

MENGEITE, $\text{Ba}(\text{Mg}, \text{Mn}^{2+})\text{Mn}^{3+}_4(\text{PO}_4)_4(\text{OH})_4 \cdot 4\text{H}_2\text{O}$, A NEW MINERAL FROM THE SPRING CREEK MINE, SOUTH AUSTRALIA, AUSTRALIA

PETER ELLIOTT[§]

Department of Earth Sciences, School of Physical Sciences, The University of Adelaide, Adelaide, South Australia 5005, Australia

South Australian Museum, North Terrace, Adelaide, South Australia 5000, Australia

ABSTRACT

Mengeite, $\text{Ba}(\text{Mg}, \text{Mn}^{2+})\text{Mn}^{3+}_4(\text{PO}_4)_4(\text{OH})_4 \cdot 4\text{H}_2\text{O}$, is a new mineral from the Spring Creek copper mine, near Wilmington, South Australia, Australia, where it occurs as dark orange-red masses to 0.8 mm across in a quartz matrix. The streak is pale salmon pink and the luster is vitreous. Mengeite is non-fluorescent and the Mohs hardness is ~3. The measured density is 3.40 g/cm³ and the calculated density is 3.43 g/cm³. Mengeite is biaxial (–) with $\alpha = 1.757(4)$, $\beta = 1.776(4)$, $\gamma = 1.781(4)$ measured in white light. Electron microprobe analyses results give the empirical formula, based on 24 O *apfu*: $\text{Ba}_{1.09}(\text{Mg}_{0.58}\text{Mn}^{2+}_{0.26}\text{Cu}_{0.10}\text{Al}_{0.02}\text{Na}_{0.01}\text{Ca}_{0.01}\text{□}_{0.09})\Sigma_{1.07}\text{Mn}^{3+}_{3.88}(\text{PO}_4)_{4.07}(\text{OH})_{3.52} \cdot 4.13\text{H}_2\text{O}$. The idealized formula is $\text{Ba}(\text{Mg}, \text{Mn}^{2+})\text{Mn}^{3+}_4(\text{PO}_4)_4(\text{OH})_4 \cdot 4\text{H}_2\text{O}$. Mengeite is triclinic, space group $P\bar{1}$, with $a = 5.4262(11)$, $b = 5.4274(11)$, $c = 16.387(3)$ Å, $\alpha = 87.61(3)$, $\beta = 98.97(3)$, $\gamma = 110.56(3)^\circ$, $V = 446.28(16)$ Å³, and $Z = 1$. The crystal structure of mengeite was solved using synchrotron single-crystal X-ray diffraction data and refined to $R1 = 0.0453$ for 2115 observed reflections with $F_0 > 4\sigma(F_0)$. It is based on $[(\text{M}_2(\text{OH})_2(\text{AsO}_4)_2]$ sheets that are linked in the *c*-direction alternately by $[\text{M}_3(\text{H}_2\text{O})_4\text{O}_2]$ octahedra and by BaO_{10} polyhedra.

Keywords: mengeite, new mineral species, phosphate, crystal structure, Spring Creek Mine, South Australia, synchrotron.

INTRODUCTION

The Spring Creek mine in Southern Flinders Ranges, South Australia, produced a minor amount of copper ore in the late 1880s and early 1900s. Although never an economic source, the mine has proven to be a prolific source of mineral specimens, particularly those collected in the 1970s and 1980s (Beyer & Elliott 1996, Kolitsch *et al.* 1999b). Of the more than 50 minerals identified at the locality, 22 are phosphates, including five for which the Spring Creek mine is the type locality: bariosincosite, $\text{BaV}^{4+}_2\text{O}_2(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O}$ (Pring *et al.* 1999); springcreekite, $\text{BaV}^{3+}_3(\text{PO}_4)_2(\text{OH}, \text{H}_2\text{O})_6$ (Kolitsch *et al.* 1999a); johntomaite, $\text{BaFe}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_3(\text{OH})_3$ (Kolitsch *et al.* 2000); strontioferloffite, $\text{SrMn}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_3(\text{OH})_3$ (Elliott 2019); and mengeite, the subject of this paper. The specimen containing mengeite was collected from the mine dumps in the mid-1980s. The name honors Johann Menge (1788–1852), geologist and linguist (Cawthorne 1859, Triebel

1963). Born in the town of Steinau, Hesse, Germany, Menge traveled to the new colony of South Australia in 1837. For the next 15 years, Menge explored the colony, documenting rock and mineral occurrences. In 1841 his booklet, *The Mineral Kingdom of South Australia*, was published. His activities encouraged an interest in the mineral wealth of South Australia and aided the discovery of major copper deposits at Burra and Kapunda. The mineral and its name have been approved by the IMA-CNMNC (IMA 2018-035). The holotype specimen of mengeite is deposited in the mineralogical collection of the South Australian Museum, Adelaide, South Australia (registration number G34744).

OCCURRENCE

The Spring Creek copper mine is situated in the South Flinders Ranges, South Australia, Australia, 10 km south of the town of Wilmington and on the

[§] Corresponding author e-mail address: peter.elliott@adelaide.edu.au

northeastern flank of Mt. Remarkable. The mine was discovered in 1860 by T. Brandon (Austin 1863). Austin reported that, in 1862, the workings comprised a drive extending for 12 feet from which five tons of ore had been recovered and sent to England. However, the mine proved to be uneconomic, and in December 1865, the mining plant, a 16 hp steam engine, and a stone crusher were sold by auction. Over the next 50 years, several companies attempted to establish the mine as a profitable venture but none was successful. The Royal Commission on Water Supply was formed in 1916 and investigated using the mine water to supply the town of Wilmington. The land was reserved from the operation of the Mining Act and in 1929, after six months of test pumping, the Hydraulic Engineers Department was given approval to pump water from the mine into the reticulation mains of the district.

The Spring Creek mine is located within the contact zone of a quartzite of the Rhynie Sandstone and a slate of the Tindelpina Shale, which are part of the Adelaide Geosyncline of late Proterozoic age (Binks *et al.* 1968). The topography of the northern end of Mt. Remarkable has been influenced by an east–west fault, and the copper mineralization lies as two intersection lodes in the fault zone. The lodes are up to 2.4 m wide with shoots of ore that pitch to the south. Mineralization occurs in a heavily brecciated hydrothermal vein. Primary ore comprises native copper and cuprite and minor chalcocite, chalcopyrite, covellite, and pyrite. Secondary minerals occur in small cavities in quartz veins and have crystallized from low-temperature hydrothermal solutions.

PHYSICAL AND OPTICAL PROPERTIES

Mengeite occurs as masses up to 0.8 mm across in a quartz matrix (Fig. 1). The color is dark orange-red; the mineral has a pale salmon pink streak. The luster is vitreous, and the mineral is non-fluorescent in both long- and short-wave ultraviolet light. Mengeite has a Mohs hardness of approximately 3 and a brittle tenacity. One excellent cleavage is observed, presumably parallel to (001) based on the crystal structure, and the fracture is uneven. The density measured by flotation in a mixture of Clerici solution and water is 3.40 g/cm^3 ; the calculated density is 3.43 g/cm^3 using the empirical formula and 3.35 g/cm^3 using the ideal formula. Mengeite is biaxial (–) with $\alpha = 1.757(4)$, $\beta = 1.776(4)$, $\gamma = 1.781(4)$ measured in white light. $2V$ was not measured: the calculated $2V$ is 53.8° . Pleochroism is $X = \text{pale gray}$, $Y = \text{pale yellow}$, $Z = \text{orange}$; $Z \gg Y > X$. The Gladstone–Dale compatibility $[1 - (K_p/K_c) =$



Fig. 1. Massive aggregate of mengeite, 0.8 mm across, in quartz.

0.03] is excellent for the empirical formula (Mandarino 1981).

CHEMICAL COMPOSITION

Quantitative chemical analyses (8 points) were obtained using a Cameca SX Five electron microprobe operating in wavelength-dispersion mode with a beam diameter of $5 \mu\text{m}$, an accelerating voltage of 15 kV, and a beam current of 20 nA. The following standards (X-ray lines) were used for calibration: baryte ($\text{BaK}\alpha$), rhodonite ($\text{MnK}\alpha$), almandine-pyrope ($\text{MgK}\alpha$), chalcopyrite ($\text{CuK}\alpha$), albite ($\text{NaK}\alpha$, $\text{AlK}\alpha$), plagioclase ($\text{CaK}\alpha$), apatite ($\text{PK}\alpha$), and gallium arsenide ($\text{AsL}\alpha$). The intensity data were corrected using the PAP procedure of Pouchou & Pichoir (1985). The results analyses are reported in Table 1. As insufficient material was available for a direct determination of H_2O , it was calculated based on results from the crystal-structure determination. The empirical formula calculated on the basis of 24 O *apfu* is $\text{Ba}_{1.09}(\text{Mg}_{0.58} \text{Mn}^{2+}_{0.26} \text{Cu}_{0.10} \text{Al}_{0.02} \text{Na}_{0.01} \text{Ca}_{0.01} \square_{0.09})_{\Sigma 1.07} \text{Mn}^{3+}_{3.88} (\text{PO}_4)_{4.07} (\text{OH})_{3.52} \cdot 4.13 \text{H}_2\text{O}$. The idealized formula is $\text{Ba}(\text{Mg}, \text{Mn}^{2+})\text{Mn}^{3+}_4(\text{PO}_4)_4(\text{OH})_4 \cdot 4\text{H}_2\text{O}$.

INFRARED SPECTROSCOPY

The infrared spectrum of powdered mengeite (Fig. 2) over the range 4000 to 650 cm^{-1} was obtained using a Nicolet 5700 FTIR spectrometer equipped with a Nicolet Continuum IR microscope and a diamond-anvil cell. The spectrum shows the characteristic absorption bands of OH-stretching at 3482 and 3142 cm^{-1} . A band at 1647 cm^{-1} is assigned to the ν_2 (δ) H_2O bending mode of H–O–H. Bands at 1173 , 1018 , and 945 cm^{-1} are assigned to ν_3 vibrations of the PO_4

TABLE 1. ANALYTICAL DATA (wt.%) FOR MENGEITE

Constituent	Mean	Range	Stand. Dev.	Probe Standard
BaO	18.32	17.52–19.07	0.50	baryte
Mn ₂ O ₃ *	33.45	32.56–33.83	0.41	rhodonite
MnO*	2.02	1.54–2.49	0.32	rhodonite
MgO	2.54	2.19–3.30	0.37	almandine
CuO	0.87	0.52–1.62	0.35	chalcopyrite
Al ₂ O ₃	0.11	0.10–0.14	0.01	albite
CaO	0.04	0.01–0.08	0.02	plagioclase
Na ₂ O	0.05	0.00–0.14	0.04	albite
P ₂ O ₅	31.57	30.98–32.08	0.40	apatite
As ₂ O ₅	0.27	0.00–0.48	0.17	gallium arsenide
H ₂ O**	11.60			
Total	100.84			

* Mn₂O₃ and MnO are calculated assuming that the *M1* and *M2* sites are occupied by Mn³⁺+Cu+Al and the *M3* site is occupied by Mg+Mn²⁺.

** Calculated from the ideal formula.

tetrahedra and the band at 839 cm⁻¹ to the ν_1 vibration of the PO₄ tetrahedra.

X-RAY POWDER DIFFRACTION

Powder X-ray diffraction data (Table 2) were collected using a Rigaku Hiflux Homelab diffractometer (phi scan, diameter = 90.0 mm, CuK α radiation, with λ = 1.54187 Å, operated at 40 kV, 30 mA). Calculated intensities were obtained using the program PowderCell (Kraus & Nolze 1996) on the basis of the refined crystal structure model. The cell parameters, refined on the basis of 26 indexed reflections using the UnitCell software of Holland & Redfern (1997), are: a = 5.4280(6), b = 5.4269(7), c = 16.390(3) Å, α = 87.72(2), β = 98.97(1), γ = 110.57(1)°, V = 446.44(9) Å³ and are similar to those obtained from the single-crystal refinement.

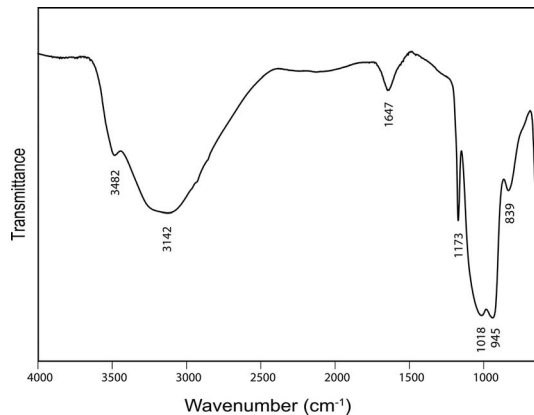


FIG. 2. The FT-IR spectrum of powdered mengeite.

STRUCTURE DETERMINATION

Single-crystal X-ray data collection and structure solution

Intensity data were collected on the macromolecular beam line MX2 of the Australian Synchrotron using an ADSC Quantum 315r detector and monochromatic radiation with a λ = 0.71080 Å. The detector-to-crystal distance was 90.15 mm. A phi scan was employed with framewidths of 1° and a counting time per frame of 1 s. Data were reduced and corrected for the Lorentz and polarization using XDS (Kabsch 2010). An absorption correction was applied using the SADABS program (Sheldrick 2000). The distribution of $|E|$ values indicated the presence of an inversion center ($|E^2 - 1|$ = 0.876); in light of this and the absence of systematic extinctions, space group *P1* was chosen for the structure solution and refinement. The positions of heavy atoms and 12 oxygen atoms were found during the initial structure solution using SHELXL-2018 (Sheldrick 2015) within the WinGX program suite (Farrugia 2012). All the O sites refined to full occupancy except for that coordinated solely to *M3*; the occupancy for this site refined to 1.76(2), suggesting the presence of a heavier atom. Given the obtained chemistry, which showed a slight excess of Ba, the site was refined as a partly occupied Ba2 site [refined site-occupancy 0.115(5)], with the occupancy being subsequently fixed to 0.045, in agreement with the chemical analytical data. A residual peak 0.79 Å from the Ba2 site was refined as a H₂O site (OW11) and completes the coordination for the *M3* site. OW11 is vacant when Ba2 is occupied. The *M3*-Ba2 distance is 2.000 Å, hence the *M3* and Ba2 sites cannot both be locally occupied. The occupancy of the *M3* site was

TABLE 2. X-RAY POWDER DIFFRACTION DATA (d IN Å) FOR MENGEITE

l_{obs}	d_{obs}	l_{calc}	d_{calc}	h	k	l
100	16.126	100	16.185	0	0	1
6	8.102	11	8.092	0	0	2
2	5.392	2	5.395	0	0	3
12	5.016	4	5.081	0	$\bar{1}$	0
		3	5.022	1	0	0
		14	5.016	1	0	1
7	4.837	5	4.828	0	1	1
4	4.587	3	4.604	1	0	$\bar{1}$
		2	4.589	1	0	2
44	4.418	26	4.409	1	1	1
2	4.270	6	4.331	0	$\bar{1}$	2
		5	4.276	0	1	2
5	4.118	3	4.099	1	1	2
7	4.047	12	4.046	0	0	4
2	3.729	4	3.989	1	0	3
		1	3.725	0	$\bar{1}$	3
3	3.654	2	3.673	0	1	3
2	3.427	3	3.646	1	1	3
		1	3.427	1	0	$\bar{3}$
14	3.246	6	3.413	1	0	4
		3	3.237	0	0	5
9	3.191	15	3.236	1	1	$\bar{3}$
12	3.145	7	3.185	1	1	4
3	3.083	12	3.144	0	$\bar{1}$	$\bar{4}$
3	2.973	1	3.079	1	$\bar{1}$	1
		1	2.976	1	$\bar{1}$	2
3	2.938	4	2.966	1	$\bar{1}$	$\bar{1}$
25	2.796	5	2.930	1	0	5
		14	2.822	1	1	$\bar{4}$
12	2.680	17	2.796	1	$\bar{1}$	3
		12	2.783	1	$\bar{1}$	2
3	2.544	9	2.778	1	1	5
		3	2.679	2	1	1
6	2.512	5	2.674	1	2	0
		2	2.667	1	2	1
2	2.491	5	2.648	2	1	0
		5	2.551	1	0	5
4	2.436	2	2.540	2	0	1
		3	2.535	2	1	3
4	2.418	2	2.515	0	2	1
		3	2.511	2	0	0
1	2.392	3	2.508	2	0	2
		3	2.504	0	$\bar{2}$	$\bar{1}$
6	2.296	1	2.491	1	2	$\bar{2}$
1	2.200	4	2.461	1	2	3
2	2.168	2	2.438	1	1	6
2	2.075	3	2.434	0	$\bar{2}$	2
1	2.053	2	2.421	2	0	3
1	1.995	4	2.414	0	2	2
1	1.970	3	2.411	2	1	$\bar{2}$
1	1.790	2	2.397	0	$\bar{1}$	6
		9	2.295	2	0	4
1	1.708	7	2.286	0	2	3
2	1.693	2	2.204	2	2	2
1	1.681	5	2.189	1	1	6
1	1.640	1	2.165	0	$\bar{2}$	4
		2	2.076	2	1	$\bar{4}$
1	1.640	4	2.073	2	2	2
		1	2.052	2	1	6
1	1.640	1	1.994	2	0	6
		3	1.967	2	2	3
1	1.640	3	1.945	1	$\bar{1}$	7
		3	1.798	0	0	9
1	1.640	2	1.789	1	3	$\bar{1}$
		2	1.713	2	0	6
1	1.640	3	1.705	2	2	7
		2	1.694	0	$\bar{3}$	0
1	1.640	5	1.679	3	1	5
		4	1.675	1	3	4
1	1.640	1	1.640	3	0	$\bar{1}$
		3	1.552	1	3	5
1	1.640	4	1.545	2	2	1
		4	1.545	2	2	1

Note: Only reflections with calculated intensities >3 are shown, unless they correspond to observed reflections.

fixed to $(\text{Mg}_{0.63}\text{Mn}^{2+}_{0.29}\square_{0.09})$ *pfu*. The refinement on the basis of 2115 unique observed reflections converged to $R1 = 0.0495$ with anisotropic-displacement parameters on all atoms except Ba2 and OW11. It was not possible to locate H atoms. The details of the data collection and refinement results are given in Table 3. The final positional and displacement parameters are given in Table 4, and selected bond lengths and angles are listed in Table 5. Table 6 provides a bond-valence analysis calculated using bond-valence parameters taken from Gagné & Hawthorne (2015)¹.

Structure description

The crystal structure of mendeite contains seven symmetrically independent cation sites. The Ba1 site is [12]-coordinated with eight bonds in the range 2.740–2.812 Å, four long bonds of 3.498 and 3.508 Å, and a $\langle\text{Ba}-\text{O}\rangle$ distance of 3.011 Å. The refined site-scattering value of 54.32 *epfu* is consistent with occupancy by Ba. The partially occupied Ba2 site is [10]-coordinated with Ba–O bonds in the range 2.737–3.472 Å and a $\langle\text{Ba}-\text{O}\rangle$ distance of 2.999 Å.

The structure contains three symmetrically independent *M* sites, *M1*, *M2*, and *M3*, each in octahedral coordination. The *M1* and *M2* sites are coordinated by four O^{2-} anions and two OH groups to form distorted octahedra with four short equatorial *M*–O distances and two longer apical distances. Such features are characteristic of Jahn-Teller distortion, as might be expected for Mn^{3+} in octahedral coordination. The *M1* and *M2* sites have refined-site-scatterings of 24.75 and 24.50 electrons per formula unit (*epfu*), respectively, consistent with their occupancy by Mn. These sites also accommodate minor Cu and Al, as shown by the chemical analysis. The *M3* site is coordinated by two O^{2-} anions and four H_2O groups. The refined scattering of 14.68 *epfu* and mean bond-length is consistent with occupancy by predominantly Mg plus minor Mn^{2+} .

The structure is based on infinite chains along $[1\bar{1}0]$ formed by $\text{M1O}_4(\text{OH})_2$ and $\text{M2O}_4(\text{OH})_2$ octahedra which share *trans* O–OH edges (Fig. 3). Chains are decorated by PO_4 tetrahedra forming sheets of composition $[\text{M}(\text{OH})(\text{PO}_4)]$ parallel to (001) (Fig. 4). Linkages between the sheets along $[010]$ is provided alternately by *X* polyhedra and $[\text{M3}(\text{H}_2\text{O})_4\text{O}_2]$ octahedra (Fig. 4). The *X* polyhedra share edges with two $\text{M1O}_4(\text{OH})_2$ octahedra, two $\text{M2O}_4(\text{OH})_2$ octahedra, and six PO_4 tetrahedra; $\text{M3}(\text{H}_2\text{O})_4\text{O}_2$ octahedra share

¹ Supplementary Data are available from the Depository of Unpublished Data on the MAC website (<http://mineralogicalassociation.ca/>), document “Mendeite, CM60, 21-00041”.

TABLE 3. CRYSTAL DATA, DATA COLLECTION, AND REFINEMENT DETAILS.

Crystal data	
Space group	$P\bar{1}$
a, b, c (Å)	5.4262(11), 5.4274(11), 16.387(3)
α, β, γ (°)	87.61(3), 98.97(3), 110.56(3)
V (Å ³), Z	446.28(16), 1
$F(000)$	429.0
μ (mm ⁻¹)	5.835
Absorption correction	multi-scan, $T_{\min}, T_{\max} = 0.273, 0.433$
Crystal dimensions (mm)	0.035 $\times$ 0.020 $\times$ 0.005
Data collection	
Diffractometer	ADSC Quantum 210r
Temperature (K)	100
Radiation Synchrotron	$\lambda = 0.71080$ Å
Crystal detector distance (mm)	90.15
Rotation axis, width (°)	$\phi, 1.0$
Total number of frames	360
Collection time per degree (s)	1.0
θ range (°)	1.258–29.572
h, k, l ranges	$-7 \rightarrow 7, -7 \rightarrow 7, -22 \rightarrow 22$
Total reflections measured	8856
Unique reflections	2115 ($R_{\text{int}} = 0.0455$)
Refinement	
Refinement on	F^2
$R1^*$ for $F_0 > 4\sigma(F_0)$	4.95%
$wR2^†$ for all F_0^2	14.01%
Reflections used $F_0^2 > 4\sigma(F_0^2)$	2115
Number of parameters refined	157
GooF	1.000
(D/s) _{max}	0.000
$Dr_{\text{max}}, Dr_{\text{min}}$ (e/Å)	3.714, -2.732

corners with two PO₄ tetrahedra. Sheets linked *via* X polyhedra are more widely separated than sheets linked *via* $[M3(H_2O)_4O_2]$ octahedra (10.3 *versus* 7.0 Å).

Hydrogen bonds

Although hydrogen atoms were not located in the difference Fourier maps, bond-valence calculations (Table 6) indicate the presence of two OH groups in the structure, each of which is shared between $M1$ and $M2$ atoms, and two H₂O groups, each of which is coordinated to the $M3$ site. The O—O distances suitable for probable hydrogen bonds are listed in Table 5. The proposed hydrogen bonding scheme is consistent with the scheme present in structures based on $[M(OH)(PO_4)]$ sheets in which positions of the H atoms have been located (*e.g.*, magnesiobermanite; Elliott 2022). The H-bonding comprises two types: (1) those involving the H₂O groups and (2) those with the OH groups of the $[M(OH)(PO_4)]$ sheet. The OH10 group is likely H-bonded to two O anions, O1 and O4,

corresponding to weak bonds according to Libowitzky (1999) and OH9 donating a H-bond accepted by OW12. Weak hydrogen bonds are also formed between OW11 and the O7 and O8 anions, with the OW12 group forming H-bonds with O6.

STRUCTURAL RELATIONS

Mengeite is a new representative of a relatively large family of minerals whose structures are based on $[M(OH)(TO_4)]$ sheets. These structures differ in the linkages between the sheets. In the tsumcorite-group minerals and synthetic isostructural compounds (*e.g.*, Krause *et al.* 1998, Mihajlovic & Effenberger 2004) and the natrochalcite-type compounds (*e.g.*, Giester & Zemann 1987, Krickl & Wildner 2007), sheets are linked *via* a large cation polyhedra (*i.e.*, those formed with Na, K, Rb, Ag, NH₄, Ca, Pb, Bi, and Tl). In the crystal structure of ercrite (Cooper *et al.* 2009), sheets are linked *via* [7]-coordinated Na polyhedra which share edges with partially occupied Mn³⁺O₄(OH)₂

TABLE 4. FRACTIONAL ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (IN Å²) FOR MENGEITE

Atom	x	y	z	U ^{eq}	U ¹¹	U ²²	U ³³	U ¹²	U ¹³	U ²³
Ba1	0	0.5	0.5	0.01203(19)	0.0148(3)	0.0120(3)	0.0118(3)	0.00191(15)	0.00133(17)	0.00821(18)
Ba2	0.735(2)	0.815(3)	0.9470(7)	0.011(3)						
M1	0.41797(16)	0.69830(15)	0.71131(5)	0.0090(2)	0.0090(4)	0.0065(4)	0.0121(4)	0.0019(3)	0.0016(3)	0.0034(3)
M2	0.08482(17)	0.80490(15)	0.28733(5)	0.0101(2)	0.0103(4)	0.0068(4)	0.0136(4)	0.0018(3)	0.0018(3)	0.0037(3)
M3	0.5	0.5	1	0.0285(6)	0.0393(16)	0.0287(13)	0.0224(12)	0.0001(10)	0.0032(11)	0.0183(12)
P1	0.6145(3)	0.8347(3)	0.40731(9)	0.0090(3)	0.0093(6)	0.0067(6)	0.0113(6)	0.0017(4)	0.0016(5)	0.0033(5)
P2	0.4499(3)	0.2269(3)	0.82570(9)	0.0107(3)	0.0118(7)	0.0091(6)	0.0122(6)	0.0010(5)	0.0015(5)	0.0052(5)
O1	0.6840(9)	0.8143(8)	0.4999(3)	0.0148(8)	0.018(2)	0.0153(19)	0.0146(19)	0.0029(15)	0.0035(17)	0.0100(16)
O2	0.2505(8)	0.3209(8)	0.6368(3)	0.0112(8)	0.0109(18)	0.0098(16)	0.0143(18)	0.0018(14)	0.0021(15)	0.0054(14)
O3	0.2796(8)	0.8729(8)	0.6200(3)	0.0102(7)	0.0093(17)	0.0082(16)	0.0138(18)	0.0024(13)	0.0002(15)	0.0046(14)
O4	0.3076(8)	0.7162(8)	0.3790(3)	0.0105(8)	0.0097(18)	0.0084(16)	0.0140(18)	0.0030(13)	0.0033(15)	0.0037(14)
O5	0.5201(11)	0.2206(10)	0.9192(3)	0.0225(10)	0.032(3)	0.026(2)	0.013(2)	0.0033(17)	0.0030(19)	0.016(2)
O6	0.1446(9)	0.1072(8)	0.8008(3)	0.0142(8)	0.0126(19)	0.0114(18)	0.020(2)	0.0030(15)	0.0037(17)	0.0060(15)
O7	0.4170(9)	0.9330(8)	0.2166(3)	0.0141(8)	0.0126(19)	0.0075(16)	0.023(2)	0.0020(15)	0.0044(17)	0.0042(14)
O8	0.5558(9)	0.5192(8)	0.7985(3)	0.0126(8)	0.0125(19)	0.0103(17)	0.0160(19)	0.0019(14)	0.0020(16)	0.0056(15)
OH9	0.0742(9)	0.5596(8)	0.7473(3)	0.0118(8)	0.0131(19)	0.0088(16)	0.0151(19)	0.0017(14)	0.0043(16)	0.0053(14)
OH10	0.7642(9)	0.8307(8)	0.6737(3)	0.0116(8)	0.0125(18)	0.0095(17)	0.0139(18)	0.0018(14)	0.0029(16)	0.0051(14)
OW11	0.7715(12)	0.8541(12)	0.9481(3)	0.0046(16)						
OW12	0.1711(18)	0.5626(18)	0.9240(4)	0.051(2)	0.066(5)	0.087(6)	0.019(3)	0.001(3)	0.008(3)	0.052(5)

TABLE 5. SELECTED INTERATOMIC DISTANCES (Å) AND POSSIBLE HYDROGEN BONDS (Å) FOR MENGEITE

Ba1	O3	2.740(4) ×2	M2	O6	1.913(4)
	O4	2.748(4) ×2		OH9	1.929(4)
	O4	2.749(4) ×2		O4	1.932(4)
	O2	2.760(4) ×2		OH10	1.948(4)
	O1	2.812(5) ×2		O7	2.186(5)
	O1	3.498(5) ×2		O2	2.255(5)
	O1	3.508(5) ×2		<M–O>	2.027
	<Ba–O>	3.011			
Ba2			M3	O5	2.096(5) ×2
	O5	2.737(13)		OW12	2.133(7) ×2
	O8	2.817(13)		OW11	2.203(6) ×2
	O5	2.823(12)		<M–O>	2.144
	OW12	2.851(16)	P1	O1	1.515(5)
	OW11	2.964(14)		O2	1.557(5)
	OW12	2.995(14)		O3	1.559(4)
	O5	3.048(14)		O4	1.560(4)
	O7	3.087(12)		<P–O>	1.548
	OW12	3.196(14)			
	O6	3.472(14)			
	<Ba–O>	2.999		P2	O5
		O6	1.545(5)		
M1	O8	1.899(4)	O7		1.549(5)
	OH9	1.927(5)	O8		1.558(4)
	O3	1.932(4)	<P–O>	1.543	
	OH10	1.950(5)			
	O7	2.194(4)			
	O2	2.251(4)			
	<M–O>	2.026			
	Possible hydrogen bonds				
OH9...OW12	2.861	OW11...O7	3.061		
OH10...O1	2.813	OW11...O8	2.944		
OH10...O4	3.000	OW12...O6	3.206		

TABLE 6. BOND-VALENCE ANALYSIS FOR MENGEITE

	Ba	Ba2*	<i>M1</i>	<i>M2</i>	<i>M3</i>	<i>P1</i>	<i>P2</i>	Sum
O1	0.23 ^{x2} ↓ 0.04 ^{x4} ↓					1.34		1.65
O2	0.27 ^{x2} ↓		0.18	0.17		1.20		1.82
O3	0.28 ^{x2} ↓		0.65			1.18		2.11
O4	0.28 ^{x2} ↓			0.64		1.18		2.10
O5		0.01 ^{x3} ↓			0.36 ^{x2} ↓		1.31	1.68
O6		0.00		0.69			1.23	1.92
O7		0.01	0.22	0.23			1.22	1.68
O8		0.01	0.72				1.20	1.93
OH9			0.65	0.65				1.20
OH10			0.60	0.60				1.30
OW11		0.01			0.33 ^{x2} ↓			0.34
OW12		0.01 ^{x2} ↓			0.34 ^{x2} ↓			0.35
Sum	2.28	0.08	3.01	2.98	2.06	4.90	4.96	

* The bond-valence sum for the Ba2 site is based on an occupancy of 0.045.

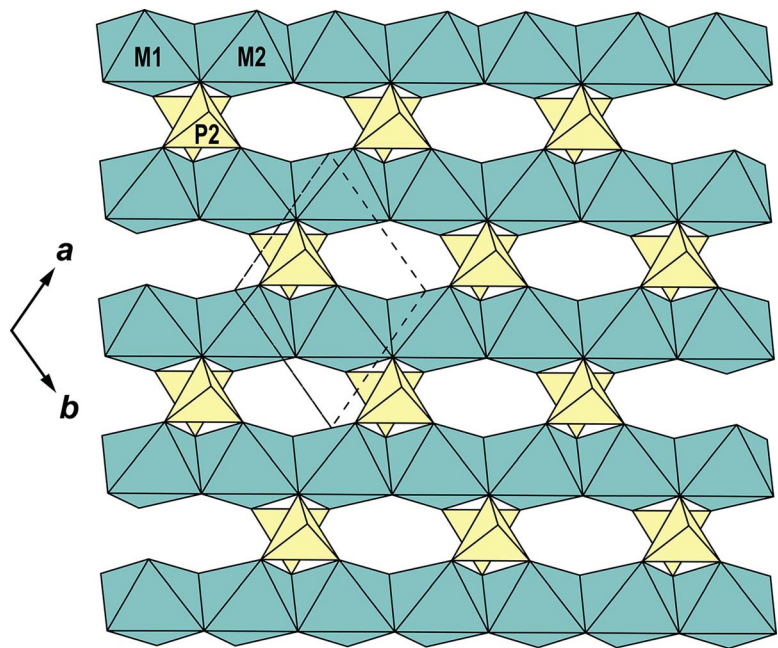


FIG. 3. The $[(M_2(OH)_2(PO_4)_2)]$ sheet in the crystal structure of menegite.

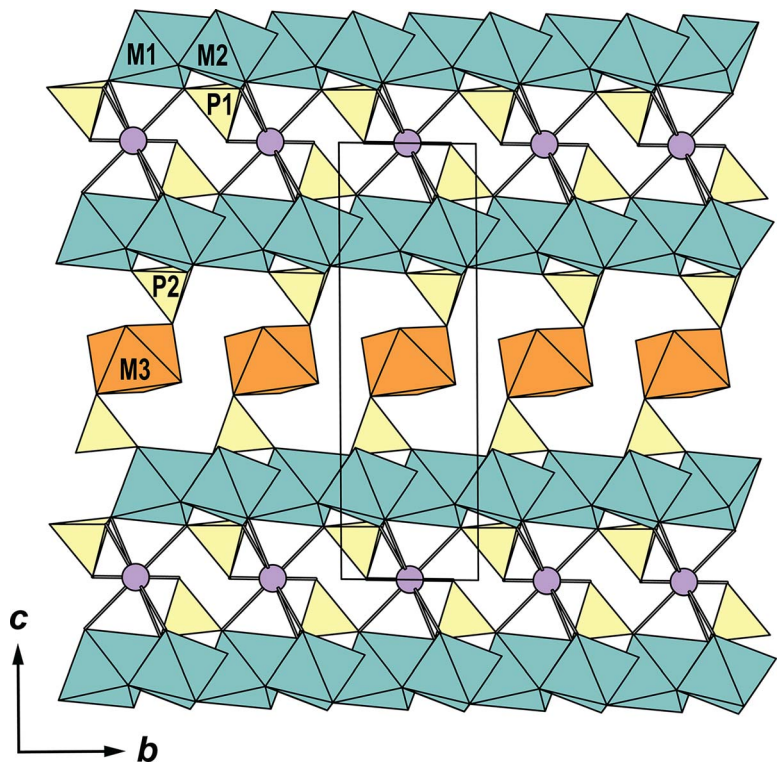


FIG. 4. The crystal structure of menegite viewed along $[100]$.

octahedra and with PO_4 tetrahedra, along with sharing corners with a second Na polyhedron. In the structures of the phosphate minerals bermanite (Kampf & Moore 1976) and magnesiobermanite (Elliott 2022), along with the arsenate mineral coralloite (Callegari *et al.* 2012), sheets are linked *via* a [6]-coordinated small cation site (Mn^{2+} and Mg). Coralloite differs in that the [6]-coordinated site corner links to TO_4 tetrahedra *via cis* O atoms as opposed to *trans* O atoms in bermanite and magnesiobermanite. Mengeite is the first of the structure type in which linkage between sheets is *via* both a large cation site and a small cation site.

ACKNOWLEDGMENTS

Ben Wade of Adelaide Microscopy, The University of Adelaide, is thanked for assistance with the microprobe analysis. The infrared spectrum was acquired with the assistance of the Forensic Science Centre, Adelaide. The single-crystal X-ray data set was collected at the macromolecular beam line MX2 at the Australian Synchrotron.

REFERENCES

- AUSTIN, J.B. (1863) The mines of South Australia; including also an account of the smelting works in that colony, together with a brief description of the country and incidents of travel in the bush, by J. B. Austin. Adelaide, C. Platts, E. S. Wigg, G. Dehane, J. Howell, W. C. Rigby, G. Mullett, 1863. Adelaide, 109p. Reprinted by Libraries Board of South Australia, Adelaide.
- BEYER, B.D. & ELLIOTT, P. (1996) Minerals from the Spring Creek mine, near Wilmington, South Australia. *Australian Journal of Mineralogy* **2**, 57–70.
- BINKS, P.J., FORBES, B.G., & MIRAMS, R.C. (1968) Ortofof sheet, S 54-1 1:250,000. Geological Survey of South Australia
- CALLEGARI, A.M., BOIOCCHI, M., CIRIOTTI, M., & BALESTRA, C. (2012) Coralloite, $\text{Mn}^{2+}\text{Mn}^{3+}_2(\text{AsO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$, a new mixed valence Mn hydrate arsenate: Crystal structure and relationships with bermanite and whitmoreite mineral groups. *American Mineralogist* **97**, 727–734.
- CAWTHORNE, W.A. (1859) Menge the Mineralogist. Adelaide, 33 p. Reprinted by Public Library of South Australia, Adelaide.
- COOPER, M.A., HAWTHORNE, F.C., & ČERNÝ, P. (2009) The crystal structure of ercitate, $\text{Na}_2(\text{H}_2\text{O})_4[\text{Mn}^{3+}_2(\text{OH})_2(\text{PO}_4)_2]$, and its relation to bermanite, $\text{Mn}^{2+}(\text{H}_2\text{O})_4[\text{Mn}^{3+}_2(\text{OH})_2(\text{PO}_4)_2]$. *Canadian Mineralogist* **33**, 889–905.
- ELLIOTT, P. (2019) Strontioperloffite, $\text{SrMn}^{2+}_2\text{Fe}^{3+}_2(\text{PO}_4)_3(\text{OH})_3$, a new bjarebyte-group mineral from the Spring Creek mine, South Australia, Australia. *European Journal of Mineralogy* **31**, 549–555.
- ELLIOTT, P. (2022) Magnesiobermanite, $\text{MgMn}^{3+}_2(\text{PO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$, the Mg analogue of bermanite: Description and crystal structure. *Mineralogical Magazine* **86**, 127–133.
- FARRUGIA, L.J. (2012) WinGX and ORTEP for Windows: An update. *Journal of Applied Crystallography* **45**, 849–854.
- GAGNÉ, O.C. & HAWTHORNE, F.C. (2015) Comprehensive derivation of bond-valence parameters for ion pairs involving oxygen. *Acta Crystallographica* **B71**, 562–578.
- GIESTER, G. & ZEMANN, J. (1987) The crystal structure of the natrochalcite-type compounds $\text{Me}^+\text{Cu}_2(\text{OH})(\text{zO}_4)_2 \cdot \text{H}_2\text{O}$ [$\text{Me}^+ = \text{Na}, \text{K}, \text{Rb}$; $z = \text{S}, \text{Se}$], with special reference to the hydrogen bonds. *Zeitschrift für Kristallographie*, **179**, 431–442.
- HOLLAND, T.J.B. & REDFERN, S.A.T. (1997) Unit cell refinement from powder diffraction data; the use of regression diagnostics. *Mineralogical Magazine* **61**, 65–77.
- KABSCH, W. (2010) XDS. *Acta Crystallographica* **D66**, 125–132.
- KAMPF, A.R. & MOORE, P.B. (1976) The crystal structure of bermanite, a hydrated manganese phosphate. *American Mineralogist* **61**, 1241–1248.
- KOLITSCH, U., TAYLOR, M.R., FALLON, G., & PRING, A. (1999a) Springcreekite, $\text{BaV}^{3+}_3(\text{PO}_4)_2(\text{OH}, \text{H}_2\text{O})_6$, a new member of the crandallite group, from the Spring Creek mine, South Australia: The first natural V^{3+} -member of the alunite family and its crystal structure. *Neues Jahrbuch für Mineralogie, Monatshefte*, 1999, 529–544.
- KOLITSCH, U., PRING, A., & ELLIOTT, P. (1999b) An update on the mineralogy of the Spring Creek mine, South Australia, including the new species springcreekite, bariosincosite and tomaite. *Australian Journal of Mineralogy* **5**, 55–62.
- KOLITSCH, U., PRING, A., & TIEKINK, E.R.T. (2000) Johntomaite, a new member of the bjarebyte group of barium phosphates: Description and structure refinement. *Mineralogy and Petrology* **70**, 1–14.
- KRAUS, W. & NOLZE, G. (1996) POWDER CELL – A program for the representation and manipulation of crystal structures and calculation of the resulting X-ray powder pattern. *Journal of Applied Crystallography* **29**, 301–303.
- KRAUSE, W., BELENDORFF, K., BERNHARDT, H.-J., MCCAMMON, C., EFFENBERGER, H., & MIKENDA, W. (1998) Crystal chemistry on the tsumcorite-group minerals. New data on ferrilotharmeyerite, tsumcorite, thometzekite, mouna-naite, helmutwinklerite, and a redefinition of gartrellite. *European Journal of Mineralogy* **10**, 179–206.
- KRICKL, R. & WILDNER, M. (2007) Crystal chemistry of synthetic Co- and Ni-analogues of natrochalcite – The shortest known hydrogen bonds among mineral-type

- compounds Part I: Single-crystal X-ray structures. *European Journal of Mineralogy* **19**, 805–816.
- LIBOWITZKY, E. (1999) Correlation of O–H stretching frequencies and O–H...O hydrogen bond lengths in minerals. *Monatshefte für Chemie* **130**, 1047–1059.
- MANDARINO, J.A. (1981) The Gladstone-Dale relationship. Part IV. The compatibility concept and its application. *Canadian Mineralogist* **19**, 441–450.
- MIHAJLOVIC, T. & EFFENBERGER, H. (2004) The first proof of protonated anion tetrahedra in the tsumcorite-type compounds. *Mineralogical Magazine* **68**, 757–767.
- POUCHOU, J.L. & PICOIR, F. (1985) “PAP” $\phi(\rho Z)$ procedure for improved quantitative microanalysis. In *Microbeam Analysis* (J.T. Armstrong, ed.). San Francisco Press, California (104–106).
- PRING, A., KOLITSCH, U., BIRCH, W.D., BEYER, B.D., ELLIOTT, P., AYYAPPAN, P., & RAMANAN, A. (1999) Barriosincosite, a new hydrated barium vanadium phosphate, from the Spring Creek Mine, South Australia. *Mineralogical Magazine* **63**, 735–741.
- SHELDRICK, G.M. (2000) SADABS Area-Detector Absorption Correction Program. Bruker AXS Inc., Madison, WI, USA.
- SHELDRICK, G.M. (2015) Crystal Structure refinement with SHELX. *Acta Crystallographica* **C71**, 3–8.
- TRIEBEL, L.A. (1963) Johann Menge: An eccentric German scientist in South Australia, 1836–1852. *Tasmanian Historical Research Association, Papers and Proceedings* **11**, 31–46.

Received April 26, 2021. Revised manuscript accepted June 1, 2022.

This manuscript was handled by Associate Editor Henrik Friis and Editors Lee Groat and Andrew McDonald.