

Meitnerite, $(\text{NH}_4)(\text{UO}_2)(\text{SO}_4)(\text{OH})\cdot 2\text{H}_2\text{O}$, a new uranyl-sulfate mineral with a sheet structure

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Abstract: Meitnerite (IMA2017-065), $(\text{NH}_4)(\text{UO}_2)(\text{SO}_4)(\text{OH})\cdot 2\text{H}_2\text{O}$, is a new mineral from the Green Lizard mine in Red Canyon, San Juan County, Utah, USA, where it occurs as a secondary alteration phase. It occurs on partially recrystallized quartz grains in association with beshtauite and gypsum. Meitnerite occurs as intergrowths of tabular crystals, flattened on $\{01\bar{1}\}$, up to about 80 μm in diameter and 30 μm thick. The mineral is slightly greenish yellow and transparent with a vitreous lustre and very pale yellow streak. It exhibits greenish-white fluorescence in 405 nm light. Crystals are brittle with irregular fracture, and a perfect cleavage on $\{01\bar{1}\}$. The Mohs' hardness is *ca.* 2. The calculated density is 3.320 $\text{g}\cdot\text{cm}^{-3}$. At room temperature, the mineral is slowly soluble in H_2O and very rapidly soluble in dilute HCl. Optically, meitnerite is biaxial (–), with $\alpha = 1.568(2)$, $\beta = 1.589(2)$, $\gamma = 1.607(2)$ (white light); $2V = 84(1)^\circ$. The dispersion is $r > v$, moderate, The optical orientation is $X^\wedge b = 26^\circ$, $Y^\wedge a = 15^\circ$, $Z^\wedge c = 53^\circ$. The pleochroism is X nearly colourless, Z pale green yellow, Y light green yellow; $X < Z < Y$. Electron-microprobe analyses gave the empirical formula $(\text{NH}_4)_{1.01}\text{Na}_{0.07}(\text{U}_{0.97}\text{O}_2)(\text{S}_{1.03}\text{O}_4)[(\text{OH})_{0.93}\text{O}_{0.07}]\cdot 2\text{H}_2\text{O}$, based on 9 O *apfu*. Meitnerite is triclinic, $P\bar{1}$, $a = 6.7964(2)$, $b = 8.0738(3)$, $c = 9.2997(7)$ Å, $\alpha = 113.284(8)$, $\beta = 99.065(7)$, $\gamma = 105.289(7)^\circ$, $V = 431.96(5)$ Å³ and $Z = 2$. The crystal structure, refined to $R_1 = 0.013$ for 1871 observed reflections [$I > 2\sigma(I)$], contains uranyl sulfate sheets based on the phosphuranylite anion topology. The interlayer region contains an NH_4^+ group and two H_2O groups.

Key-words: meitnerite; new mineral; crystal structure; uranyl sulfate; phosphuranylite anion topology; Green Lizard mine, Red Canyon, Utah, USA.

1. Introduction

Uranium mining in Red Canyon in the White Canyon district of south-eastern Utah (USA) ceased nearly four decades ago. In the intervening years, the relatively high humidity underground has produced a wide variety of secondary phases in efflorescent crusts on tunnel walls. Our interest in the secondary mineralization of the Blue Lizard mine began about six years ago. Our investigations have now yielded 18 new mineral species from that mine, with several others still under study. We have more recently expanded our efforts to several nearby mines including the Green Lizard, Giveaway-Simplot and Markey mines, which all have geology and mineralogy similar to the Blue Lizard mine. We have provided a brief synopsis of the history of uranium mining in the area in our descriptive paper on shumwayite, a new mineral found at both the Green Lizard and Giveaway-Simplot mines (Kampf *et al.*, 2017). Herein, we describe meitnerite, the fourth new mineral species from the Green Lizard mine.

Meitnerite is named for Austrian-Swedish physicist Lise Meitner (1878–1968) who, with Otto Hahn and his assistant Fritz Straßmann, was responsible for the discovery of nuclear fission (of uranium) in 1938 and explained the physical process. In 1926 Meitner became Professor of Physics at the University of Berlin, and in 1936 was appointed head of the physics department at the Kaiser Wilhelm Institute. Increased anti-Jewish activities by the Nazi regime forced her to flee to Sweden whose citizenship she adopted. Less well known is that in 1922, prior to the determination of nuclear fission with Hahn, Meitner discovered the Auger effect a year prior to its independent discovery by Pierre Auger who is often credited with the discovery. In her later life, Meitner was recognized with many awards and honors and, in 1997, chemical element 109 was named meitnerium; however, she was overlooked in 1944 when the Nobel Prize in Chemistry was awarded to Otto Hahn alone for the discovery of nuclear fission.

The new mineral and its name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical

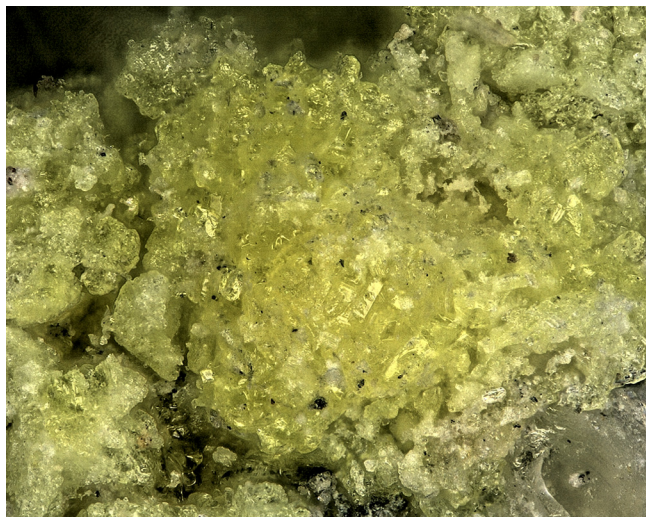


Fig. 1. Intergrowth of greenish-yellow meitnerite tablets (centre) on and surrounded by yellowish-green beshtauite with gypsum on quartz. The field of view is 0.8 mm across.

Association (IMA2017-065). The description is based on one holotype specimen, which is deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue number 66623.

2. Occurrence

Meitnerite was discovered on a specimen collected underground in the Green Lizard Mine (37°34'37.10" N 110°17'52.80" W) 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 geology is similar to that of the Blue Lizard mine (Chenoweth, 1993; Kampf *et al.*, 2015a). Mineralized channels are in the Shinarump member of the Chinle Formation (late Triassic). The Shinarump member consists of medium- to coarse-grained sandstone, conglomeratic sandstone beds and thick siltstone lenses. Accumulations of wood and other plant material in the channels provided reducing environments that caused the deposition of the ore minerals, which are found as replacements of the 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. The NH_4^+ , essential to meitnerite and several other secondary phases (see below), presumably derives from the organic matter noted above.

Meitnerite is a very rare mineral, found on only one small specimen in association with beshtauite (Pekov *et al.*, 2014) and gypsum on quartz. Besides meitnerite and beshtauite, other secondary NH_4 -bearing phases found in the Green Lizard mine include ammoniozippeite (Kampf *et al.*, 2018a), boussingaultite, greenlizardite (Kampf *et al.*, 2018b). Other secondary minerals found in the Green

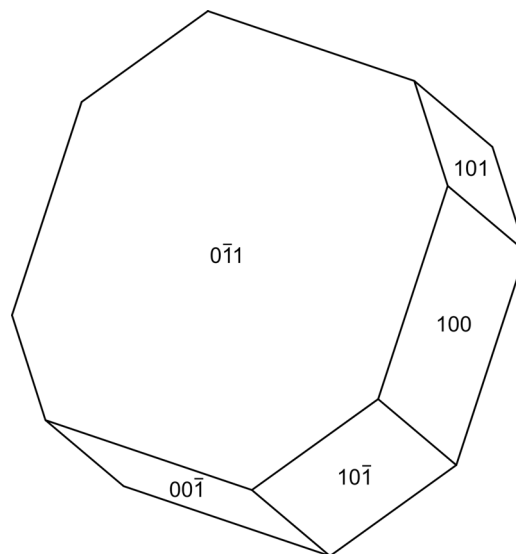


Fig. 2. Crystal drawing of meitnerite; clinographic projection in non-standard orientation.

Lizard mine assemblage include arsenuranospathite, bobcockite (Kampf *et al.*, 2015b), calcite, dickite, fermiite (Kampf *et al.*, 2015c), johannite, magnesioleydetite (Kampf *et al.*, 2018c), metakahlerite, nováčekite-II, natrozippeite, oppenheimerite (Kampf *et al.*, 2015c), plášilite (Kampf *et al.*, 2015a), rozenite, shumwayite (Kampf *et al.*, 2017), straßmannite (Kampf *et al.*, 2018c), sulfur, wetherillite (Kampf *et al.*, 2015b) and other potentially new uranyl sulfate minerals, currently under study.

3. Physical and optical properties

Meitnerite occurs as intergrowths of tabular crystals up to about 80 μm in diameter and 30 μm thick (Fig. 1). Tablets are flattened on $\{01\bar{1}\}$; the forms $\{01\bar{1}\}$ and $\{001\}$ were measured by reflected-light goniometry and the additional forms $\{100\}$, $\{101\}$ and $\{101\bar{1}\}$ (Fig. 2) are likely based upon crystal morphology observed during optical and single-crystal X-ray diffraction studies. No twinning was observed. Crystals are slightly greenish yellow and transparent with a vitreous lustre and very pale yellow streak. The mineral fluoresces greenish white in 405 nm light. Crystals are brittle with irregular fracture and a perfect $\{01\bar{1}\}$ cleavage. The Mohs' hardness is estimated to be about 2. The density could not be measured because of the scarcity and small size of crystals, and their solubility in Clerici solution. The calculated density is 3.320 $\text{g}\cdot\text{cm}^{-3}$, based on the empirical formula. At room temperature, the mineral is slowly soluble in H_2O and very rapidly soluble in dilute HCl. Optically, meitnerite is biaxial (–), with the indices of refraction $\alpha=1.568(2)$, $\beta=1.589(2)$ and $\gamma=1.607(2)$ measured in white light. The $2V$ measured directly on a spindle stage is $84(1)^\circ$; the calculated $2V$ is 84.5° . The dispersion is $r > v$, moderate. The optical orientation is $X \wedge \mathbf{b}=26^\circ$, $Y \wedge \mathbf{a}=15^\circ$, $Z \wedge \mathbf{c}=53^\circ$. The pleochroism is X nearly colourless, Z pale green

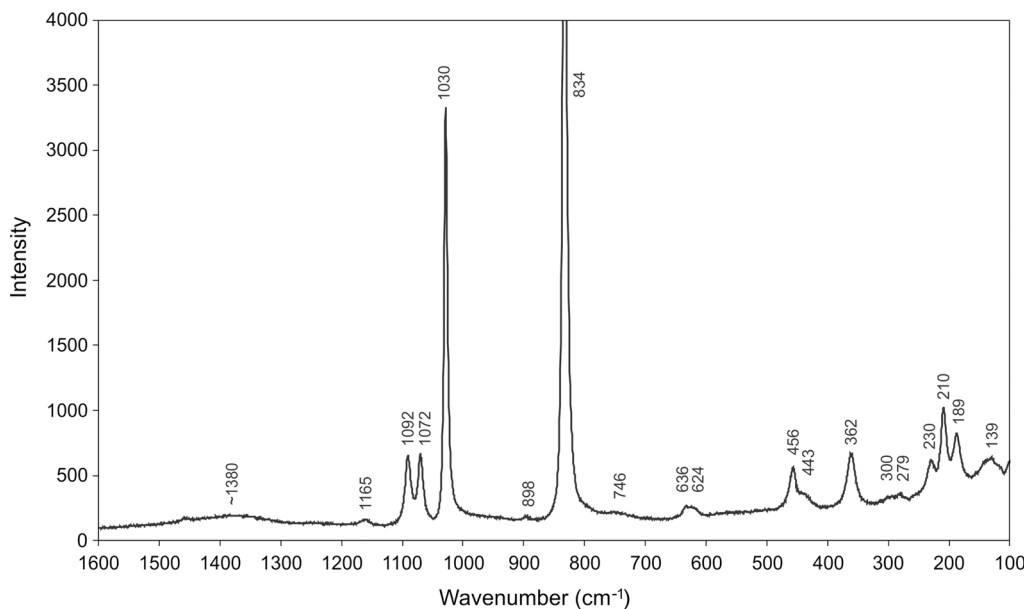


Fig. 3. Raman spectrum of meitnerite recorded using a 785 nm diode laser.

yellow, Y light green yellow; $X < Z < Y$. The Gladstone–Dale compatibility, $1 - (K_P/K_C)$, (Mandarino, 2007) is -0.014 (superior) based upon the empirical formula and -0.009 (superior) based on the ideal formula, in both cases using $k(\text{UO}_3) = 0.118$, as provided by Mandarino (1976).

4. Raman spectroscopy

Raman spectroscopy was conducted on a Horiba XploRA PLUS. Pronounced fluorescence was observed using a 532 nm diode laser; consequently, a 785 nm diode laser was utilized. The spectrum, recorded from 1600 to 100 cm^{-1} , is shown in Fig. 3.

The rather broad band centred at approximately 1380 cm^{-1} is related to the ν_2 (δ) H–N–H bending vibration of the NH_4^+ cations. The weak band at 1165 cm^{-1} and the strong bands at 1092 and 1072 cm^{-1} are attributed to split triply degenerate ν_3 antisymmetric stretching vibrations of the SO_4 tetrahedra. A sharp intensive band at 1030 cm^{-1} is assigned to the ν_1 symmetric stretching vibration of the SO_4 tetrahedra. A very weak band at 898 cm^{-1} may be assigned to the ν_3 antisymmetric stretching vibration of the uranyl ion, UO_2^{2+} . A very strong band at 834 cm^{-1} is assigned the ν_1 symmetric U–O stretching vibration of the UO_2^{2+} . A very weak band at 746 cm^{-1} can be attributed to the libration mode of the H_2O molecule. The inferred U–O bond-lengths (after Bartlett & Cooney 1989) for the uranyl ion of $\sim 1.78 \text{ \AA}$ (from ν_1) and 1.74 (from ν_3) are in line with those derived from the X-ray study (this study). The value inferred from the ν_3 , active in Raman due to lowering of the factor group, should be considered an approximation only.

Weak Raman composite bands at 636 and 624 cm^{-1} are attributed to the ν_4 (δ) triply degenerated antisymmetric stretching vibrations of SO_4 tetrahedra. The Raman band at 456 with a shoulder at 443 cm^{-1} is related to the split ν_2 (δ) doubly degenerate bending vibrations of the SO_4 group.

The band at 362 cm^{-1} can be attributed to Na–O stretching vibrations (cf. Kampf *et al.*, 2015b,c; Plášil *et al.*, 2010, 2016; Volkovich *et al.*, 1998), as the Na content is probably variable among the studied crystals (see chemical analysis). It might also be related to the $\nu_{\text{Rotational}}$ of the NH_4^+ (Heyns *et al.*, 1987). There are two other peaks, at 300 and 279 cm^{-1} , that can be connected with these modes. The two-component strong Raman band at 210 and 189 cm^{-1} , and most probably also a band at 230 cm^{-1} , are related to the overlapping ν_2 (δ) doubly degenerate bending vibration of the UO_2^{2+} and U–O_{eq}–ligand stretching modes (cf. Bullock & Parret, 1970; Ohwada, 1976; Brittain *et al.*, 1985; Plášil *et al.*, 2010). The weak band at 139 cm^{-1} can be assigned to unclassified lattice modes, most probably skeletal vibrations of the whole sheets of polyhedra.

5. Chemical composition

Chemical analyses 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. Analytical conditions were 15 kV accelerating voltage, 10 nA beam current and a beam diameter of $5 \mu\text{m}$. Counting times were 30 s on peak and 30 s on background for each element. Raw X-ray intensities were corrected for matrix effects with a $\varphi\rho(z)$ algorithm (Pouchou & Pichoir, 1991). A time-dependent intensity correction was applied to Na; the N intensity was time independent. The N concentration was corrected for the partial overlap of the U N4–N6 emission line on the N $K\alpha$ peak.

Meitnerite was very challenging to analyze. It was not possible to obtain a good polish and some beam damage was noted. A total of ten analyses on four crystals were attempted; however, only one analysis was deemed of sufficient quality to report. Because insufficient material is

Table 1. Chemical composition (wt%) for meitnerite based on one analysis.

Constituent	Analysis	Probe standard	Normalized
(NH ₄) ₂ O	5.53	syn. Cr ₂ N	6.07
Na ₂ O	0.41	albite	0.45
SO ₃	17.44	celestine	19.13
UO ₃	58.40	syn. UO ₂	64.06
H ₂ O*			10.29
Total			100.00

* Based on structure.

available for a direct determination of H₂O, it has been calculated based upon the structure determination. The results for the single good analysis are given in Table 1. In spite of the chemical analytical problems, including the very low total for the one reported analysis, the excellent structure refinement (see below), which allowed the location of all H atoms, leaves no doubt regarding the essential composition of the mineral. The superior Gladstone-Dale compatibility provides further support.

Table 2. Powder X-ray diffraction data (*d* in Å) for meitnerite. Only calculated lines with *I* > 2 are listed.

<i>I</i> _{obs}	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>I</i> _{calc}	<i>hkl</i>	<i>I</i> _{obs}	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>I</i> _{calc}	<i>hkl</i>
100	7.15	7.1331	100	0 $\bar{1}$ 1			2.2477	2	$\bar{2}$ 22
		6.9208	2	010	7	2.242	2.2403	2	$\bar{2}$ 32
30	6.36	6.2632	21	100			2.2329	3	$\bar{3}$ 10
			18	$\bar{1}$ 01	6	2.207	2.2131	2	$\bar{2}$ 13
36	5.85	{ 5.8776	18	$\bar{1}$ 10			2.2101	4	013
		{ 5.7939	14	$\bar{1}$ $\bar{1}$ 1			2.1802	3	$\bar{2}$ 11
21	5.038	4.9921	11	$\bar{1}$ $\bar{1}$ 1	10	2.172	2.1759	2	$\bar{2}$ $\bar{2}$ 1
15	4.483	4.4647	17	011			2.1644	3	$\bar{3}$ 20
14	4.390	4.3798	12	002			2.1445	4	$\bar{1}$ 33
15	4.085	4.0805	3	$\bar{1}$ 02	10	2.138	2.1424	3	$\bar{1}$ 31
		4.0022	3	0 $\bar{2}$ 1			2.1314	4	$\bar{3}$ 02
10	3.873	{ 3.8911	11	$\bar{1}$ $\bar{1}$ 2			2.1025	2	$\bar{2}$ 23
		{ 3.8516	7	$\bar{1}$ $\bar{2}$ 1			2.0877	2	$\bar{3}$ 00
8	3.818	3.7813	17	0 $\bar{2}$ 2	10	2.0809	2.0807	2	$\bar{2}$ 31
19	3.569	3.5666	5	$\bar{1}$ $\bar{1}$ 2			2.0743	2	$\bar{1}$ $\bar{2}$ 4
		3.5247	12	020			2.0671	3	$\bar{3}$ $\bar{1}$ 1
18	3.451	3.4604	19	$\bar{2}$ 10	4	2.0517	2.0463	2	$\bar{2}$ $\bar{1}$ 4
20	3.340	3.3392	15	$\bar{2}$ 01			2.0402	2	004
17	3.257	{ 3.2640	3	$\bar{1}$ $\bar{2}$ 2	5	1.9844	1.9809	2	$\bar{1}$ 41
		{ 3.2605	15	$\bar{1}$ 12	2	1.9436	1.9311	2	$\bar{1}$ 43
12	3.185	3.1749	14	111	10	1.9274	1.9277	7	$\bar{3}$ 22
21	3.075	3.0749	3	0 $\bar{1}$ 3			1.9114	4	$\bar{1}$ 23
13	3.040	{ 3.0529	14	102	6	1.9063	1.9093	2	043
		{ 3.0335	11	$\bar{1}$ 21	11	1.8899	1.8928	3	$\bar{3}$ 01
10	3.001	2.9911	2	012			1.8886	4	$\bar{3}$ 13
		2.9694	4	$\bar{1}$ $\bar{2}$ 2			1.8848	3	113
		2.9598	2	0 $\bar{2}$ 3			1.8610	2	$\bar{1}$ 14
7	2.872	2.8723	5	$\bar{2}$ 21	7	1.8487	1.8560	3	$\bar{1}$ 22
11	2.826	{ 2.8305	9	$\bar{1}$ 03			1.8345	4	$\bar{3}$ 31
		{ 2.8178	5	$\bar{2}$ 12	11	1.8293	1.8334	3	$\bar{3}$ $\bar{1}$ 2
		{ 2.7118	4	$\bar{2}$ $\bar{1}$ 2			1.8318	2	$\bar{1}$ 32
7	2.706	{ 2.6983	4	201			1.8256	3	310
		{ 2.6716	4	$\bar{1}$ 20			1.8064	2	203
11	2.647	{ 2.6522	6	$\bar{2}$ 21			1.7904	2	104
		{ 2.6396	2	$\bar{1}$ $\bar{2}$ 3	10	1.7863	1.7874	2	$\bar{2}$ 43
		{ 2.6245	3	$\bar{1}$ 32			1.7833	3	044
		{ 2.5872	2	0 $\bar{3}$ 2			1.7787	2	023
8	2.576	{ 2.5775	4	$\bar{1}$ $\bar{1}$ 3			1.7383	2	$\bar{3}$ 04
		{ 2.5744	3	0 $\bar{3}$ 1	5	1.7424	1.7332	2	$\bar{1}$ 42
		2.5466	3	$\bar{2}$ 10			1.7223	2	$\bar{1}$ 35
		2.5318	5	$\bar{2}$ $\bar{1}$ 2	7	1.7223	1.7190	2	131
2	2.473	2.4730	5	0 $\bar{3}$ 3					
5	2.377	2.3777	3	$\bar{2}$ 30	8	1.6995	1.7094	2	$\bar{2}$ 34
		{ 2.2918	2	$\bar{1}$ $\bar{1}$ 4			1.6965	2	411
7	2.286	{ 2.2822	3	0 $\bar{2}$ 4			1.6696	2	$\bar{4}$ 20
		{ 2.2713	2	$\bar{3}$ 11	13	1.6672	1.6660	4	$\bar{3}$ 21
		{ 2.2522					1.6629	2	$\bar{1}$ 41
							1.6563	2	$\bar{3}$ 40

Table 3. Data collection and structure refinement details for meitnerite.

Diffractometer	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	(NH ₄)(UO ₂)(SO ₄)(OH)·2H ₂ O
Space group	$P\bar{1}$
Unit-cell dimensions	$a = 6.7964(3)$ Å $\alpha = 113.284(8)^\circ$ $b = 8.0738(3)$ Å $\beta = 99.065(7)^\circ$ $c = 9.2997(7)$ Å $\gamma = 105.289(7)^\circ$
V	$431.96(5)$ Å ³
Z	2
Density (for above formula)	3.361 g·cm ⁻³
Absorption coefficient	19.052 mm ⁻¹
$F(000)$	392
Crystal size	$60 \times 50 \times 30$ µm
θ range	4.49 to 27.46°
Index ranges	$-8 \leq h \leq 8$, $-10 \leq k \leq 10$, $-12 \leq l \leq 12$
Reflections collected/unique	7547/1931; $R_{\text{int}} = 0.024$
Reflections with $I > 2\sigma I$	1871
Completeness to $\theta = 27.46^\circ$	98.0%
Refinement method	Full-matrix least-squares on F^2
Parameter/restraints	136/17
GoF	1.106
Final R indices [$F > 4\sigma(F)$]	$R_1 = 0.0132$, $wR_2 = 0.0305$
R indices (all data)	$R_1 = 0.0138$, $wR_2 = 0.0307$
Largest diff. peak/hole	$+1.15/-0.72$ e Å ⁻³

$$R_{\text{int}} = \frac{\sum |F_o^2 - F_o^2(\text{mean})|}{\sum [F_o^2]}. \text{GoF} = S = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{(n - p)} \right\}^{1/2}.$$

$$R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}, wR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]} \right\}^{1/2}.$$

$$w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP] \text{ where } a \text{ is } 0.0155, b \text{ is } 0.1432 \text{ and } P \text{ is } [2F_c^2 + \text{Max}(F_o^2, 0)]/3.$$

The empirical formula (calculated on the basis of 9 O *apfu*) is (NH₄)_{1.01}Na_{0.07}(U_{0.97}O₂)(S_{1.03}O₄)[(OH)_{0.93}O_{0.07}]·2H₂O. The ideal formula is (NH₄)(UO₂)(SO₄)(OH)·2H₂O, which requires (NH₄)₂O 5.96, SO₃ 18.31, UO₃ 65.43, and H₂O 10.30, total 100 wt%.

6. X-ray crystallography and crystal-structure determination

Powder X-ray diffraction data for meitnerite were obtained on a Rigaku R-Axis Rapid II curved-imaging-plate microdiffractometer utilising monochromatised MoK α radiation. 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.). Data are given in Table 2. The unit-cell parameters refined from the powder data using JADE 2010 with whole-pattern fitting are $a = 6.774(8)$, $b = 8.031(7)$, $c = 9.269(7)$ Å, $\alpha = 113.22(4)$, $\beta = 99.11(4)$, $\gamma = 105.37(4)^\circ$ and $V = 426.7(7)$ Å³.

Single-crystal structure data were obtained on the same instrument noted above. The Rigaku CrystalClear software package was used for processing of structure data, including the application of an empirical multi-scan absorption correction using ABCOR (Higashi, 2001). The structure was solved using SIR2011 (Burla *et al.*, 2012). SHELXL-2013 (Sheldrick, 2015) was used for the

refinement of the structure. Difference Fourier syntheses located all H atom positions, which were then refined with soft restraints of 0.82(3) Å on the O–H distances and 1.30(3) Å 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 3, atom coordinates and displacement parameters in Table 4, selected bond distances in Table 5 and a bond valence analysis in Table 6. The Crystallography Information File (CIF), including reflection data, is available online as Supplementary Material linked to this article on the GSW website of the journal, <https://pubs.geoscienceworld.org/eurjmin>.

7. Discussion of the structure

The U sites in the structure of meitnerite are surrounded by seven O atoms forming a squat UO₇ pentagonal bipyramid. This is the most typical coordination for U⁶⁺, particularly in uranyl sulfates, where the two short apical bonds of the bipyramid constitute the UO₂ uranyl group. In the structure of meitnerite, pairs of pentagonal bipyramids share a common edge, forming dimers. The dimers are linked by sharing corners with SO₄ groups, yielding a [(UO₂)₂(SO₄)₂(OH)₂]²⁻ sheet parallel to {01 $\bar{1}$ } (Fig. 4). This sheet is based on the phosphuranylite anion topology (Burns, 2005), with a ring symbol 6¹5²4²3² (Krivovichev & Burns, 2007). The sheets in johannite, Cu(UO₂)₂(OH)₂(SO₄)₂·8H₂O (Mereiter, 1982), deliensite, Fe(UO₂)₂(SO₄)₂(OH)₂·7H₂O (Plášil *et al.*, 2012), plášilite, Na(UO₂)(SO₄)(OH)·2H₂O (Kampf *et al.*, 2015a) and greenlizardite, (NH₄)Na(UO₂)₂(SO₄)₂(OH)₂·4H₂O (Kampf *et al.*, 2018b), are topologically identical to that in meitnerite; however, these sheets are geometrical isomers, differing in the orientation of the SO₄ groups (Fig. 5). Note that the sheets in meitnerite and johannite are the same geometrical isomer, differing in relatively minor canting of the tetrahedra.

The interlayer region in the meitnerite structure contains an NH₄⁺ group and two H₂O groups (OW8 and OW9). The NH₄⁺ coordinates to eight O sites; six are O atoms in adjacent uranyl-sulfate sheets and two are the interlayer H₂O groups. The NH₄–O bonds and hydrogen bonding serve to link the uranyl-sulfate sheets to one another (Fig. 6). The aforementioned minerals with [(UO₂)₂(SO₄)₂(OH)₂]²⁻ sheets differ in their interlayer constituents and the ways in which these constituents link the sheets together.

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Table 4. Atom coordinates and displacement parameters ($\text{\AA}^2$) for meitnerite.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
U	0.38491(2)	0.29830(2)	0.27561(2)	0.01300(4)
S	0.79886(10)	0.16444(9)	0.08914(8)	0.01497(13)
O1	0.7477(4)	0.2395(3)	−0.0256(3)	0.0273(5)
O2	0.0232(3)	0.2696(3)	0.1904(3)	0.0301(5)
O3	0.6644(3)	0.1890(3)	0.2006(2)	0.0216(4)
O4	0.2374(3)	0.0438(3)	−0.0025(2)	0.0200(4)
O5	0.4513(4)	0.4721(3)	0.2025(3)	0.0259(5)
O6	0.3238(4)	0.1259(3)	0.3512(3)	0.0273(5)
OH7	0.3098(3)	0.5094(3)	0.4991(3)	0.0230(5)
H7	0.241(6)	0.570(5)	0.479(5)	0.028
OW8	0.9331(4)	0.2701(4)	0.5354(3)	0.0345(6)
HW8a	0.962(6)	0.286(6)	0.628(3)	0.041
HW8b	1.033(6)	0.325(6)	0.519(5)	0.041
OW9	1.1019(5)	0.3358(4)	0.8494(3)	0.0366(6)
HW9a	1.170(6)	0.441(4)	0.917(5)	0.044
HW9b	0.998(5)	0.291(6)	0.869(5)	0.044
N	0.6508(5)	−0.1181(5)	0.2985(4)	0.0365(7)
HNa	0.612(6)	−0.156(5)	0.372(4)	0.044
HNb	0.737(5)	0.006(3)	0.364(4)	0.044
HNc	0.721(5)	−0.189(5)	0.249(4)	0.044
HNd	0.541(4)	−0.126(5)	0.234(4)	0.044

	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ²³	<i>U</i> ¹³	<i>U</i> ¹²
U	0.01115(6)	0.01165(6)	0.01072(6)	0.00051(4)	0.00251(4)	0.00357(4)
S	0.0103(3)	0.0138(3)	0.0128(3)	−0.0006(3)	0.0023(2)	0.0035(2)
O1	0.0304(12)	0.0259(12)	0.0249(12)	0.0117(10)	0.0071(9)	0.0096(10)
O2	0.0108(10)	0.0272(12)	0.0300(12)	−0.0045(10)	−0.0005(9)	0.0051(9)
O3	0.0183(10)	0.0272(11)	0.0174(10)	0.0048(9)	0.0087(8)	0.0121(9)
O4	0.0201(10)	0.0154(10)	0.0149(10)	−0.0009(8)	0.0022(8)	0.0060(8)
O5	0.0272(12)	0.0204(11)	0.0293(12)	0.0124(10)	0.0069(10)	0.0067(9)
O6	0.0347(13)	0.0261(12)	0.0248(12)	0.0135(10)	0.0142(10)	0.0106(10)
OH7	0.0164(10)	0.0257(11)	0.0164(10)	−0.0021(9)	0.0003(8)	0.0128(9)
OW8	0.0355(14)	0.0399(15)	0.0291(13)	0.0159(12)	0.0102(11)	0.0145(12)
OW9	0.0420(15)	0.0329(14)	0.0316(14)	0.0139(11)	0.0125(12)	0.0088(12)
N	0.0397(18)	0.0282(16)	0.0440(19)	0.0194(15)	0.0096(15)	0.0129(14)

Table 5. Selected bond distances ($\text{\AA}$) and angles ($^\circ$) for meitnerite.

N–OW9	2.860(4)	U–O5	1.775(2)	S–O1	1.460(2)
N–OW8	2.897(4)	U–O6	1.779(2)	S–O2	1.471(2)
N–O5	2.916(4)	U–OH7	2.337(2)	S–O3	1.477(2)
N–O3	2.945(4)	U–OH7	2.341(2)	S–O4	1.478(2)
N–O1	3.034(4)	U–O2	2.380(2)	$\langle \text{S–O} \rangle$	1.472
N–O4	3.200(4)	U–O3	2.385(2)		
N–O6	3.261(4)	U–O4	2.410(2)		
N–O6	3.308(4)	$\langle \text{U–O}_{\text{Ur}} \rangle$	1.777		
$\langle \text{N–O} \rangle$	3.053	$\langle \text{U–O}_{\text{eq}} \rangle$	2.371		

Hydrogen bonds					
<i>D–H...A</i>	<i>D–H</i>	<i>H...A</i>	<i>D...A</i>	<i>$\langle \text{D–H–A} \rangle$</i>	
OH7–H7...OW8	0.81(2)	2.00(3)	2.799(4)	171(4)	
OW8–HW8a...OW9	0.80(2)	1.96(3)	2.743(4)	166(4)	
OW8–HW8b...OH7	0.78(2)	2.15(3)	2.929(4)	173(5)	
OW9–HW9a...O1	0.78(2)	2.23(3)	2.945(4)	152(4)	
OW9–HW9b...O1	0.79(2)	2.12(3)	2.891(4)	166(4)	

Table 6. Bond-valence analysis for meitnerite. Values are expressed in valence units.*

	NH ₄	U	S	Hydrogen bonds		Σ
				Accepted	Donated	
O1	0.11		1.55	0.14, 0.16		1.96
O2		0.49	1.50			1.99
O3	0.14	0.49	1.48			2.11
O4	0.07	0.46	1.48			2.01
O5	0.15	1.77				1.92
O6	0.06, 0.05	1.76				1.87
OH7		0.54, 0.54		0.15	−0.18	1.05
OW8	0.16			0.18	−0.21, −0.15	−0.02
OW9	0.18			0.21	−0.14, −0.16	0.09
Σ	0.92	6.05	6.01			

* NH₄⁺–O bond valence parameters from Garcia-Rodriguez *et al.* (2000). U⁶⁺–O and S⁶⁺–O bond valence parameters are from Gagné & Hawthorne (2015). Hydrogen-bond strengths based on O–O bond lengths from Ferraris & Ivaldi (1988).

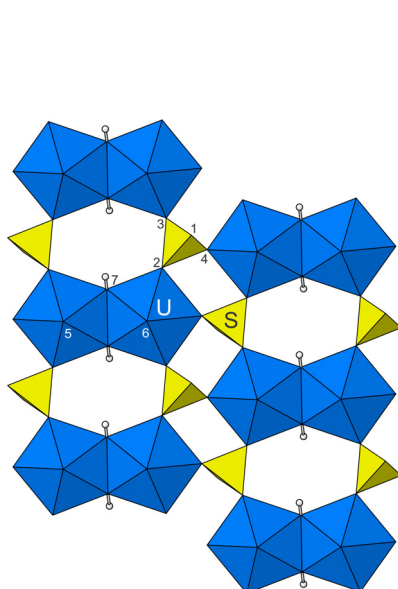


Fig. 4. The uranyl-sulfate sheet in the structure of meitnerite viewed on {011} with [100] vertical. The O sites in the sheet are numbered.

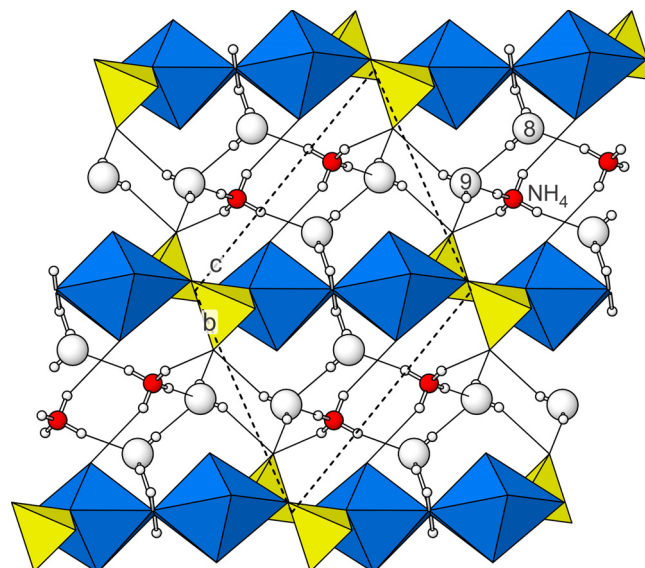


Fig. 6. The structure of meitnerite viewed down **a**. The O sites in the interlayer region are numbered. O–H bonds are shown as sticks; hydrogen bonds are shown as thin black lines. Note that bonds between NH₄ H atoms and nearest O atoms are also shown as thin black lines, even though NH₄ group is treated as a spherical atom in Tables 5 and 6. The unit-cell outline is shown by dashed lines.

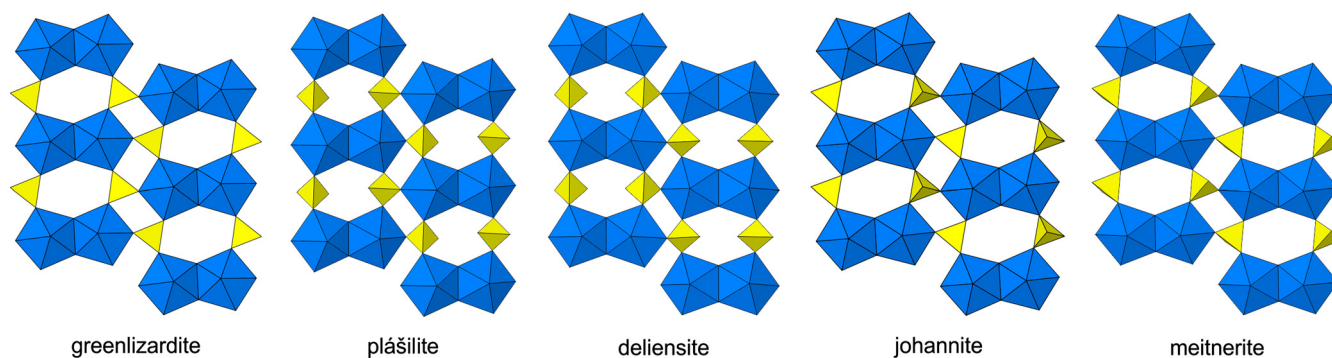


Fig. 5. The uranyl-sulfate sheets in the structures of greenlizardite, plášilite, deliensite, johannite and meitnerite.

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