

## Alfredopetrovite, a new selenite mineral from the El Dragón mine, Bolivia

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**Abstract:** Alfredopetrovite,  $\text{Al}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$ , is a new secondary selenite mineral from the El Dragón mine, Antonio Quijarro Province, Potosí Department, Bolivia. The mineral occurs in vugs in a matrix of Co-rich krut'aite–penroseite, dolomite and goethite. Associated minerals are: ahlfeldite, allophane, calcite, chalcomenite, favreauite, felsőbányaite, malachite and molybdomenite. Crystals occur in drusy/scaly coatings and compact balls, the latter to 0.5 mm in diameter. Individual crystals are up to about 0.1 mm across. The Mohs hardness of alfredopetrovite is 2½; it has no cleavage, curved fracture and a vitreous lustre. The calculated density based on the empirical formula is 2.504 g cm<sup>-3</sup>. Alfredopetrovite is uniaxial (+), with  $\omega = 1.554(2)$  and  $\varepsilon = 1.566(2)$  (white light), and exhibits no pleochroism. Electron microprobe analyses gave the empirical formula  $\text{Al}_{1.94}\text{Cu}_{0.07}\text{Ni}_{0.03}\text{Co}_{0.01}\text{Se}_{2.95}\text{O}_{15}\text{H}_{12.16}$ , based on 15 O *apfu*. Alfredopetrovite is hexagonal, space group  $P\bar{6}2c$ , with the unit-cell parameters:  $a = 8.818(3)$  Å,  $c = 10.721(2)$  Å,  $V = 722.0(5)$  Å<sup>3</sup> and  $Z = 2$ . The eight strongest lines in the X-ray powder diffraction pattern are [ $d_{\text{obs}}/\text{Å}$  ( $I$ ) ( $hkl$ ): 7.63(55)(100), 6.22(55)(101), 5.37(26)(002), 4.398(40)(110,102), 3.404(100)(112), 2.783(50)(211), 2.606(22)(203), and 1.6609(26)(410,322,314,116)]. The crystal structure was refined to  $R_1 = 0.0268$  for 240 observed reflections [ $F_o > 4\sigma F$ ]. The structure is comprised of fairly regular  $\text{AlO}_6$  octahedra and  $\text{Se}^{4+}\text{O}_3$  triangular pyramids. Three  $\text{Se}^{4+}\text{O}_3$  pyramids link two adjacent  $\text{AlO}_6$  octahedra forming a  $[\text{Al}(\text{H}_2\text{O})_3]_2(\text{Se}^{4+}\text{O}_3)_3$  cluster structural unit. These structural units are bonded to one another only *via* hydrogen bonds yielding a structure with relatively large channels along [001]. The configuration of the cluster is similar to that of the distinctive unit in the NASICON structure, commonly referred to as a *lantern unit*.

**Key-words:** alfredopetrovite; new mineral; selenite; crystal structure; NASICON structure; El Dragón mine, Bolivia.

### 1. Introduction

The new mineral alfredopetrovite was first recognized during the characterization of the recently described mineral favreauite,  $\text{PbBiCu}_6\text{O}_4(\text{SeO}_3)_4(\text{OH}) \cdot \text{H}_2\text{O}$  (Mills *et al.*, 2014). Detailed study of the minerals associated with favreauite revealed rather indistinct colourless to blue, scaly crystal aggregates on two of the cotype specimens of favreauite. Subsequent examination of additional small pieces turned up several more examples of the new species.

The species is named for Mr. Alfredo Petrov (born 1955). Mr Petrov is a British-born geologist/mineralogist of Russian and German extraction with a bachelor's degree in geology (1982) from San Diego State University (USA) who has lived much of his adult life in Bolivia. He is an avid mineral collector and renowned mineral connoisseur, specializing in rare species, especially from Bolivia, many of which he

has self-collected or obtained by visiting mines and miners. After receiving his degree, he worked as a geologist for the Bolivian government for more than a decade and since then has done free-lance consulting work for both the Bolivian government and mining corporations. Mr. Petrov was the first person to decipher the origin of the several Alto Chapare danburite–boracite–povondraite–magesioriebeckite occurrences in Bolivia as being leached saltdome caprocks (Žáček *et al.*, 1998, 2000), and the Cerro Sapo sodalite deposit, also in Bolivia, as being a carbonatite dyke, rather than a hydrothermal ankerite vein (Hyrsl & Petrov, 1999; Petrov, 2009).

Mr. Petrov generously gives back to the mineralogical community, writing articles for numerous publications including *Rocks and Minerals*, *Mineralogical Record*, *Mineral News* and *Lapis*, and serving as an active manager for *Mindat.org*. He also freely provides specimens for scientific research.

The compound name “alfredopetrovite” has been chosen rather than the simpler “petrovite” because of the similarity of the latter to petrovicite, which also occurs at the El Dragón mine. The mineral and name were approved by the IMA–CNMNC (IMA2015–026) prior to publication. The description is based upon five small cotype specimens. Four cotypes are deposited in the collections of the Natural History Museum of Los Angeles County, Los Angeles, USA: catalogue numbers 64111 (also a cotype for favreaute), 65578, 65579 and 65580. One cotype specimen is housed in the Geosciences collections at Museum Victoria, Australia, registration number M53004 (also a cotype for favreaute).

## 2. Occurrence

The new mineral alfredopetrovite occurs at the El Dragón mine, Antonio Quijarro Province, Potosí Department, Bolivia (19°49'15"S, 65°55'0"W). The most detailed description of the El Dragón mine is given by Grundmann *et al.* (1990), and more recent information is provided by Paar *et al.* (2012). The El Dragón mine exploited a telethermal deposit consisting of a single selenide vein hosted by sandstones and shales. The principle ore mineral was krut'aite,  $\text{CuSe}_2$ , varying in composition to penroseite,  $\text{NiSe}_2$ , and commonly containing a significant amount of Co. Later solutions rich in Bi, Pb and Hg resulted in the crystallization of phases such as clausthalite, petrovicite, watkinsonite, and the recently described minerals eldragónite,  $\text{Cu}_6\text{BiSe}_4(\text{Se}_2)$  (Paar *et al.*, 2012) and grundmannite,  $\text{CuBiSe}_2$  (Förster *et al.*, 2016). Oxidation produced a wide range of secondary phases, including several rare selenites, such as the recently described mineral favreaute,  $\text{PbBiCu}_6\text{O}_4(\text{SeO}_3)_4(\text{OH}) \cdot \text{H}_2\text{O}$  (Mills *et al.*, 2014) and the new mineral alfredopetrovite, described herein.

The new mineral occurs in vugs in a matrix composed mostly of Co-rich krut'aite–penroseite, dolomite and goethite. Other secondary minerals found in direct association with alfredopetrovite are ahlfeldite, allophane, calcite, chalcocite, favreaute, felsöbányaite, malachite and molybdomenite.

## 3. Physical and optical properties

Alfredopetrovite occurs in drusy/scaly coatings (Fig. 1) and compact balls (Fig. 2), the latter to 0.5 mm in diameter. Individual crystals are up to about 0.1 mm across. No forms could be determined because the crystals occur in intergrowths. No twinning was observed. Crystals are colourless and transparent with a vitreous lustre and white streak. Crystals can transmit the colours of phases on which they are growing, giving them different apparent colour. In particular, alfredopetrovite commonly seems to show a blue colour when overgrowing chalcocite. Crystals are brittle with a smooth, curved fracture, and

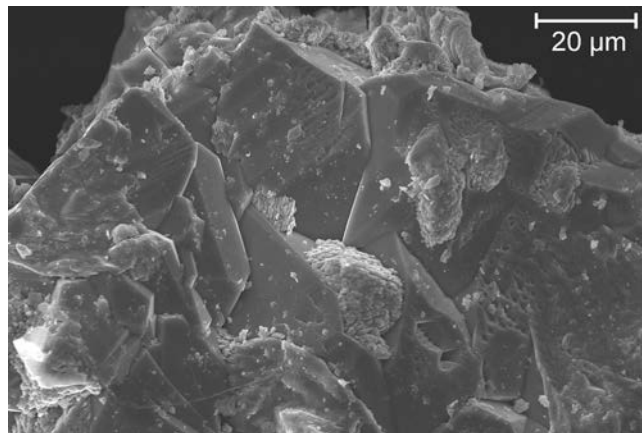


Fig. 1. SEM image of intergrown alfredopetrovite crystals with ahlfeldite (NHMLAC#65578).

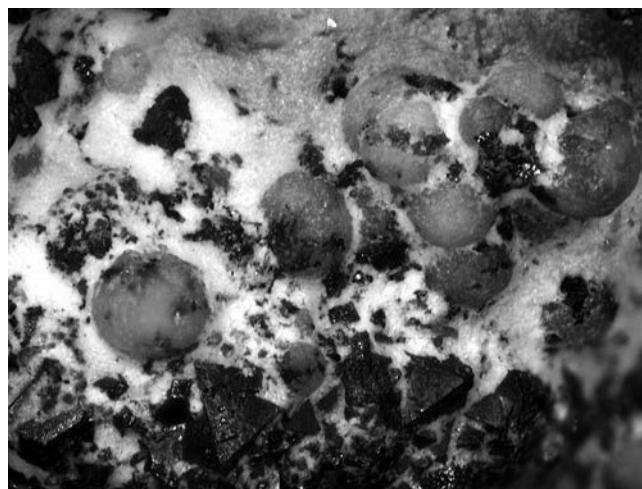


Fig. 2. Compact balls of alfredopetrovite (gray) with felsöbányaite (white) on krut'aite–penroseite (black); field of view = 3 mm across (NHMLAC#65580).

have no apparent cleavage. The Mohs' hardness is 2½, based upon scratch tests.

The density could not be measured because individual crystal fragments are virtually invisible in density liquids and crystal clusters contain admixed ahlfeldite and/or felsöbányaite. The calculated density is  $2.504 \text{ g cm}^{-3}$ , based on the empirical formula. Optically, alfredopetrovite crystals are uniaxial (+), with  $\omega = 1.554(2)$  and  $\epsilon = 1.566(2)$ , measured in white light, and are nonpleochroic. The Gladstone–Dale compatibility (Mandarino, 2007) is 0.014, in the range of superior compatibility, based upon the empirical formula.

## 4. Chemical composition

Chemical analyses (3) of alfredopetrovite were carried out using a Cameca SX-50 electron microprobe in the Department of Geology and Geophysics at the University

of Utah utilizing Probe for EPMA software (WDS mode, 15 kV, 10 nA and 8  $\mu\text{m}$  beam diameter). Raw X-ray intensities were corrected for matrix effects with a  $\phi(\rho z)$  algorithm (Pouchou & Pichoir, 1991). No other elements were detected in EDS analyses.

There was moderate damage from the electron beam, but this did not seem to affect the relative proportions of cations. However, as is typical of highly hydrated phases with weakly held  $\text{H}_2\text{O}$ , alfredopetrovite partially dehydrates under vacuum either during carbon coating or in the microprobe chamber. This  $\text{H}_2\text{O}$  loss results in higher concentrations for the remaining constituents than are to be expected for the fully hydrated phase. Because insufficient material is available for a direct determination of  $\text{H}_2\text{O}$ , it has been calculated based upon the structure determination. The analysed constituents have then been normalized to provide a total of 100 % when combined with the calculated  $\text{H}_2\text{O}$ . Analytical data are given in Table 1.

The empirical formula for alfredopetrovite (based on 15 O atoms per formula unit, *apfu*) is  $\text{Al}_{1.94}\text{Cu}_{0.07}\text{Ni}_{0.03}\text{Co}_{0.01}\text{Se}_{2.95}\text{O}_{15}\text{H}_{12.16}$ . The simplified formula is  $\text{Al}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$ , which requires  $\text{Al}_2\text{O}_3$  18.78,  $\text{SeO}_2$  61.31 and  $\text{H}_2\text{O}$  19.91 wt%, total 100 wt%.

Table 1. Analytical data for alfredopetrovite.

Const.	wt%	Range	SD	Norm. wt%	Standard
CuO	1.27	1.04–1.46	0.21	1.09	Cu metal
CoO	0.12	0.10–0.15	0.03	0.10	Co metal
NiO	0.51	0.35–0.68	0.17	0.44	Ni metal
$\text{Al}_2\text{O}_3$	20.99	20.41–22.04	0.92	18.12	albite
$\text{SeO}_2$	69.63	68.83–70.36	0.77	60.12	ZnSe (syn)
$\text{H}_2\text{O}_{\text{calc}}$	23.30			20.12	
Total	115.82			99.99	

## 5. X-ray crystallography and crystal-structure determination

Powder X-ray diffraction data for alfredopetrovite were obtained on a Rigaku R-Axis Rapid II curved-imaging-plate microdiffractometer utilising monochromatised  $\text{MoK}\alpha$  radiation. A Gandolfi-like motion on the  $\phi$  and  $\omega$  axes was used to randomize the sample. Observed  $d$  spacings 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

Table 2. Powder X-ray data for alfredopetrovite ( $d$ -spacings in Å).

$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$	$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$
55	7.63	7.6366	73	1 0 0	5	1.7487	1.7520	5	3 2 0
55	6.22	6.2200	64	1 0 1	8	1.7203	1.7212	8	2 1 5
26	5.37	5.3605	30	0 0 2	6	1.7019	1.7026	5	2 2 4
40	4.398	{4.4090 4.3875}	35 9	1 1 0 1 0 2	26	1.6609	{1.6664 1.6653 1.6618 1.6560}	6 7 8 5	4 1 0 3 2 2 3 1 4 1 1 6
13	3.817	3.8183	11	2 0 0	11	1.6436	{1.6467 1.6399 1.6184}	8 2 1	4 1 1 3 0 5 2 0 6
19	3.595	3.5970	19	2 0 1	5	1.5882	1.5913	5	4 1 2
100	3.404	3.4052	100	1 1 2			1.5731	1	3 2 3
8	3.246	3.2368	8	1 0 3			1.5550	1	4 0 4
6	3.104	3.1100	6	2 0 2			1.5273	1	5 0 0
8	2.886	2.8864	9	2 1 0	18	1.5088	{1.5193 1.5103 1.5068 1.4697}	4 7 6 1	2 1 6 4 1 3 3 1 5 3 3 0
50	2.783	2.7871	58	2 1 1	8	1.4638	1.4665	8	3 2 4
4	2.673	2.6803	5	0 0 4			1.4432	1	4 2 0
22	2.606	2.6092	25	2 0 3			1.4259	1	4 0 5
14	2.539	2.5414	15	2 1 2			{1.4215 1.4174 1.4152}	3 3 3	2 0 7 3 3 2 4 1 4
		2.5290	1	1 0 4	3	1.3918	1.3936	3	4 2 2
		2.4767	1	3 0 1			{1.3657 1.3605 1.3567 1.3529}	2 2 1 4	3 1 6 5 1 1 3 2 5 2 1 7
14	2.290	2.2903	12	1 1 4	8	1.3546	1.3401	1	0 0 8
4	2.242	2.2454	3	2 1 3			1.3288	2	5 1 2
		2.2045	1	2 2 0			1.3158	5	4 1 5
11	2.193	2.1937	10	2 0 4	7	1.3165			
5	2.1137	2.1180	5	3 1 0					
15	2.0701	{2.0779 2.0733 2.0644 2.0388}	6 9 1 2	3 1 1 3 0 3 1 0 5 2 2 2	10	1.4171	{1.4174 1.4152 1.3936}	3 3 3	3 3 2 4 1 4 4 2 2
19	1.9667	{1.9698 1.9641 1.9092}	17 3 3	3 1 2 2 1 4 4 0 0	8	1.3546	{1.3657 1.3605 1.3567 1.3529}	2 2 1 4	3 1 6 5 1 1 3 2 5 2 1 7
3	1.8638	1.8696	2	2 0 5			1.3401	1	0 0 8
		1.8458	3	3 0 4			1.3288	2	5 1 2
11	1.8234	1.8220	11	3 1 3	7	1.3165	1.3158	5	4 1 5
6	1.7906	{1.7985 1.7868}	1 5	4 0 2 0 0 6					

powder data using JADE 2010 with whole-pattern fitting are:  $a = 8.7978(14)$ ,  $c = 10.7184(18)$  Å and  $V = 718.5(3)$ , which are in good agreement with the single-crystal study below.

Single-crystal structure data were obtained on the same instrument noted above. The relatively small size and poor diffracting power of the crystal fragment used limited the resolution of the data to 1.04 Å ( $\theta = 20^\circ$ ). 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 by direct methods using SIR2004 (Burla *et al.*, 2005); SHELXL-2013 (Sheldrick, 2008) was used for the refinement of the structure.

Table 3. Crystal data and structure refinement for alfredopetrovite.

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation/power	MoK $\alpha$ ( $\lambda = 0.71075$ Å) /50 kV, 40 mA
Temperature	298(2) K
Structural formula	[Al(H <sub>2</sub> O) <sub>3</sub> ] <sub>2</sub> (Se <sup>4+</sup> O <sub>3</sub> ) <sub>3</sub>
Space group	$P\bar{6}2c$
Unit-cell dimensions	$a = 8.818(3)$ Å $c = 10.721(2)$ Å
$V$	722.0(5) Å <sup>3</sup>
$Z$	2
Density (for above formula)	2.497 g/cm <sup>3</sup>
Absorption coefficient	7.835 mm <sup>-1</sup>
$F(000)$	520
Crystal size	80 × 40 × 40 µm
$\theta$ range	3.28–19.95°
Index ranges	$-8 \leq h \leq 8$ , $-8 \leq k \leq 8$ , $-9 \leq l \leq 10$
Reflections collected/unique	1817/246 [ $R_{\text{int}} = 0.064$ ]
Reflections with $F_o > 4\sigma F$	240
Completeness to $\theta = 19.95^\circ$	99.4 %
Max. and min. transmission	0.573 and 0.745
Refinement method	Full-matrix least-squares on $F^2$
Parameters refined	40
GoF	1.073
Final $R$ indices [ $F_o > 4\sigma F$ ]	$R_1 = 0.0268$ , $wR_2 = 0.0633$
$R$ indices (all data)	$R_1 = 0.0288$ , $wR_2 = 0.0649$
Absolute structure parameter	-0.01(2)
Largest diff. peak/hole	+0.34/-0.39 e/Å <sup>3</sup>

\* $R_{\text{int}} = \sum |F_o^2 - F_c^2(\text{mean})| / \sum [F_o^2]$ . GoF =  $S = \{ \sum [w(F_o^2 - F_c^2)^2] / (n-p) \}^{1/2}$ .  $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ .  $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$ .  $w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$  where  $a$  is 0.0424,  $b$  is 0.1809 and  $P$  is  $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$ .

Table 4. Atom fractional coordinates and displacement parameters (Å<sup>2</sup>) for alfredopetrovite.

	$x$	$y$	$z$	$U_{\text{eq}}$	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Al	0.3333	0.6667	0.5331(6)	0.0223(15)	0.021(2)	0.021(2)	0.024(4)	0	0	0.0106(10)
Se	0.61798(18)	0.74258(17)	0.7500	0.0259(7)	0.0260(11)	0.0292(10)	0.0225(10)	0	0	0.0138(9)
OW1	0.3148(10)	0.4820(10)	0.4278(7)	0.030(2)	0.035(5)	0.037(5)	0.027(5)	-0.017(4)	-0.012(4)	0.025(4)
H1	0.390(8)	0.457(11)	0.401(9)	0.036						
H2	0.240(9)	0.439(13)	0.373(7)	0.036						
O2	0.4866(8)	0.6210(8)	0.6274(6)	0.026(2)	0.032(5)	0.031(5)	0.016(4)	-0.007(3)	-0.009(3)	0.017(4)
O3	0.7667(11)	0.6772(14)	0.7500	0.033(3)	0.027(6)	0.054(7)	0.031(7)	0	0	0.030(6)

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  $U_{\text{eq}}$  of each H set to 1.2 times that of the donor O atom. Details of data collection and structure refinement are provided in Table 3. Fractional coordinates and atom displacement parameters are provided in Table 4, selected interatomic distances in Table 5 and bond valences in Table 6.

## 6. Discussion of the structure

The structure of alfredopetrovite is the same as that of synthetic  $\text{Al}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$  (Morris *et al.*, 1991, 1992). The structure is comprised of fairly regular  $\text{AlO}_6$  octahedra and  $\text{Se}^{4+}\text{O}_3$  triangular pyramids. The Al is coordinated to three  $\text{H}_2\text{O}$  groups on the same side of the octahedron. The opposite vertices are O atoms shared with  $\text{Se}^{4+}\text{O}_3$  pyramids. Two of the O atoms of the  $\text{Se}^{4+}\text{O}_3$  pyramid are shared with  $\text{AlO}_6$  octahedra and the third O atom is unshared. Three  $\text{Se}^{4+}\text{O}_3$  pyramids link two

Table 5. Selected bond distances (Å) and angles (°) in alfredopetrovite.

Al–O2 (×3)	1.886(7)	Se–O3	1.676(9)	
Al–OW1 (×3)	1.920(8)	Se–O2 (×2)	1.726(6)	
<Al–O>	1.903	<Se–O>	1.709	
Hydrogen bonds				
D–H $\cdots$ A	D–H	H $\cdots$ A	D $\cdots$ A	<DHA
OW1–H1A $\cdots$ O2	0.85(4)	1.94(4)	2.744(9)	157(8)
OW1–H1B $\cdots$ O3	0.82(4)	1.79(4)	2.601(9)	171(10)

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

	OW1	O2	O3	$\Sigma$
Al	0.48 × 3 →	0.53 × 3 →		3.03
Se		1.26 × 2 →	1.44	3.96
H1	0.81	0.19		1.00
H2	0.75		0.25 × 2 ↓	1.00
$\Sigma$	2.04	1.98	1.94	

Bond multiplicities are indicated by × ↓ →. Bond-valence parameters are from Brown & Altermatt (1985). Hydrogen bond strengths are based on O $\cdots$ O distances.

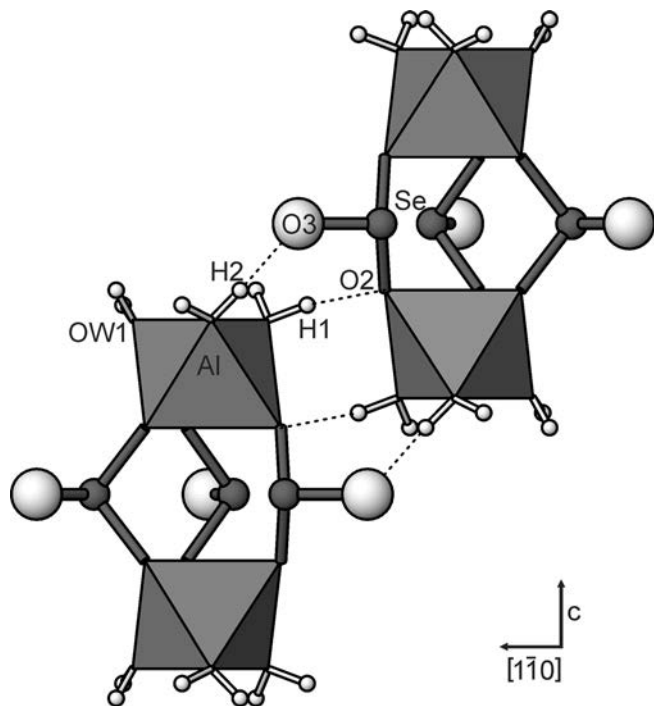


Fig. 3. Two adjacent clusters in the structure of alfredopetrovite viewed down  $[110]$  with  $[001]$  vertical. Hydrogen bonds are shown as dashed lines.

adjacent  $\text{AlO}_6$  octahedra forming a  $[\text{Al}(\text{H}_2\text{O})_3]_2(\text{Se}^{4+}\text{O}_3)_3$  cluster structural unit. These structural units are bonded to one another only *via* hydrogen bonds (Fig. 3) yielding a structure with relatively large channels along  $[001]$  (Fig. 4). Based upon the geometry of the  $\text{Se}^{4+}\text{O}_3$  group, the lone electron pair of the  $\text{Se}^{4+}$  atom projects into the channel around its periphery.

The configuration of the  $[\text{Al}(\text{H}_2\text{O})_3]_2(\text{Se}^{4+}\text{O}_3)_3$  cluster in the structure of alfredopetrovite is similar to that of the distinctive unit in the NASICON (sodium super-ionic conductor) structure (*cf.* Anantharamulu *et al.*, 2011), commonly referred to as a *lantern unit* because of its similarity in appearance to a lantern. The lantern unit in the structure of alfredopetrovite differs principally in that the octahedra are bridged by selenite pyramids rather than by tetrahedra (silicate, phosphate, *etc.*).

Similar lantern units, in which the octahedra are linked by phosphate groups, are found in the structure of the mineral camaronesite,  $[\text{Fe}^{3+}(\text{H}_2\text{O})_2(\text{PO}_3\text{OH})]_2(\text{SO}_4) \cdot 1-2\text{H}_2\text{O}$  (Kampf *et al.*, 2013), while doubled lantern units are found in the structures of taranakite,  $\text{K}_3\text{Al}_5(\text{PO}_3\text{OH})_6(\text{PO}_4)_2 \cdot 18\text{H}_2\text{O}$  (Dick *et al.*, 1998), and the sulphates coquimbite and paracoquimbite,  $\text{Fe}^{3+}_2(\text{SO}_4)_3 \cdot 9\text{H}_2\text{O}$  (Fang & Robinson, 1970; Robinson & Fang, 1971; Hawthorne *et al.*, 2000). In all of these structures, the lantern units are linked to one another by additional polyhedra. As noted by Krivovichev (2004), the only phase besides  $\text{Al}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$  (alfredopetrovite) with a structure containing an unlinked cluster with this topology, is the synthetic phase  $\text{Al}_2(\text{PO}_4)(\text{PO}_2(\text{OH})_2)_3 \cdot 6\text{H}_2\text{O}$  (Kniep & Wilms, 1979).

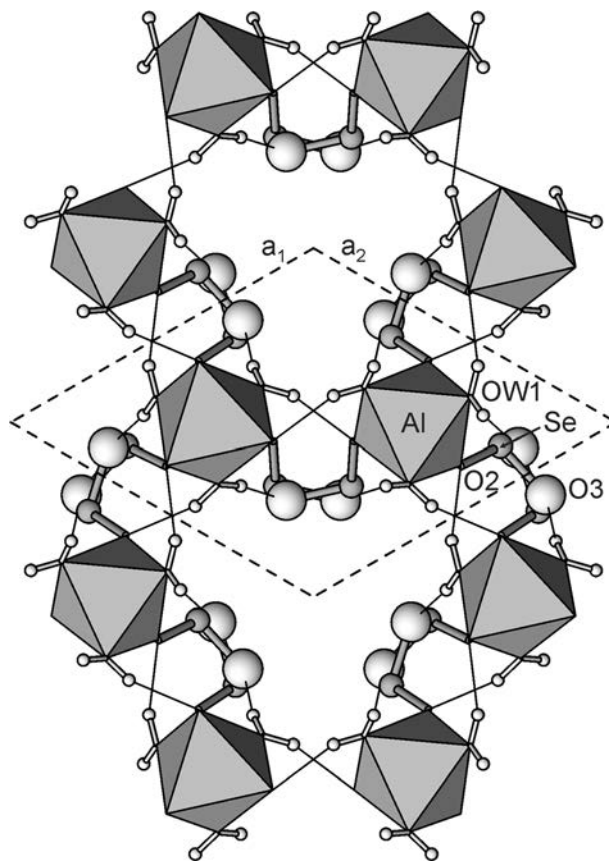


Fig. 4. The structure of alfredopetrovite viewed down  $[001]$ . Hydrogen bonds are shown as solid lines. Unit cell outline is shown with dashed lines.

The mineral to which alfredopetrovite is most similar compositionally is mandarinoite,  $\text{Fe}^{3+}_2(\text{Se}^{4+}\text{O}_3)_3 \cdot 6\text{H}_2\text{O}$ , which is chemically its Fe analogue. However, the structure of mandarinoite is quite different from that of alfredopetrovite. The structure of mandarinoite consists of a corner-sharing framework of  $\text{Fe}^{3+}\text{O}_6$  octahedra and  $\text{Se}^{4+}\text{O}_3$  pyramids, which contains large voids that are occupied by the  $\text{H}_2\text{O}$  groups (Hawthorne, 1984).

**Acknowledgements:** The paper benefited from comments by two anonymous reviewers. This study was funded by the John Jago Trelawney Endowment to the Mineral Sciences Department of the Natural History Museum of Los Angeles County.

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Received 18 August 2015

Modified version received 19 September 2015

Accepted 29 September 2015