) 2.422(2) 2.318(3)	S1-O1 S1-O2 S1-O3 ⁱⁱ S1-O4 < <i>S</i> 1-O>	1.448(3) 1.454(3) 1.468(3) 1.509(2) 1.470	$S3-O9^{iv} \\ S3-O10^{v} \\ S3-O11^{iv} \\ S3-O12 \\ < S3-O>$	1.446(3) 1.467(3) 1.483(3) 1.489(3) 1.471
$\begin{array}{l} U = 011\\ U = 012\\ < U = 0_{Ur} >\\ < U = 0_{eq} > \end{array}$	2.382(3) 1.769 2.384	S2-O5 S2-O6 S2-O7 <s2-o8 <<i>S</i>2-<i>O</i>8</s2-o8 	1.452(3) 1.473(3) 1.482(3) 1.497(2) 1.476	S4-013 S4-014 S4-015 S4-0h16 < <i>S4-0</i> >	1.435(4) 1.454(3) 1.460(3) 1.562(3) 1.478
Na1–O2 Na1–O2 ^{vi} Na1–O3 Na1–O3 ^{vi} Na1–O14 ⁱⁱ Na1–O14 ^{vii} < <i>Na1–O</i> >	2.347(3) 2.347(3) 2.272(3) 2.272(3) 2.772(3) 2.772(3) 2.46	$\begin{array}{l} Na2-O1^{vi}\\ Na2-O2^{iii}\\ Na2-O3\\ Na2-O10\\ Na2-O14\\ Na2-O14\\ Na2-O14^{ii}\\ Na2-O15\\ <\!\!Na2-O\!\!> \end{array}$	2.379(3) 2.955(3) 2.363(3) 2.383(3) 2.652(4) 2.696(4) 2.420(3) 2.56	Na3-O6 Na3-O6 ^{viii} Na3-O7 ⁱⁱ Na3-O7 ⁱ Na3-O8 ⁱⁱ Na3-O8 ⁱ Na3-O18 ⁱⁱⁱ Na3-O18 ⁱ <i>Na3-O</i> 8 ⁱ	2.365(3) 2.365(3) 2.747(3) 2.747(3) 2.447(2) 2.447(2) 2.857(3) 2.857(3) 2.60
Na4–O2 Na4–O3 Na4–O4 ⁱⁱⁱ Na4–O9 Na4–O10 Na4–O14 ⁱⁱ Na4–O17 < <i>Na4–O</i> >	2.368(4) 2.374(3) 2.756(3) 2.322(4) 2.451(3) 2.791(3) 2.562(3) 2.52	$\begin{array}{l} Na5-O5^{ix} \\ Na5-O6^{x} \\ Na5-O9^{ii} \\ Na5-O10^{ii} \\ Na5-O12^{iv} \\ Na5-O13^{xi} \\ Na5-O18^{xii} \\ <\!Na5-O8 \end{array}$	2.515(3) 2.735(3) 2.447(3) 2.460(3) 2.676(3) 2.420(3) 2.627(3) 2.55	$\begin{array}{l} Na6-O1 \\ Na6-O5 \\ Na6-O13^{xiii} \\ Na6-O15^{xiv} \\ Na6-O15^{vi} \\ Na6-Oh16^{vii} \\ Na6-Oh19 \\ <\!\!Na6-O\!\!> \end{array}$	2.929(4) 2.302(3) 2.512(4) 2.807(4) 2.422(3) 2.526(3) 2.491(4) 2.57
$\begin{array}{c} 01-02\\ 01-03^{ii}\\ 01-04\\ 01-0h16^{vii}\\ 01-0w19\\ 02-03^{ii}\\ 02-04\\ 03-04^{iii}\\ 04-07\\ 04-011\\ 04-017\\ 05-06\\ 05-07\\ 05-08 \end{array}$	$\begin{array}{c} 2.406(5)\\ 2.401(4)\\ 2.398(4)\\ 2.995(4)\\ 2.909(4)\\ 2.383(4)\\ 2.426(3)\\ 2.384(3)\\ 2.789(3)\\ 2.834(4)\\ 2.883(4)\\ 2.420(4)\\ 2.394(4)\\ 2.404(4) \end{array}$	$\begin{array}{c} 06{-}07\\ 06{-}08\\ 06{-}018^{i}\\ 06{-}0w19^{iii}\\ 07{-}08\\ 07{-}08^{i}\\ 07{-}018\\ 08{-}012^{i}\\ 08{-}018^{i}\\ 09{-}011^{ii}\\ 09{-}011^{iii}\\ 09{-}011^{iii}\\ 010{-}011^{iiii}\\ 010{-}012^{v} \end{array}$	2.429(4) 2.433(3) 2.893(3) 2.762(4) 2.382(3) 2.811(4) 2.880(4) 2.738(4) 2.944(4) 2.425(4) 2.410(4) 2.416(4) 2.380(4) 2.388(4)	$\begin{array}{c} 011-012\\ 011-012^{iv}\\ 011-018\\ 012-017\\ 013-014\\ 013-015\\ 013-0h16\\ 014-015\\ 014-0h16\\ 015-0h16\\ 0h16-0w19^{vi}\\ 017-018^{iii} \end{array}$	2.861(4) 2.389(4) 2.873(4) 2.924(4) 2.411(5) 2.436(4) 2.351(4) 2.403(4) 2.424(4) 2.430(4) 2.535(5) 2.852(4)

Symmetry codes: (i) -x+1, -y+2, -z+1; (ii) x+1, y, z; (iii) x-1, y, z; (iv) -x+1, -y+1, -z+1; (v) -x, -y+1, -z+1; (vi) -x, -y+1, -z+1; (vii) -x, -y+1, -z; (viii) -x, -y+1, -z; (viii) -x, -y+2, -z+1; (ix) x, y-1, z; (x) x+1, y-1, z; (xi) x+2, y, z; (xii) -x+2, -y+1, -z+1; (xiii) x+2, y+1, z; (xiv) x+1, y+1, z.

 $(H_2O)](H_2O)$ (Ling *et al.*, 2010); however, it differs in that one vertex of the uranyl pentagonal bipyramid is occupied by H_2O rather than being linked to an SO₄ group. The orientation of the tetrahedral units in that structure may be written

as ...*dduu*.... There are several structures of inorganic uranyl sulfates containing uranylsulfate clusters, where the U:S ratio is 1:4 (Hayden and Burns, 2002a,b; Burns and Hayden, 2002); However, these structures

$D-\mathrm{H}\cdots A$	<i>D</i> -Н (Å)	$\mathbf{H}\cdots \mathbf{A}(\mathbf{\mathring{A}})$	D-A (Å)]	D-H···A angle (°)
Oh16-H16····Ow19 ^{vi}	0.83(4)	1.71(4)	2.535(5)	172(5)
Ow19-H19a····O6 ⁱⁱ	0.91(4)	1.88(4)	2.762(4)	163(5)
Ow19-H19bO4	0.86(5)	2.25(5)	3.075(5)	160(5)

TABLE 6. Hydrogen-bond geometry in the structure of meisserite.

Symmetry codes: (ii) x+1, y, z; (vi) -x, -y+1, -z.

contain bidentate linkages between uranyl pentagonal bipyramids and sulfate tetrahedra, which have not been observed in the structures of natural minerals. The protonated sulfate group is rare in mineral structures (Hawthorne *et al.*, 2000). Those minerals known to contain SO₃OH groups in their structures include matteuccite (Catti *et al.*, 1975), mercallite (Payan and Haser, 1976), letovicite (Leclair *et al.*, 1985) and mitryaevaite (Ankinovich *et al.*, 1997; Cahill *et al.*, 2001). Prior to the discovery of meisserite and several other new Na-bearing uranyl-sulfate minerals at the Blue Lizard mine, natrozippeite, Na₅[(UO₂)₈(SO₄)₄O₅(OH)₃](H₂O)₁₂ (Frondel *et al.*, 1976; Burns *et al.*, 2003), was the only known Na-bearing uranyl-sulfate mineral. That made the identification of natrozippeite in the geological material seemingly "straightforward", often based only on qualitative EDS analyses (see e.g. Stefaniak *et al.*, 2009). With the discovery of



FIG. 3. The crystal structure of meisserite viewed along [100]. The infinite chains composed of uranyl pentagonal bipyramids (blue) and sulfate tetrahedra (yellow) are linked by $Na\Phi_n$ polyhedra and S4 sulfate tetrahedra into a 3D framework with additional linkage provided by hydrogen bonds (blue dashed lines).

	U	S1	S2	S3	$\mathbf{S4}$	Na1	Na2	Na3	Na4	Na5	Na6	H16	H19a	H19b	ΣBV
01 02 03	0 50	1.61 1.58 1.52 1.36				$\begin{array}{c} 0.23\times2 \\ 0.28\times2 \\ \end{array}$	0.21 0.04 0.22		0.22 0.21		0.05			017	1.87 2.07 2.23 2.13
006 006 006	0.48	06.1	1.59 1.50 1.47					0.22×2 0.08×2 0.18×2	0.00	0.15 0.08	0.26		0.25	11.0	2.13 2.00 2.03 2.03
010	050			1.62 1.53			0.21	→1 < 01.0	0.25 0.17	$0.18 \\ 0.17$					2.05 2.08 2.08
012	0.52			1.44	1.67					$0.09 \\ 0.19$	0.15				2.05 2.05 2.01
014 015 0H16	1 73				1.18 1.18	$0.07 \times 2 \downarrow$	0.19, U.U	~	0.07	11 0	0.25 0.14	0.76			1.84 2.07 2.08 1.07
018 0w19	1.70							$0.06 \times 2 \downarrow$	01.0	11.0	0.16	0.30	0.70	0.73	1.76 1.89
ΣBV	6.02	6.07	5.97	6.05	6.01	1.16	1.06	1.08	1.13	0.97	1.01	1.06	0.95	06.0	
Values are taken from	given in va Burns <i>et al</i>	lence units	s (vu). ΣB Na ⁺ -O. S ⁶	V = sum o $^{6+}-O bonc$	of bond-v	/alences inc hs taken fr	cident at tl om Brown	he atomic si and Altern	te; ×2↓ = 1985	= multiplic	sity. U^{6+} -	O bond str 9. $h = 0.92$	rengths (r _c 4) from Bi	= 2.045, 1	b = 0.51

TABLE 7. The bond-valence analysis for meisserite.

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meisserite, as well as the other new Na-bearing uranyl sulfates, the identification of Na-bearing uranyl sulfates in natural environments will clearly involve more demanding analytical study, and earlier identifications, based primarily on composition, require reassessment.

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