

Alwilkinsite-(Y), a new rare-earth uranyl sulfate mineral from the Blue Lizard mine, San Juan County, Utah, USA

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[Received 20 April 2016; Accepted 28 July 2016; Associate Editor: Michael Rumsey]

ABSTRACT

The new mineral alwilkinsite-(Y) (IMA2015-097), $Y(H_2O)_7[(UO_2)_3(SO_4)_2O(OH)_3] \cdot 7H_2O$, was found in the Blue Lizard mine, San Juan County, Utah, USA, where it occurs as a secondary alteration phase. The mineral is slightly flexible before brittle failure with splintery fracture and perfect cleavage parallel to [010], has Mohs hardness of $\sim 2-2\frac{1}{2}$, exhibits dull greenish-grey fluorescence and has a calculated density of 3.371 g cm^{-3} . Alwilkinsite-(Y) occurs as yellowish-green needles, elongate on [010], with domatic terminations and exhibits the forms {102}, {301} and {124}. It is optically biaxial (+) with $\alpha = 1.573(1)$, $\beta = 1.581(1)$, $\gamma = 1.601(1)$ (white light), the measured $2V$ is $65.3(1)^\circ$, the dispersion is $r < v$ (weak), the optical orientation is $X = c$, $Y = a$, $Z = b$ and there is no pleochroism. Electron microprobe analyses yielded the empirical formula $(Y_{0.66}Dy_{0.08}Gd_{0.06}Er_{0.05}Nd_{0.03}Yb_{0.03}Sm_{0.02}Ce_{0.01})_{\Sigma 0.94}(H_2O)_7[(UO_2)_3(S_{1.01}O_4)_2O(OH)_3] \cdot 7H_2O$. The eight strongest powder X-ray diffraction lines are [d_{obs} Å(l)(hkl)]: 9.88(100)(101,002), 7.47(13)(102), 5.621(17)(103,201), 4.483(18)(104), 3.886(14)(130,222), 3.322(46) (multiple), 3.223(13)(multiple) and 3.145(16)(034). Alwilkinsite-(Y) is orthorhombic, $P2_12_12_1$, $a = 11.6194(5)$, $b = 12.4250(6)$, $c = 19.4495(14)$ Å, $V = 2807.9(3)$ Å³ and $Z = 4$. The structure of alwilkinsite-(Y) ($R_1 = 0.042$ for $4244 F_o > 4\sigma F$) contains edge-sharing chains of uranyl bipyramids with outlying sulfate tetrahedra that are similar to the chain linkages within the uranyl sulfate sheets of the zippeite structure. Short segments of the uranyl sulfate chains in the alwilkinsite-(Y) structure have the same topology as portions of the uranyl sulfate linkages in uranopilite. Alwilkinsite-(Y) is named for Alan (Al) J. Wilkins, MD (born 1955), the discoverer of the mineral.

KEYWORDS: alwilkinsite-(Y), new mineral, uranyl sulfate, crystal structure, Blue Lizard mine, Utah, USA.

Introduction

ALWILKINSITE-(Y) is the twelfth new uranyl sulfate and the fourteenth new mineral overall to be first described from the Blue Lizard uranium mine in

southeast Utah (Table 1). In an accompanying paper, the fifteenth new mineral from this deposit, chinleite-(Y) $NaY(SO_4)_2 \cdot H_2O$ is described (Kampf *et al.*, 2017a). Alwilkinsite-(Y) is the only new mineral from the Blue Lizard mine that does not contain essential Na and is one of only two new rare-earth-bearing phases to be described from the mine, the other being chinleite-(Y). It is only the second known rare-earth uranyl sulfate mineral,

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<https://doi.org/10.1180/minmag.2016.080.139>

TABLE 1. New mineral species described from the Blue Lizard mine.

Mineral	Structural Formula	Reference
cobaltblöndite	$\text{Na}_2\text{Co}(\text{SO}_4)_2(\text{H}_2\text{O})_4$	Kasatkin <i>et al.</i> (2013)
manganoblöndite	$\text{Na}_2\text{Mn}(\text{SO}_4)_2(\text{H}_2\text{O})_4$	Kasatkin <i>et al.</i> (2013)
meisserite	$\text{Na}_5(\text{SO}_3\text{OH})(\text{H}_2\text{O})[(\text{UO}_2)(\text{SO}_4)_3]$	Plášil <i>et al.</i> (2013)
belakovskiiite	$\text{Na}_7(\text{SO}_3\text{OH})(\text{H}_2\text{O})_3[(\text{UO}_2)(\text{SO}_4)_4(\text{H}_2\text{O})]$	Kampf <i>et al.</i> (2014)
bluelizardite	$\text{Na}_7\text{Cl}(\text{H}_2\text{O})_2[(\text{UO}_2)(\text{SO}_4)_4]$	Plášil <i>et al.</i> (2014)
plášilite	$\text{Na}(\text{H}_2\text{O})_2[(\text{UO}_2)(\text{SO}_4)(\text{OH})]$	Kampf <i>et al.</i> (2015a)
bobcookite	$\text{Na}(\text{H}_2\text{O})_2\text{Al}(\text{H}_2\text{O})_6[(\text{UO}_2)_2(\text{SO}_4)_4(\text{H}_2\text{O})_2] \cdot 8\text{H}_2\text{O}$	Kampf <i>et al.</i> (2015b)
wetherillite	$\text{Na}_2(\text{H}_2\text{O})_6(\text{Mg,Zn})(\text{H}_2\text{O})_6[(\text{UO}_2)_2(\text{SO}_4)_4(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$	Kampf <i>et al.</i> (2015b)
fermiite	$\text{Na}_4(\text{H}_2\text{O})_3[(\text{UO}_2)(\text{SO}_4)_3]$	Kampf <i>et al.</i> (2015c)
oppenheimerite	$\text{Na}_2(\text{H}_2\text{O})_2[(\text{UO}_2)(\text{SO}_4)_2(\text{H}_2\text{O})]$	Kampf <i>et al.</i> (2015c)
klaprothite	$\text{Na}_6(\text{H}_2\text{O})_4[(\text{UO}_2)(\text{SO}_4)_4]$	Kampf <i>et al.</i> (2017b)
péligotite	$\text{Na}_6(\text{H}_2\text{O})_4[(\text{UO}_2)(\text{SO}_4)_4]$	Kampf <i>et al.</i> (2017b)
ottohahnite	$\text{Na}_6(\text{H}_2\text{O})_7[(\text{UO}_2)_2(\text{SO}_4)_5] \cdot 1.5\text{H}_2\text{O}$	Kampf <i>et al.</i> (2017b)
alwilkinsite-(Y)	$\text{Y}(\text{H}_2\text{O})_7[(\text{UO}_2)_3(\text{SO}_4)_2\text{O}(\text{OH})_3] \cdot 7\text{H}_2\text{O}$	This study
chinleite-(Y)	$\text{NaY}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$	Kampf <i>et al.</i> (2017a)

the first being the zippeite-group mineral sejkoraite-(Y), described by Plášil *et al.* (2011) from Jáchymov, Czech Republic.

Alwilkinsite-(Y) is named in honour of Alan (Al) J. Wilkins, MD (born 1955) of Coto de Caza, California. Dr. Wilkins has had a keen interest in microminerals for nearly 20 years and has been very active in the amateur mineral community. He is one of a group of sophisticated and dedicated collectors who in recent years have provided many specimens for scientific research, especially from the Blue Bell claims and Otto Mountain in California (USA), the Silver Coin mine in Nevada (USA) and the Blue Lizard mine in Utah (USA), which have resulted in the descriptions of

numerous new mineral species. Dr. Wilkins collected and provided the only specimen known of the new mineral described herein. He has given permission for the naming of the mineral in his honour. Note that the compound name ‘alwilkinsite’ is proposed rather than the simpler ‘wilkinsite’ to avoid possible confusion with the existing mineral species wilkinsonite.

The new mineral and name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA2015-097). The description is based on one holotype specimen deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue number 65629.



FIG. 1. Alwilkinsite-(Y) with gypsum and natrozippeite on quartz; field of view: 1 mm across.

Occurrence

Alwilkinsite-(Y) 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). The Blue Lizard mine is located ~72 km west of the town of Blanding, Utah, and ~22 km southeast of Good Hope Bay on Lake Powell. Information on the history and geology of the deposit is taken largely from Chenoweth (1993).

Mineralized channels are in the Shinarump member of the Chinle Formation. The Shinarump member consists of medium- to coarse-grained

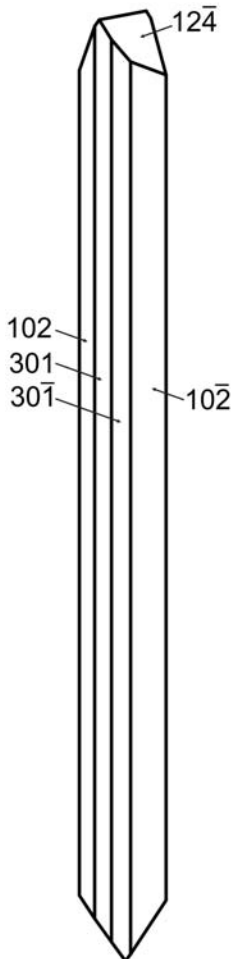


FIG. 2. Crystal drawing of alwilkinsite-(Y), clinographic projection in nonstandard orientation, [010] vertical.

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 in 1978, 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.

Alwilkinsite-(Y) is a very rare mineral, known only from one micromount specimen. On that specimen there are only a few groupings of crystals, as described below. The other secondary minerals found in direct association with alwilkinsite-(Y) are calcite, dickite, gypsum, johannite, natrozippeite and zinczippeite. The bulk of the matrix is



FIG. 3. Bundles of alwilkinsite-(Y) needles with gypsum and natrozippeite on quartz; field of view: 1 mm across.

comprised of subhedral to euhedral, equant quartz crystals that are recrystallized counterparts of the original grains of the sandstone. Other minerals remaining from the original sandstone include feldspar and rare detrital almandine and zircon. An exhaustive list of other secondary minerals found in our studies of the Blue Lizard secondary assemblages can be found in Kampf *et al.* (2017b).

Alwilkinsite-(Y) and the other minerals in the secondary assemblages in the Blue Lizard mine formed at ambient temperature by evaporative processes at the surface of a rock with high relative porosity. The environment is relatively oxidizing (high Eh) and solutions are generally acidic (low pH). The high molar proportion of H₂O in alwilkinsite-(Y) suggests that it formed at moderately high relative humidity. A detailed discussion of the origin and conditions of formation of the uranyl sulfate assemblages at the Blue Lizard mine was provided by Plášil *et al.* (2014) and was more recently summarized by Kampf *et al.* (2017b). As noted above, the only Y-bearing phases thus far observed are the very rare new minerals alwilkinsite-(Y) and chinleite-(Y). The Y, as well as other rare-earth elements (REEs) found in lesser amounts, in these minerals probably existed in the sandstones of the Chinle Formation prior to the deposition of the U ores. Shoemaker *et al.* (1959) noted that Y is intrinsic to the rocks of the Chinle Formation and Newman (1962) suggested that the source of the above-average concentrations of Y in certain areas may be Precambrian rocks of the ancestral Uncompahgre highland. It is also likely that some Y and other REEs were introduced along with U in the ore-forming solutions.

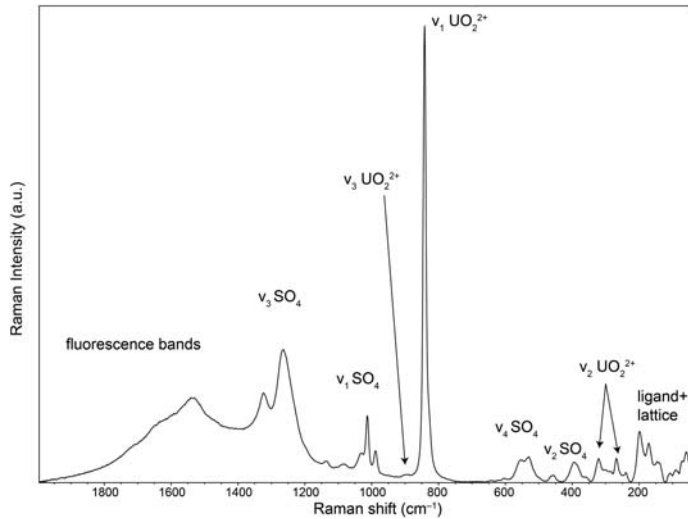


FIG. 4. The Raman spectrum of alwilkinsite-(Y) measured with a red (NIR) laser.

Physical and optical properties

Alwilkinsite-(Y) crystals are long, thin prisms (Fig. 1), elongate on [010], with domatic terminations and exhibit the forms {102}, {301} and {124} (Fig. 2). Prisms are up to ~0.5 mm long and are sometimes intergrown in subparallel bundles (Fig. 3). No twinning was observed.

Crystals are yellow green and transparent with a vitreous lustre. The streak is pale yellow green. The mineral fluoresces greenish grey under a 405 nm laser. (Note that the Blue Lizard uranyl sulfates

typically exhibit very similar fluorescence under the 405 nm laser, as they do under both longwave and shortwave ultraviolet radiation. For sparsely distributed microscopic crystals, the 405 nm laser is the most practical tool for observing fluorescence.) The Mohs hardness is estimated to be between 2 and 2½, based upon the behaviour of crystals when broken. Crystals are slightly flexible before brittle failure with at least one perfect cleavage parallel to [010], possibly {102}, and have splintery fracture. The mineral is insoluble in H₂O, but easily soluble in dilute HCl, in both cases at room temperature. The

TABLE 2. Chemical composition (in wt.%) for alwilkinsite-(Y).

Constituent	Mean	Range	Stand. Dev.	Probe standard (Line)
CaO	0.01	0.00–0.07	0.03	Wollastonite ($K\alpha$)
Y ₂ O ₃	5.49	5.11–5.69	0.21	YPO ₄ ($L\alpha$)
Ce ₂ O ₃	0.15	0.12–0.17	0.02	CePO ₄ ($L\alpha$)
Nd ₂ O ₃	0.38	0.33–0.42	0.03	NdPO ₄ ($L\beta$)
Sm ₂ O ₃	0.29	0.20–0.36	0.06	SmPO ₄ ($L\alpha$)
Gd ₂ O ₃	0.76	0.61–0.94	0.11	GdPO ₄ ($L\alpha$)
Dy ₂ O ₃	1.11	1.10–1.17	0.06	DyPO ₄ ($L\alpha$)
Er ₂ O ₃	0.67	0.45–0.76	0.06	ErPO ₄ ($L\alpha$)
Yb ₂ O ₃	0.37	0.27–0.50	0.06	YbPO ₄ ($L\alpha$)
SO ₃	11.97	10.31–12.41	0.77	SrSO ₄ ($K\alpha$)
UO ₃	63.25	61.06–64.94	1.48	uranophane ($M\alpha$)
H ₂ O*	20.59			
Total	105.04			

*Based on the structure.

TABLE 3. Powder X-ray data (d in Å) for alwilkinsite-(Y).

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
		10.4708	1	0 1 1										
100	9.88	{ 9.9749	63	1 0 1	3	2.563	{ 2.5760	1	2 2 6	9	1.8605	{ 1.8672	4	5 1 6
		{ 9.7248	37	0 0 2			{ 2.5527	1	0 3 6			{ 1.8626	1	4 4 5
3	7.82	{ 7.7784	4	1 1 1			{ 2.5364	1	0 2 7			{ 1.8523	2	0 5 7
13	7.47	{ 7.4575	11	1 0 2	4	2.495	{ 2.5066	3	2 0 7			{ 1.8438	1	3 3 8
9	6.38	{ 6.3942	8	1 1 2			{ 2.4937	1	4 0 4			{ 1.8421	1	3 5 5
17	5.621	{ 5.6615	12	1 0 3			{ 2.4858	1	3 0 6			{ 1.8276	1	5 4 2
		{ 5.5667	6	2 0 1			{ 2.4780	1	1 2 7	5	1.8281	{ 1.8262	1	3 4 7
7	5.252	{ 5.2734	3	1 2 1			{ 2.4382	1	4 2 3			{ 1.8182	1	3 6 1
		{ 5.2628	2	2 1 0			{ 2.4312	1	0 0 8			{ 1.8163	1	6 2 2
11	5.151	{ 5.2354	1	0 2 2	3	2.412	{ 2.4113	1	1 5 1			{ 1.8130	1	4 5 3
		{ 5.1519	10	1 1 3			{ 2.4076	1	0 5 2	7	1.8069	{ 1.8104	1	2 6 4
2	4.654	{ 4.9875	1	2 0 2			{ 2.4046	1	3 4 1			{ 1.8070	1	5 2 6
18	4.483	{ 4.6285	3	2 1 2			{ 2.3866	1	2 4 4			{ 1.8057	2	3 2 9
6	4.314	{ 4.4855	16	1 0 4			{ 2.3576	1	1 5 2			{ 1.7973	1	5 3 5
3	4.137	{ 4.3267	7	2 0 3			{ 2.3513	1	3 4 2			{ 1.7857	1	4 2 8
		{ 4.1458	2	2 2 1	3	2.336	{ 2.3372	1	1 1 8			{ 1.7806	1	6 1 4
		{ 4.0860	1	2 1 3			{ 2.3275	1	4 0 5	4	1.7678	{ 1.7681	2	2 2 10
14	3.886	{ 3.9012	8	1 3 0			{ 2.3142	1	4 2 4			{ 1.7647	1	2 5 7
		{ 3.8892	1	2 2 2			{ 2.2879	2	3 3 5			{ 1.7578	2	3 6 3
7	3.807	{ 3.8251	5	1 3 1	8	2.275	{ 2.2848	1	2 5 0	5	1.7456	{ 1.7437	1	2 6 5
		{ 3.8105	1	0 3 2			{ 2.2755	1	1 5 3			{ 1.7406	1	1 3 10
8	3.639	{ 3.6976	2	3 1 0			{ 2.2692	2	2 5 1			{ 1.7379	1	5 4 4
		{ 3.6366	2	1 2 4	3	2.218	{ 2.2632	2	1 3 7			{ 1.7281	2	6 2 4
8	3.580	{ 3.6208	4	1 3 2			{ 2.2237	2	5 1 2	7	1.7192	{ 1.7258	1	1 6 6
		{ 3.5982	2	3 0 2			{ 2.2213	1	3 1 7			{ 1.7187	2	1 5 8
		{ 3.5714	3	2 1 4			{ 2.1688	1	3 4 4			{ 1.7172	1	4 1 9
		{ 3.5505	2	2 2 3			{ 2.1631	1	5 2 1			{ 1.7096	1	3 6 4
		{ 3.4903	1	0 3 3			{ 2.1545	1	5 1 3			{ 1.7001	2	4 3 8
46	3.322	{ 3.3427	9	1 3 3	8	2.124	{ 2.1364	3	4 3 4	7	1.6918	{ 1.6987	1	4 5 5
		{ 3.3229	21	2 3 1			{ 2.1291	1	0 1 9			{ 1.6934	1	6 3 3
		{ 3.2969	3	0 2 5			{ 2.1240	1	5 2 2			{ 1.6909	1	5 5 1
		{ 3.2867	4	3 2 0			{ 2.1219	2	3 2 7			{ 1.6862	1	4 6 0
13	3.223	{ 3.2408	3	3 2 1	3	2.0839	{ 2.1095	1	2 2 8	4	1.6627	{ 1.6647	1	5 1 8
		{ 3.2323	4	2 0 5			{ 2.0966	1	0 3 8			{ 1.6614	1	4 6 2
		{ 3.2120	3	3 1 3			{ 2.0923	1	2 4 6			{ 1.6420	1	5 5 3
		{ 3.1971	2	2 2 4			{ 2.0708	2	0 6 0			{ 1.6394	1	7 1 1
16	3.145	{ 3.1863	1	2 3 2	9	2.0596	{ 2.0679	1	2 5 4			{ 1.6374	1	5 3 7
		{ 3.1529	9	0 3 4			{ 2.0633	3	1 3 8	3	1.6308	{ 1.6317	1	4 5 6
		{ 3.1224	1	1 0 6			{ 2.0609	1	1 5 5			{ 1.6307	1	0 5 9
		{ 3.1137	2	3 2 2			{ 2.0387	1	1 6 0			{ 1.6138	1	5 4 6
12	3.029	{ 3.0429	3	1 3 4	9	2.0195	{ 2.0276	2	1 6 1			{ 1.6128	1	3 4 9
		{ 3.0295	7	3 0 4			{ 2.0254	1	0 6 2			{ 1.6085	1	3 0 11
11	2.978	{ 2.9919	7	2 3 3			{ 2.0164	3	4 4 3			{ 1.6037	1	7 2 0
		{ 2.9658	2	1 4 1			{ 2.0103	1	1 2 9			{ 1.6027	1	2 7 4
		{ 2.9433	1	3 1 4			{ 1.9991	1	2 1 9			{ 1.5965	2	2 6 7
3	2.905	{ 2.9049	2	4 0 0			{ 1.9953	1	1 6 2			{ 1.5947	1	7 1 3
		{ 2.8739	1	0 2 6			{ 1.9866	1	5 2 4	10	1.5958	{ 1.5930	1	6 4 3
		{ 2.8674	3	2 2 5	9	1.9820	{ 1.9823	5	3 3 7			{ 1.5919	1	3 7 2
6	2.848	{ 2.8289	4	3 3 0			{ 1.9722	1	0 5 6			{ 1.5887	1	6 0 7
							{ 1.9698	1	5 1 5			{ 1.5859	1	2 4 10

(continued)

TABLE 3. (contd.)

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
8	2.799	2.7991	3	4 1 1	6	1.9408	1.9546	1	3 2 8	6	1.5603	1.5759	1	6 1 7
		2.7898	3	1 2 6			1.9448	3	1 6 3			1.5700	1	2 5 9
		2.7833	1	4 0 2			1.9409	1	2 6 1			1.5660	1	2 3 11
10	2.751	2.7600	3	2 1 6	6	1.9111	1.9343	1	5 3 3	3	1.5233	1.5641	1	4 2 10
		2.7546	3	1 3 5			1.9213	2	3 5 4			1.5618	1	4 5 7
		2.7446	1	3 0 5			1.9175	2	4 3 6			1.5571	1	3 2 11
6	2.698	2.7393	1	2 4 0	5	1.8828	1.9135	1	6 1 0	4	1.5034	1.5346	1	1 8 1
		2.7163	3	3 3 2			1.8994	1	5 2 5			1.5275	1	6 5 0
		2.7115	1	0 1 7			1.8958	2	1 1 10			1.5185	1	1 5 10
		2.7023	1	1 0 7			1.8887	1	5 0 6			1.5100	1	4 7 1
		2.6800	3	3 1 5			1.8801	2	1 6 4			1.5056	1	4 3 10
		2.6367	1	2 4 2			1.8775	1	6 1 2			1.5039	1	5 6 3
		2.5926	2	4 1 3										

density could not be measured because the mineral is soluble in Clerici solution. The calculated density is 3.371 g cm⁻³ based on the empirical formula and single-crystal cell parameters.

Optically, alwilkinsite-(Y) is biaxial (+), with $\alpha = 1.573(1)$, $\beta = 1.581(1)$, $\gamma = 1.601(1)$ (measured in white light). The 2V measured using spindle-stage extinction data with EXCALIBR (Gunter

TABLE 4. Data collection and structure refinement details for alwilkinsite-(Y).*

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation/power	MoK α ($\lambda = 0.71075 \text{ \AA}$)/50 kV, 40 mA
Temperature	298(2) K
Structural formula	(Y _{0.66} Dy _{0.34})[(UO ₂) ₃ (SO ₄) ₂ O(OH) ₃](H ₂ O) ₇ ·7H ₂ O
Space group	$P2_12_12_1$
Unit-cell dimensions	$a = 11.6194(5) \text{ \AA}$ $b = 12.4250(6) \text{ \AA}$ $c = 19.4495(14) \text{ \AA}$
V	2807.9(3) \AA^3
Z	4
Density (for above formula)	3.401 g cm ⁻³
Absorption coefficient	19.781 mm ⁻¹
$F(000)$	2576.5
Crystal size (μm)	5 × 5 × 100
θ range	3.19 to 25.03°
Index ranges	-10 ≤ h ≤ 13, -14 ≤ k ≤ 13, -23 ≤ l ≤ 23
Reflections collected/unique	12598/4893; $R_{\text{int}} = 0.074$
Reflections with $F > 4\sigma(F)$	4244
Completeness to $\theta = 25.03^\circ$	99.5%
Refinement method	Full-matrix least-squares on F^2
Restraints/parameters	0/344
Goof	1.024
Final R indices [$F > 4\sigma(F)$]	$R_1 = 0.0422$, $wR_2 = 0.0830$
R indices (all data)	$R_1 = 0.0535$, $wR_2 = 0.0876$
Absolute structure parameter	-0.002(11)
Largest diff. peak/hole	+1.72/-1.75 e \AA^{-3}

* $R_{\text{int}} = \Sigma |F_o^2 - F_c^2(\text{mean})| / \Sigma [F_o^2]$. Goof = $S = \{ \Sigma [w(F_o^2 - F_c^2)^2] / (n-p) \}^{1/2}$. $R_1 = \Sigma |F_o| / \Sigma F_o$. $wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$; $w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0302, b is 0 and P is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.

TABLE 5. Atom coordinates and displacement parameters (\AA^2) for alwilkinsite-(Y).

	<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>
Y*	0.14324(14)	0.17466(13)	0.42601(8)	0.0201(6)	0.0181(10)	0.0243(10)	0.0180(9)	0.0009(7)	0.0001(7)	0.0010(8)
U1	0.61542(7)	0.34108(6)	0.28129(4)	0.0170(2)	0.0179(4)	0.0133(4)	0.0198(4)	-0.0007(4)	-0.0031(4)	0.0014(4)
U2	0.35441(7)	0.48448(6)	0.19984(4)	0.0163(2)	0.0166(4)	0.0138(4)	0.0185(4)	0.0001(3)	-0.0025(3)	-0.0006(3)
U3	0.55600(7)	0.63142(6)	0.32771(4)	0.0158(2)	0.0183(4)	0.0133(4)	0.0157(4)	-0.0001(4)	-0.0010(4)	-0.0002(3)
S1	0.7905(5)	0.7794(5)	0.4039(3)	0.0239(14)	0.029(4)	0.017(3)	0.025(3)	0.000(3)	-0.009(3)	-0.002(3)
S2	0.8680(5)	0.1883(4)	0.3340(3)	0.0193(12)	0.015(3)	0.018(3)	0.025(3)	0.001(2)	0.000(2)	-0.002(2)
O1	0.8717(15)	0.7484(13)	0.3499(9)	0.040(5)	0.031(11)	0.036(10)	0.053(11)	-0.007(9)	0.018(9)	0.002(8)
O2	0.8442(15)	0.7839(13)	0.4720(8)	0.038(4)	0.033(10)	0.036(10)	0.044(11)	0.004(9)	-0.023(9)	-0.012(9)
O3	0.7381(14)	0.8857(12)	0.3888(8)	0.032(4)	0.027(10)	0.023(9)	0.044(10)	0.022(8)	-0.013(8)	0.000(7)
O4	0.6950(13)	0.6996(11)	0.4081(7)	0.020(3)	0.026(9)	0.014(8)	0.019(8)	0.002(7)	-0.002(7)	0.005(7)
O5	0.9221(14)	0.2081(13)	0.2686(8)	0.033(4)	0.024(9)	0.045(10)	0.032(9)	0.007(8)	-0.002(8)	0.006(8)
O6	0.8205(15)	0.0798(13)	0.3344(10)	0.043(5)	0.036(11)	0.025(9)	0.068(13)	0.016(10)	-0.015(10)	-0.006(8)
O7	0.7770(13)	0.2662(12)	0.3478(7)	0.024(4)	0.023(9)	0.036(9)	0.014(8)	-0.004(7)	-0.006(7)	0.011(7)
O8	0.9515(12)	0.1976(12)	0.3917(7)	0.024(4)	0.007(7)	0.036(9)	0.029(9)	0.000(8)	0.000(7)	-0.003(7)
O9	0.7164(13)	0.3910(12)	0.2210(8)	0.028(4)	0.028(9)	0.030(9)	0.026(9)	-0.005(8)	-0.008(7)	-0.006(7)
O10	0.5167(12)	0.2856(11)	0.3420(8)	0.024(4)	0.020(9)	0.013(8)	0.039(10)	-0.008(7)	0.001(7)	-0.005(6)
O11	0.4343(13)	0.5491(11)	0.1343(8)	0.025(4)	0.012(8)	0.014(8)	0.051(10)	-0.001(7)	-0.003(8)	0.001(7)
O12	0.2678(14)	0.4188(13)	0.2635(8)	0.033(4)	0.021(9)	0.037(10)	0.040(11)	-0.004(8)	-0.005(8)	0.000(8)
O13	0.4618(13)	0.6114(11)	0.3989(7)	0.023(4)	0.018(9)	0.023(8)	0.027(8)	0.001(7)	-0.001(7)	-0.008(7)
O14	0.6516(14)	0.6620(13)	0.2569(8)	0.032(4)	0.031(9)	0.034(10)	0.032(9)	0.015(8)	0.001(8)	-0.006(9)
O15	0.5009(12)	0.4855(12)	0.2712(7)	0.021(3)						
OH1	0.6331(10)	0.1567(10)	0.2361(6)	0.014(3)	0.010(7)	0.012(7)	0.021(7)	0.006(6)	0.001(6)	0.004(6)
OH2	0.4805(12)	0.3232(11)	0.1809(7)	0.024(4)	0.030(9)	0.018(8)	0.025(9)	0.005(7)	-0.005(7)	0.008(7)
OH3	0.6670(12)	0.4787(11)	0.3616(7)	0.020(3)	0.022(8)	0.012(7)	0.026(8)	0.004(7)	0.005(6)	0.009(6)
OW1	0.0691(16)	0.0774(13)	0.5165(8)	0.038(4)	0.048(12)	0.044(11)	0.021(9)	0.010(8)	0.000(8)	-0.002(9)
OW2	0.1074(18)	-0.0023(14)	0.3879(8)	0.051(5)	0.087(16)	0.037(11)	0.030(10)	0.003(9)	0.012(10)	0.009(11)
OW3	0.1434(12)	0.1910(12)	0.3054(7)	0.029(4)	0.016(7)	0.050(11)	0.021(8)	0.004(7)	0.003(7)	0.010(7)
OW4	0.2364(16)	0.3391(15)	0.3990(8)	0.044(5)	0.050(12)	0.042(11)	0.041(10)	0.012(10)	0.001(9)	-0.004(10)
OW5	0.2844(15)	0.1780(17)	0.5149(7)	0.047(5)	0.045(11)	0.091(16)	0.007(8)	-0.003(9)	-0.005(8)	-0.017(11)
OW6	0.3240(15)	0.1043(16)	0.3878(9)	0.049(6)	0.020(10)	0.077(15)	0.050(12)	0.000(11)	0.009(8)	0.025(10)
OW7	0.0615(18)	0.3051(12)	0.5069(8)	0.043(5)	0.068(13)	0.031(10)	0.032(10)	-0.006(8)	-0.003(9)	0.017(9)
OW8	0.9899(16)	0.4294(14)	0.2362(11)	0.049(5)	0.033(11)	0.037(11)	0.077(15)	0.008(11)	0.008(10)	0.000(8)
OW9	0.0921(15)	0.8077(12)	0.4564(8)	0.037(4)	0.049(12)	0.025(10)	0.036(10)	0.005(8)	0.000(9)	0.000(8)
OW10	0.9005(17)	0.6164(15)	0.5655(9)	0.048(5)	0.055(13)	0.057(12)	0.034(10)	0.008(9)	-0.019(9)	-0.012(10)
OW11	0.9026(16)	0.5281(13)	0.3537(9)	0.047(5)	0.052(13)	0.029(10)	0.059(12)	0.005(9)	0.001(10)	0.000(9)

(continued)

TABLE 5. (*contd.*)

	<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>
OW12	0.1874(17)	0.6498(17)	0.3608(9)	0.056(5)	0.059(13)	0.067(14)	0.042(11)	0.004(11)	0.020(10)	-0.013(12)
OW13	0.046(2)	0.5147(16)	0.4677(11)	0.066(6)	0.073(15)	0.049(13)	0.076(15)	0.000(12)	0.011(12)	0.017(13)
OW14	0.3338(15)	0.4818(14)	0.4959(9)	0.042(5)	0.042(11)	0.037(11)	0.048(11)	-0.012(9)	0.016(9)	-0.011(9)

* Refined occupancy of Y site is Y/Dy = 0.661/0.339(10)

et al., 2004) is 65.3(1)°; the calculated 2V is 65.3°. Dispersion is $r > v$, weak. No pleochroism was observed. The optical orientation is $X = \mathbf{c}$, $Y = \mathbf{a}$, $Z = \mathbf{b}$.

Raman spectroscopy

The Raman spectrum of alwilkinsite-(Y) is shown in Fig. 4. The strong fluorescence of the material (due to the presence of Y and REEs) required the use of a 780 nm laser for collection of the Raman data. As a result, it was not possible to acquire the O–H stretching region of the spectrum. The broad bands at $\sim 1600 \text{ cm}^{-1}$ are the result of the fluorescence; assignment of some of them as ν_2 (δ) H_2O is unlikely. A similar effect was observed in sejkoraite-(Y) (Plášil *et al.*, 2011). A broader Raman band of medium intensity at 1265 cm^{-1} and also weak bands at 1135 and 1080 cm^{-1} are attributed to the split triply degenerate ν_3 antisymmetric stretching vibrations of the (SO_4) tetrahedra. The Raman band at 1325 cm^{-1} is probably an overtone or a combination band. Sharp Raman bands at 1035 , 1015 and 990 cm^{-1} are attributed to the ν_1 symmetric stretching vibrations of (SO_4) tetrahedra.

A very weak Raman band at 900 cm^{-1} is attributed to the ν_3 antisymmetric stretching vibration of the uranyl ion, $(\text{UO}_2)^{2+}$. The very strong Raman band at 840 cm^{-1} is attributed to the ν_1 symmetric stretching vibration of the uranyl ion. The inferred U–O bond lengths (after Bartlett and Cooney, 1989) for the uranyl ion of 1.77 \AA (ν_1) and 1.79 \AA (ν_3) are consistent with those obtained in the structure determination (see below).

Medium-weak Raman bands at 605 , 555 and 530 cm^{-1} are attributed to the ν_4 (δ) triply degenerate antisymmetric stretching vibrations of the (SO_4) tetrahedra. Weak bands at 465 and 455 cm^{-1} and a broader band at $\sim 380 \text{ cm}^{-1}$, consisting of at least two overlapping bands centred at 395 and 378 cm^{-1} , are related to the split ν_2 (δ) doubly degenerate bending vibrations of the (SO_4) . A suite of overlapping bands below 300 cm^{-1} (320 , 288 , 268 , 240 cm^{-1}) is associated with the ν_2 (δ) doubly degenerate bending vibrations of the UO_2^{2+} (e.g. Bullock and Parret, 1970; Ohwada, 1976; Brittain *et al.*, 1985; Plášil *et al.*, 2010). The high number of bands reflects the large number of symmetrically nonequivalent U sites in the structure. More intense splitting bands at 200 and 170 cm^{-1} are assigned to the U–O_{eq}–ligand stretching (Bullock and Parret, 1970; Plášil *et al.*, 2010). Weak bands at

TABLE 6. Selected bond distances (Å) for alwilkinsite-(Y).

U1–O9	1.771(16)	Y–OW1	2.303(16)	Hydrogen bonds	
U1–O10	1.784(15)	Y–O8	2.343(15)	OH1–OW12	2.81(2)
U1–O15	2.243(13)	Y–OW3	2.355(14)	OH2–OW10	2.74(2)
U1–OH3	2.392(14)	Y–OW2	2.357(18)	OH3–OW11	2.81(2)
U1–OH1	2.462(13)	Y–OW4	2.371(18)	OW1–OH3	2.72(2)
U1–O7	2.463(14)	Y–OW5	2.384(16)	OW1–OW14	2.84(3)
U1–OH2	2.514(14)	Y–OW6	2.393(16)	OW2–OW8	2.80(3)
<U–O _{Ur} >	1.778	Y–OW7	2.451(16)	OW2–OW9	2.72(2)
<U–O _{eq} >	2.415	<Y–O>	2.370	OW3–O5	2.68(2)
				OW3–O14	2.70(2)
U2–O11	1.770(16)	S1–O1	1.463(17)	OW4–O12	2.84(2)
U2–O12	1.792(17)	S1–O2	1.465(16)	OW4–OW14	2.83(2)
U2–O15	2.196(13)	S1–O3	1.484(16)	OW5–O8	3.08(2)
U2–O3	2.373(14)	S1–O4	1.490(16)	OW5–OW7	3.26(3)
U2–O6	2.445(16)	<S1–O>	1.461	OW6–O11	2.92(2)
U2–OH1	2.480(12)			OW6–O14	2.92(2)
U2–OH2	2.509(14)	S2–O5	1.439(16)	OW7–O10	3.19(2)
<U–O _{Ur} >	1.781	S2–O6	1.457(16)	OW7–O11	3.07(2)
<U–O _{eq} >	2.401	S2–O7	1.459(15)	OW8–O1	3.23(2)
		S2–O8	1.488(15)	OW8–O9	3.23(2)
U3–O13	1.783(15)	<S2–O>	1.476	OW9–O2	2.91(2)
U3–O14	1.809(15)			OW9–O4	2.90(2)
U3–O15	2.215(14)			OW10–O2	2.84(2)
U3–OH3	2.387(13)			OW10–OW13	2.84(3)
U3–O4	2.402(14)			OW11–O1	2.76(2)
U3–OH2	2.426(14)			OW11–OW13	2.78(3)
U3–OH1	2.543(12)			OW12–O5	2.91(3)
<U–O _{Ur} >	1.796			OW12–OW9	2.92(3)
<U–O _{eq} >	2.395			OW13–OW10	2.84(3)
				OW13–OW11	2.78(3)
				OW14–O2	2.98(2)
				OW14–O13	2.89(2)

145, 135, 108, 90, 72 and 60 cm⁻¹ are attributed to –O_{eq}–U–O_{eq}– bending (Ohwada, 1976) and to unclassified lattice modes, most probably skeletal vibrations of the entire chains of polyhedra.

Composition

Chemical analyses (seven points on several crystals) were undertaken using a Cameca SX100 electron microprobe (WDS mode, 15 kV, 10 nA, 10 μm beam diameter). Because insufficient material is available for a direct determination of H₂O, it was calculated by stoichiometry. As is typical of highly hydrated phases with weakly held H₂O, alwilkinsite-(Y) partially dehydrates under vacuum during carbon coating and in the microprobe chamber. This H₂O loss results in higher concentrations for the remaining constituents than are to be expected for the

fully hydrated phase; hence, the high analytical total when the calculated H₂O is included. Lanthanum, Pr, Tb, Ho, Tm and Lu were sought, but their contents were below the detection limit of the electron microprobe. No other elements with Z > 8 were observed. Analytical data are given in Table 2.

The empirical formula (calculated on the basis of 3 U and 32 O atoms per formula unit) is (Y_{0.66}Dy_{0.08}Gd_{0.06}Er_{0.05}Nd_{0.03}Yb_{0.03}Sm_{0.02}Ce_{0.01})_{Σ0.94}(H₂O)₇[(UO₂)₃(S_{1.01}O₄)₂O(OH)₃]:7H₂O. The ideal structural formula is Y(H₂O)₇[(UO₂)₃(SO₄)₂O(OH)₃]:7H₂O, which requires Y₂O₃ 8.01, UO₃ 60.84, SO₃ 11.35 and H₂O 19.80, total 100 wt.%.

The Gladstone-Dale compatibility index I – (K_p/K_c) for the empirical formula is –0.015, in the superior range (Mandarino, 2007), using k(UO₃) = 0.118, as provided by Mandarino (1976).

TABLE 7. Bond-valence analysis for alwilkinsite-(Y). Values are expressed in valence units.*

	Y	U1	U2	U3	S1	S2	Hydrogen bonds	Σ
O1					1.55		+0.20, +0.10	1.85
O2					1.54		+0.15, +0.17, +0.13	1.99
O3			0.54		1.46			2.00
O4				0.51	1.44		+0.15	2.10
O5						1.65	+0.24, +0.15	2.04
O6			0.47			1.57		2.04
O7		0.45				1.56		2.01
O8	0.41					1.44	+0.12	1.97
O9		1.72					+0.10	1.82
O10		1.67					+0.10	1.77
O11			1.72				+0.15, +0.12	1.99
O12			1.65				+0.17	1.82
O13				1.68			+0.15	1.83
O14				1.59			+0.23, +0.15	1.97
O15		0.69	0.76	0.73				2.18
OH1		0.45	0.44	0.39			-0.18	1.10
OH2		0.41	0.41	0.49			-0.20	1.11
OH3		0.52		0.52			+0.22, -0.18	1.08
OW1	0.46						-0.22, -0.17	0.07
OW2	0.39						-0.18, -0.22	-0.01
OW3	0.39						-0.24, -0.23	-0.08
OW4	0.38						-0.17, -0.17	0.04
OW5	0.36						-0.10, -0.12	0.14
OW6	0.35						-0.15, -0.15	0.05
OW7	0.30						+0.10, -0.12, -0.10	0.18
OW8							+0.18, -0.10, -0.10	-0.02
OW9							+0.22, +0.15, -0.15, -0.15	0.07
OW10							+0.20, +0.17, -0.17, -0.17	0.03
OW11							+0.18, +0.19, -0.20, -0.19	-0.02
OW12							+0.18, -0.15, -0.15	-0.12
OW13							+0.19, +0.17, -0.17, -0.19	0.00
OW14							+0.17, +0.17, -0.13, -0.15	0.06
Σ	3.04	5.91	5.99	5.91	5.99	6.22		

* S^{6+} -O bond-valence parameter from Brown and Altermatt (1985); Y^{3+} -O from Krivovichev (2012); U^{6+} -O from Burns *et al.* (1997); hydrogen-bond strengths based on O-O bond lengths from Ferraris and Ivaldi (1988).

X-ray crystallography and structure refinement

Powder X-ray studies were done using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatized $MoK\alpha$ radiation ($\lambda = 0.71075 \text{ \AA}$). A Gandolfi-like motion on the ϕ and ω axes was used to randomize the sample and observed d -values and intensities were derived by profile fitting using *JADE 2010* software (Materials Data, Inc.). The powder data presented in Table 3 show good agreement with the pattern calculated from the structure determination.

Unit-cell parameters refined from the powder data using *JADE 2010* with whole pattern fitting are: $a = 11.5874(10)$, $b = 12.4171(10)$, $c = 19.4242(17) \text{ \AA}$ and $V = 2794.8(4) \text{ \AA}^3$.

The single-crystal structure data for alwilkinsite-(Y) were collected at room temperature on a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, also using monochromatized $MoK\alpha$ radiation. The data were processed using the Rigaku *CrystalClear* software package and an empirical (multi-scan) absorption correction was applied using the *ABSCOR* program (Higashi, 2001) in the *CrystalClear* software suite. The

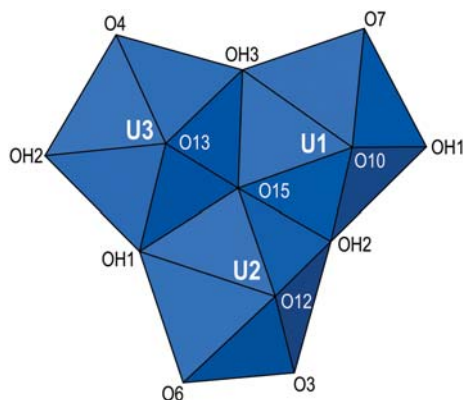


FIG. 5. The $[(\text{UO}_2)_3\text{O}_5(\text{OH})_5]^{9-}$ uranyl trimer in the structure of alwilkinsite-(Y).

structure was solved by direct methods using *SIR2011* (Burla *et al.*, 2012). *SHELXL-2013* (Sheldrick, 2008) was used for the refinement of the structure. The Y site was refined with joint occupancy by Y and Dy, yielding a site scattering value of 192.61 electrons per formula unit (epfu). While significantly higher than that expected based on the chemical analysis, 175.92 epfu, it is still consistent with strong dominance of Y in this site. A difference-Fourier synthesis failed to locate the H atom positions. All atoms were refined with anisotropic-displacement parameters, except for O15 which yielded a negative displacement parameter along the *c* axis; consequently, it was refined with an isotropic displacement parameter in the final cycles. Data collection and refinement details are given in Table 4, atom coordinates and displacement parameters in Table 5, selected bond distances in Table 6, and a bond-valence analysis in Table 7. For the bond-valence analysis, calculations are based upon full occupancy of the Y site by Y. (Note that the weighted average of the bond-valence parameters for the REEs are close to the bond-valence parameters for Y.)

Description and discussion of the structure

The three U sites in the structure of alwilkinsite-(Y) are each surrounded by seven O atoms, forming squat UO_7 pentagonal bipyramids. This is the most typical coordination for U^{6+} , particularly in uranyl sulfates. The two apical O atoms of each bipyramid form short bonds with the U, and this unit comprises the UO_2^{2+} uranyl group. The five equatorial O atoms complete each of the U

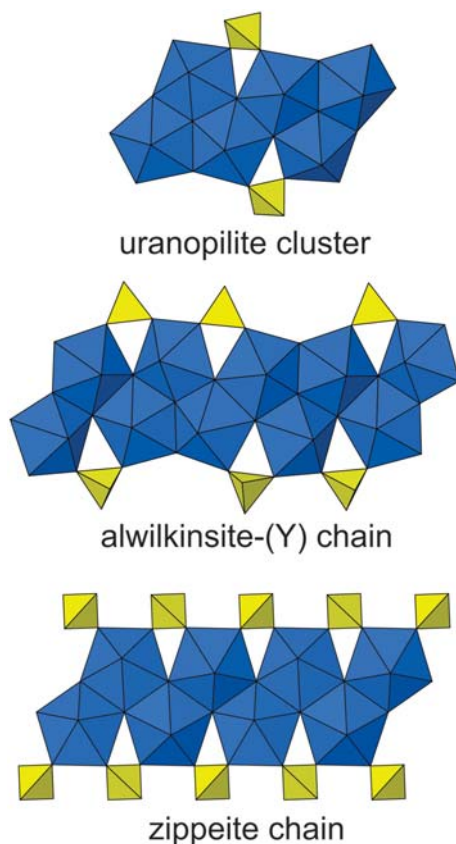


FIG. 6. The edge-sharing uranyl chain decorated by sulfate groups in the structure of alwilkinsite-(Y) compared to the cluster (part of the infinite chain) in the uranopilite structure and the chain in the zippeite structure.

coordinations. The three different UO_7 bipyramids in the structure share a single O atom (O15) and each bipyramid shares two edges (O15–OH1, O15–OH2 and/or O15–OH3) with each of the two other bipyramids to form a $[(\text{UO}_2)_3\text{O}_5(\text{OH})_5]^{9-}$ trimer (Fig. 5). The trimers are linked to one another through OH1–OH2 shared edges between U1 and U3 polyhedra in adjacent trimers to form a chain along [010]. The chain is decorated by two different SO_4 tetrahedra (SiO_4 and S2O_4), which each share corners with UO_7 bipyramids in adjacent trimers. This decorated chain (Fig. 6) has the formula $[(\text{UO}_2)_3(\text{SO}_4)_2\text{O}(\text{OH})_3]^{3-}$. The SiO_4 tetrahedron has two unshared corners, while the S2O_4 tetrahedron shares one corner with the $\text{YO}(\text{H}_2\text{O})_7$ polyhedron and has one unshared corner. The decorated chain with linked Y polyhedron forms a

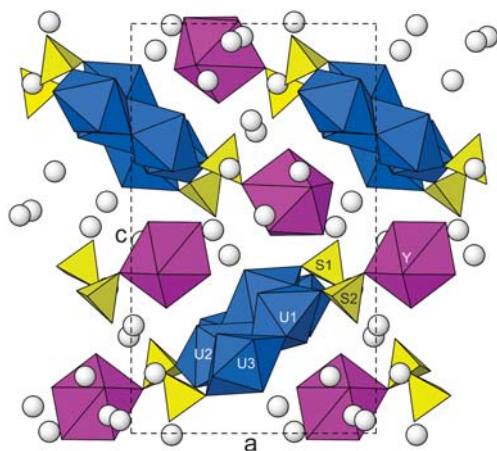


FIG. 7. The structure of alwilkinsite-(Y) viewed along [010], the chain direction. The O atoms of isolated H₂O groups are shown as white spheres. Unit-cell outlines are shown as dashed lines. The complicated hydrogen bond network is not shown; the scheme proposed (Table 6) was based upon a detailed evaluation of O–O distances and geometries, and using an analysis of bond-valence balance (Table 7).

neutral unit of formula $Y(H_2O)_7[(UO_2)_3(SO_4)_2O(OH)_3]$ (Fig. 7). Seven additional isolated H₂O groups complete the complement of structural components. The $Y(H_2O)_7[(UO_2)_3(SO_4)_2O(OH)_3]$ units and isolated H₂O groups are linked only *via* hydrogen bonds. The hydrogen bonding scheme proposed in Table 6 should be considered tentative because, lacking H atom locations, the choices of many of the hydrogen bonds are ambiguous.

There are numerous structures of uranyl sulfates that are based upon chains of polyhedra (cf. Burns, 2005); however, none contain chains with a topology identical to that in the structure of alwilkinsite-(Y). As noted above, the only other known rare-earth uranyl sulfate mineral, sejkoraite-(Y), belongs to the zippeite group. The uranyl sulfate sheet of the zippeite topology contains edge-sharing chains of UO₇ pentagonal bipyramids with outlying SO₄ tetrahedra that somewhat resemble the chain in the alwilkinsite-(Y) structure (Fig. 6); however, the zippeite-type chains do not contain uranyl trimers. The uranyl sulfate chain in the uranopilite structure (in which the chain linkage is through SO₄ tetrahedra) contains a cluster consisting of two uranyl trimers sharing an edge and further decorated by SO₄ tetrahedra. The topology of this cluster is the same as the topology of a section of the alwilkinsite-(Y) chain (Fig. 6).

Although uranopilite has not been recognized in the secondary assemblages at the Blue Lizard mine, it is worth noting that uranyl sulfates, including uranopilite, zippeite-related phases and alwilkinsite-(Y), can be involved in complex hydrolysis reactions. Later phases can be derived from earlier ones by dissolution and hydrolysis in which structures are broken down and reassembled, preserving some distinctive structural features.

Acknowledgements

Two anonymous reviewers and Editorial Board Member Mike Rumsey are thanked for their constructive comments on the manuscript. A portion of this study was funded by the John Jago Trelawney Endowment to the Mineral Sciences Department of the Natural History Museum of Los Angeles County. This research was also financially supported by GACR post-doctoral Grant no. 13-31276P to J.P. and by the long-term project DKRVO 2016-02 of the Ministry of Culture of the Czech Republic (National Museum 00023272) to J.Č.

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