

Chongite, $\text{Ca}_3\text{Mg}_2(\text{AsO}_4)_2(\text{AsO}_3\text{OH})_2 \cdot 4\text{H}_2\text{O}$, a new arsenate member of the hureaulite group from the Torrecillas mine, Iquique Province, Chile

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[Received 27 September 2015; Accepted 24 November 2015; Associate Editor: Stuart Mills]

ABSTRACT

The new mineral chongite (IMA2015–039), $\text{Ca}_3\text{Mg}_2(\text{AsO}_4)_2(\text{AsO}_3\text{OH})_2 \cdot 4\text{H}_2\text{O}$, was found at the Torrecillas mine, Iquique Province, Chile, where it occurs as a secondary alteration phase in association with native arsenic, arsenolite, gajardoite, talmessite and torrecillasite. Chongite occurs as prismatic crystals up to ~1 mm long grouped in tightly intergrown radial aggregates up to 2 mm in diameter. Crystals are transparent, with vitreous lustre and white streak. The Mohs hardness is ~3½, tenacity is brittle and fracture is conchoidal. Cleavage is good on {100}. The measured density is 3.09(2) g/cm³ and the calculated density is 3.087 g/cm³. Optically, chongite is biaxial (–) with $\alpha = 1.612(1)$, $\beta = 1.626(1)$, $\gamma = 1.635(1)$ and $2V = 76.9(1)^\circ$ (measured in white light). Dispersion is $r < v$, distinct. The optical orientation is $X = b$; $Z \wedge a = 27^\circ$ in obtuse angle β . The mineral is slowly soluble in dilute HCl at room temperature. The empirical formula, determined from electron-microprobe analyses, is $(\text{Ca}_{2.90}\text{Mg}_{1.93}\text{Mn}_{0.14})_{\Sigma 4.97}\text{As}_4\text{O}_{20}\text{H}_{10.07}$. Chongite is monoclinic, $C2/c$, $a = 18.5879(6)$, $b = 9.3660(3)$, $c = 9.9622(7)$ Å, $\beta = 96.916(7)^\circ$, $V = 1721.75(14)$ Å³ and $Z = 4$. The eight strongest powder X-ray diffraction lines are [d_{obs} Å(hkl)]: 8.35(29)(110), 4.644(62)($\bar{3}11, 020, 400, \bar{2}02$), 4.396(26)(311), 3.372(62)(022, 312, $\bar{5}11$), 3.275(100)(420, $\bar{2}22, \bar{4}21$), 3.113(57)(222), 2.384(30)(711, 530, $\bar{7}12$) and 1.7990(22)($\bar{9}13, 334, \bar{5}34$). The structure determination ($R_1 = 1.56\%$ for 1849 $F_o > 4\sigma F$ reflections) confirms that chongite is a member of the hureaulite group.

KEYWORDS: chongite, new mineral, arsenate, crystal structure, hureaulite group, Torrecillas mine, Chile.

Introduction

THE Torrecillas mine, in the northern Atacama Desert of Chile, is a small, long-inactive arsenic mine probably discovered and first mined during the guano mining boom of the early 19th century (Mortimer, *et al.*, 1971). It was clearly never a significant producer and was probably finally abandoned several years prior to 1950 (Pimentel, 1978). In recent years, our investigations on the

minerals of this unusual deposit have yielded many new and potentially new mineral species. To date, the descriptions of four new minerals have been published: leverettite (Kampf *et al.*, 2013a), magnesiokoritnigite (Kampf *et al.*, 2013b), torrecillasite (Kampf *et al.*, 2014a) and canutite (Kampf *et al.*, 2014b). Herein, we describe the new mineral chongite and, in an accompanying paper, we describe the associated new mineral gajardoite (Kampf *et al.*, 2016; IMA2015–039). Several other potentially new minerals are currently under study.

The new mineral chongite (/ˈʒɒŋ aɪt/) honours Dr. Guillermo Chong Díaz (b. 1936). Dr. Chong is a prominent Chilean geologist and academician

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DOI: 10.1180/minmag.2016.080.064

whose research has focused largely on the Atacama Desert. During his approximately 50-year career, he has some 250 publications and meeting presentations, including serving as lead author for the chapter on Industrial Minerals and Rocks in *The Geology of Chile* published by the Geological Society of London in 2007. Dr. Chong is currently a professor in the Department of Geological Sciences at Universidad Católica del Norte in Antofagasta, Chile. He is Director (and founder) of the Museo Geológico Prof. Humberto Fuenzalida Villegas. He also founded the Museo Geológico de San Francisco de Chiu Chiu and the Museo del Desierto de Atacama. During his illustrious career, he has received numerous awards and honours. Dr. Chong has agreed to the naming of this mineral in his honour.

The new mineral and the name have been approved by the International Mineralogical Association (IMA2015-039). The description is based upon one holotype and two cotype specimens that are deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue numbers 65585, 65586 and 65587, respectively. These are the same as the holotype and cotypes for gajardoite.

Occurrence

The Torrecillas mine is located on Torrecillas Hill, Iquique Province, Tarapacá Region, Chile (approximately 20°58'13"S, 70°8'17"W). Four different rock units are exposed on the hill. The Coastal Range Batholith (mainly gabbros) extends from the seashore to the Pan-American Road along the base of Torrecillas Hill. At the foot of Torrecillas Hill is a small area of contact metamorphic rocks in which garnet crystals occur in metamorphosed shales. Higher on the hill, the rocks are predominantly andesites and porphyritic lavas of the Jurassic La Negra Formation. The Torrecillas deposit, in which the new mineral is found, consists of two main veins rich in secondary arsenic and copper minerals that intersect metamorphosed marine shales and lavas. These mineralized veins are genetically related to the aforementioned andesites and porphyritic lavas of the Jurassic La Negra Formation. More information on the geology and mineralogy of the area is provided by Gutiérrez (1975).

The rare secondary chlorides, arsenates and arsenites have been found at three main sites on the hill: an upper pit measuring ~8 m long and 3 m deep, a lower pit ~100 m from the upper pit and measuring

~5 m long and 3 m deep, and a mine shaft adjacent to the lower pit and lower on the hill. Chongite was found by a collecting party consisting of three of the authors (ARK, MD and AAMD) along with Jochen Schlüter and Joe Marty in February 2014 at a small excavation a few metres above the shaft.

The new mineral is a secondary alteration phase occurring in association with native arsenic, arsenolite, gajardoite, talmessite and torrecillasite (Kampf *et al.*, 2014a). The secondary assemblages at the Torrecillas deposit are interpreted as having formed from the oxidation of native arsenic and other As-bearing primary phases, followed by later alteration by saline fluids derived from evaporating meteoric water under hyperarid conditions (*cf.* Cameron *et al.*, 2007).

Physical and optical properties

Chongite occurs as prismatic crystals up to ~1 mm long grouped in tightly intergrown radial aggregates up to ~2 mm in diameter (Fig. 1). Prisms are elongated on [001] and exhibit the forms {100}, {110}, {111}, {11 $\bar{1}$ }, {20 $\bar{1}$ } and {311} (Fig. 2). No twinning was observed. Crystals are transparent, with vitreous lustre and white streak. The mineral does not fluoresce in longwave or shortwave ultraviolet light. The Mohs hardness is ~3½, based on scratch tests. The tenacity is brittle and the fracture is conchoidal. Cleavage is good on {100}. The density measured by floatation in Clerici solution is 3.09(2) g/cm³ and the calculated density is 3.087 g/cm³. Optically, chongite is biaxial (-) with $\alpha = 1.612(1)$, $\beta = 1.626(1)$ and $\gamma = 1.635(1)$ measured in white light. The 2V measured using extinction data and *EXCALIBRW* (Gunter *et al.*, 2004) is 76.9(1)°. The calculated 2V



FIG. 1. Chongite crystals. Field of view: 1 mm across.

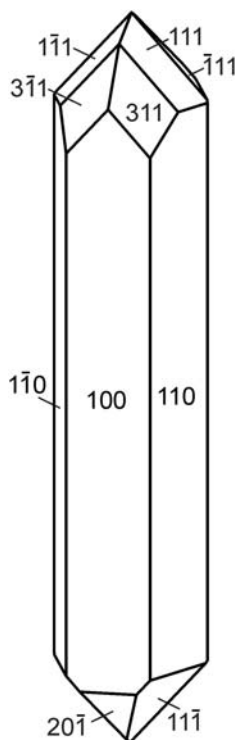


FIG. 2. Crystal drawing of chongite, clinographic projection in standard orientation.

is 76.9° . Dispersion is $r < v$, distinct. The optical orientation is $X = b$; $Z \wedge a = 27^\circ$ in the obtuse angle β . Chongite is nonpleochroic. The mineral is slowly soluble in dilute HCl at room temperature.

Composition

Quantitative analyses (12 points on 4 crystals) were performed at the University of Utah using a Cameca SX-50 electron microprobe with four wavelength-dispersive spectrometers utilizing *Probe for EPMA* software. Analytical conditions were 15 kV accelerating voltage, 10 nA beam current and a beam diameter of 12 μm . Chongite exhibited visible beam damage under the electron beam. Counting times were 20 s on peak and 10 s on + and - background. Background positions were selected specifically to account for the proximity of the $\text{AsL}\alpha_1$ and $\text{MgK}\alpha_{1,2}$ peaks. No other elements were detected by EDS and other possible elements were sought by EPMA, but none were above the detection limits. Raw X-ray intensities were corrected for matrix effects with a $\phi(\rho z)$ (PAP)

TABLE 1. Analytical data (wt.%) for chongite.

Constituent	Mean	Range	SD	Standard
CaO	19.96	19.43–20.29	0.23	diopside
MgO	9.55	9.32–9.96	0.23	diopside
MnO	1.18	0.86–1.67	0.24	rhodonite
As_2O_5	56.42	56.09–57.04	0.36	syn. GaAs
H_2O^*	11.13			
Total	98.24			

*Calculated on the basis of As = 4 apfu, charge balance and O = 20 apfu.

SD – standard deviation.

algorithm (Pouchou and Pichoir, 1991). Because insufficient material was available for a direct determination of H_2O , the amount of water was calculated on the basis of As = 4 atoms per formula unit (apfu), charge balance and O = 20 apfu, as determined by the crystal structure analysis (see below). Analytical data are given in Table 1.

The empirical formula is $(\text{Ca}_{2.90}\text{Mg}_{1.93}\text{Mn}_{0.14})_{\Sigma 4.97}\text{As}_4\text{O}_{20}\text{H}_{10.07}$. The simplified structural formula is $\text{Ca}_3\text{Mg}_2(\text{AsO}_4)_2(\text{AsO}_3\text{OH})_2 \cdot 4\text{H}_2\text{O}$, which requires CaO 21.07, MgO 10.09, As_2O_5 57.56, H_2O 11.28, total 100 wt.%. The Gladstone-Dale compatibility $1 - (K_p/K_c)$ for the empirical formula is -0.031 in the range of excellent compatibility (Mandarino, 2007).

X-ray crystallography and structure refinement

Both powder and single-crystal X-ray studies were carried out using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer, with monochromatic $\text{MoK}\alpha$ radiation. For the powder-diffraction study 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 2 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 $a = 18.580(11)$, $b = 9.357(11)$, $c = 9.957(11)$ \AA , $\beta = 96.918(9)^\circ$ and $V = 1718(3)$ \AA^3 .

The *Rigaku CrystalClear* software package was used for processing structure data, including the application of an empirical absorption correction using *ABSCOR* (Higashi, 2001). The structure was

TABLE 2. Powder X-ray data for chongite.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	h	k	l	I_{obs}	d_{obs}	d_{calc}	I_{calc}	h	k	l
9	9.39	9.2263	10	2	0	0	21	2.0753	2.0879	6	4	4	0
29	8.35	8.3518	22	1	1	0			2.0846	3	5	3	2
12	6.55	6.5595	7	1	1	1			2.0720	4	3	3	3
7	6.12	6.2160	5	1	1	1			2.0626	6	4	2	4
62	4.644	4.7621	8	3	1	1	9	2.0118	2.0141	5	7	3	0
		4.6830	18	0	2	0			2.0071	3	5	3	3
		4.6132	13	4	0	0			1.9829	3	8	2	1
		4.5948	23	2	0	2	6	1.8450	1.8639	2	5	3	3
26	4.396	4.3847	27	3	1	1			1.8630	2	6	4	0
16	4.160	4.1759	4	2	2	0			1.8394	2	8	2	2
		4.1550	15	2	0	2			1.8355	3	1	5	1
15	3.927	3.9244	13	2	2	1	22	1.7990	1.8087	4	9	1	3
5	3.775	3.7740	9	2	2	1			1.8006	6	3	3	4
62	3.372	3.4002	13	0	2	2			1.7868	8	5	3	4
		3.3972	7	3	1	2	20	1.7135	1.7179	8	9	3	1
		3.3625	46	5	1	1			1.7138	3	9	3	0
100	3.275	3.2864	11	4	2	0			1.7040	4	3	5	2
		3.2798	72	2	2	2			1.7001	6	0	4	4
		3.2020	17	4	2	1	10	1.6879	1.6812	4	10	2	2
		3.1872	4	4	0	2			1.6751	4	6	4	3
		3.1366	4	5	1	1	20	1.6591	1.6604	4	10	2	1
57	3.113	3.1080	45	2	2	2			1.6575	5	2	0	6
19	3.008	3.0108	21	1	1	3			1.6524	4	7	3	3
10	2.904	2.9114	9	3	1	3	13	1.6410	1.6490	5	1	3	5
		2.8522	5	4	2	2			1.6364	3	5	1	5
6	2.781	2.7839	4	3	3	0			1.6308	3	1	5	3
		2.7187	4	3	3	1	7	1.5947	1.6006	4	1	1	6
16	2.692	2.6957	7	0	2	3			1.5838	3	5	3	5
		2.6830	9	5	1	2	18	1.5632	1.5683	7	10	2	2
6	2.651	2.6425	6	3	3	1			1.5625	4	2	2	6
4	2.533	2.5295	4	7	1	1			1.5570	4	5	5	2
11	2.466	2.4724	12	0	0	4			1.5548	3	0	2	6
		2.4292	5	6	2	1	16	1.5369	1.5419	4	0	6	1
30	2.384	2.3920	17	7	1	1			1.5377	7	12	0	0
		2.3835	10	5	3	0			1.5269	5	7	5	0
		2.3720	7	7	1	2	9	1.5106	1.5135	4	2	4	5
17	2.296	2.3066	8	8	0	0			1.5054	3	2	2	6
		2.2974	9	4	0	4			1.4982	4	9	1	5
		2.2728	3	1	3	3			1.4956	3	7	3	4
		2.2265	4	2	4	1	14	1.4878	1.4885	4	7	5	2
13	2.1986	2.1979	7	2	4	1			1.4800	3	9	3	4
		2.1864	7	0	2	4	11	1.4618	1.4697	3	2	4	5
5	2.1404	2.1454	3	3	1	4			1.4618	3	7	1	6
		2.1339	5	7	1	3			1.4610	3	12	2	0

Only calculated lines with $I_{\text{calc}} > 3$ are included, except those needed to index the observed line at 1.8450 Å.

solved by direct methods using *SIR2011* (Burla *et al.*, 2012) and then the atom coordinates were transformed to conform with those of *sainfeldite* (Ferarris and Abbona, 1972), *miguelromeroite* and *villyaellenite* (Kampf, 2009), with which *chongite* is isostructural. *SHELXL-2013* (Sheldrick, 2015)

was used for the refinement of the structure. A difference-Fourier synthesis 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.

TABLE 3. Data collection and structure refinement details for chongite.

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	Ca(Mg _{1.92} Mn _{0.08}) _{Σ2} Ca ₂ (AsO ₄) ₂ (AsO ₃ OH) ₂ ·4H ₂ O
Space group	C2/c
Unit-cell dimensions	$a = 18.5879(6)$ Å $b = 9.3660(3)$ Å $c = 9.9622(7)$ Å $\beta = 96.916(7)^\circ$
<i>V</i>	1721.75(14) Å ³
<i>Z</i>	4
Density (for above formula)	3.090 g/cm ³
Absorption coefficient	8.817 mm ⁻¹
<i>F</i> (000)	1547.9
Crystal size (μ m)	100 × 80 × 40
θ range ($^\circ$)	3.11 to 27.47
Index ranges	$-24 \leq h \leq 24$, $-12 \leq k \leq 12$, $-12 \leq l \leq 10$
Refls collected/unique	7873/1964; $R_{\text{int}} = 0.0205$
Reflections with $F > 4\sigma(F)$	1849
Completeness to $\theta = 27.47^\circ$	99.1%
Max. and min. transmission	0.719 and 0.473
Refinement method	Full-matrix least-squares on F^2
Parameters/restraints	148/7
Goof	1.124
Final <i>R</i> indices [$F_o > 4\sigma(F)$]	$R_1 = 0.0156$, $wR_2 = 0.0326$
<i>R</i> indices (all data)	$R_1 = 0.0178$, $wR_2 = 0.0334$
Largest diff. peak/hole	+0.67/-0.42 e/Å ³

* $R_{\text{int}} = \Sigma|F_o^2 - F_c^2(\text{mean})|/\Sigma[F_o^2]$. Goof = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0104, b is 3.3407 and P is $[2F_c^2 + \text{Max}(F_o^2, 0)]/3$.

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.

Discussion

Chongite is a member of the hureaulite group and is isostructural with other members of the group (Table 7). The general formula of these phases is $M1M2M3_2[T1O_4]_2[T2O_3(OH)]_2 \cdot 4H_2O$ { $T = P, As$ }, where the *M1*, *M2* and *M3* octahedra form an octahedral edge-sharing pentamer. Pentamers are linked into a loose framework by sharing corners with octahedra in adjacent pentamers and are further linked via TO_4 and TO_3OH tetrahedra (Fig. 3). This structure type was originally solved by Moore and Araki (1973) for the PO_4 analogue hureaulite. In the structure of chongite, the *M1* and

M3 sites refine to full occupancy by Ca and the *M2* site refines to $Mg_{0.963}Mn_{0.037}$. Bond lengths and bond-valence calculations further confirm these assignments.

The labelling of the cation sites is consistent among the published structure determinations of all of the hureaulite-group minerals; however, the O (and H) labelling varies among some of the structures. The site assignments are consistent for the chongite, miguelromeroite and villyaellenite structures. For all three structures, H atom positions have been determined and yield the same hydrogen bonding scheme provided in Table 5. The H atom positions were also determined for the sainfeldite structure and, although the labelling of the O and H atoms is not the same as for the above structures, the hydrogen bonding scheme is the same. The structure determinations for the two remaining members of the hureaulite group, hureaulite and nyholmite,

TABLE 4. Atom coordinates and displacement parameters (\AA^2) for chongite.

	x/a	y/b	z/c	U_{eq}	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
$M1^*$	0.5000	0.38565(6)	0.7500	0.00819(11)	0.0074(3)	0.0092(3)	0.0079(3)	0	0.00079(19)	0
$M2^*$	0.31319(3)	0.08177(7)	0.18672(6)	0.0087(2)	0.0085(4)	0.0084(3)	0.0089(4)	0.0016(2)	0.0008(2)	0.0001(2)
$M3^*$	0.32451(2)	0.46965(4)	0.13727(4)	0.00973(9)	0.00826(18)	0.00925(19)	0.01188(19)	-0.00265(15)	0.00207(14)	-0.00102(14)
As1	0.41477(2)	0.30629(2)	0.40820(2)	0.00763(6)	0.00732(10)	0.00853(10)	0.00688(10)	-0.00045(7)	0.00024(7)	0.00033(7)
As2	0.66224(2)	0.22868(2)	0.61869(2)	0.00594(5)	0.00615(9)	0.00563(9)	0.00598(10)	0.00000(7)	0.00054(6)	0.00027(7)
O1	0.42612(8)	0.43046(16)	0.29395(15)	0.0150(3)	0.0139(7)	0.0159(8)	0.0151(7)	0.0074(6)	0.0017(6)	-0.0015(6)
O2	0.33804(8)	0.21906(16)	0.35288(14)	0.0139(3)	0.0111(7)	0.0176(7)	0.0127(7)	-0.0033(6)	0.0007(5)	-0.0045(6)
O3	0.41126(8)	0.37721(16)	0.56128(14)	0.0141(3)	0.0137(7)	0.0181(8)	0.0100(7)	-0.0063(6)	-0.0006(5)	0.0044(6)
O4	0.66752(7)	0.23807(14)	0.45096(13)	0.0102(3)	0.0145(7)	0.0101(7)	0.0061(6)	0.0003(5)	0.0015(5)	0.0004(5)
O5	0.70620(7)	0.08341(14)	0.68394(14)	0.0101(3)	0.0102(7)	0.0084(6)	0.0118(7)	0.0042(6)	0.0014(5)	0.0029(5)
O6	0.70372(7)	0.37389(15)	0.69137(15)	0.0121(3)	0.0107(7)	0.0091(7)	0.0167(7)	-0.0061(6)	0.0023(5)	-0.0014(5)
O7	0.57413(7)	0.22336(15)	0.64605(14)	0.0109(3)	0.0066(6)	0.0130(7)	0.0131(7)	0.0001(6)	0.0015(5)	0.0003(5)
OH	0.48529(8)	0.18616(17)	0.42157(16)	0.0177(3)	0.0167(8)	0.0206(8)	0.0144(8)	-0.0049(6)	-0.0041(6)	0.0102(6)
H	0.5128(13)	0.198(3)	0.493(2)	0.021						
OW1	0.23471(8)	0.41841(16)	0.46616(15)	0.0141(3)	0.0168(8)	0.0148(8)	0.0118(8)	-0.0003(6)	0.0053(6)	0.0006(6)
H1a	0.2063(12)	0.385(3)	0.509(2)	0.017						
H1b	0.2506(13)	0.362(3)	0.420(2)	0.017						
OW2	0.58612(8)	0.00090(18)	0.82841(17)	0.0195(3)	0.0139(8)	0.0195(8)	0.0258(9)	0.0115(7)	0.0058(6)	0.0017(6)
H2a	0.5738(14)	0.061(2)	0.777(2)	0.023						
H2b	0.5554(13)	-0.045(3)	0.850(3)	0.023						

* $M1$ = Ca; $M2$ = Mg 0.963(3) + Mn 0.037(3); $M3$ = Ca.

CHONGITE, NEW HUREAULITE-GROUP ARSENATE FROM TORRECILLAS MINE, CHILE

TABLE 5. Selected bond distances (Å) and angles (°) for chongite.

M1–O1(×2)	2.2778(15)	M2–OW2	2.0476(17)	M3–O1	2.3299(15)
M1–O3(×2)	2.3483(14)	M2–O4	2.0667(15)	M3–O3	2.3503(15)
M1–O7(×2)	2.3718(14)	M2–O5	2.0726(15)	M3–O4	2.3517(14)
<M1–O>	2.333	M2–O6	2.0828(15)	M3–O5	2.3550(14)
As1–O1	1.6584(14)	M2–O2	2.1031(15)	M3–O6	2.3565(14)
As1–O3	1.6719(14)	M2–OW1	2.2642(16)	M3–OW1	2.4711(16)
As1–O2	1.6781(14)	<M2–O>	2.106	<M3–O>	2.369
As1–OH	1.7204(15)	Hydrogen bonding			
<As1–O>	1.682	D–H···A	D–H	H···A	D···A
As2–O5	1.6773(13)	OH–H···O7	0.84(2)	1.80(2)	2.638(2)
As2–O6	1.6835(14)	OW1–H1a···O2	0.79(2)	1.94(2)	2.706(2)
As2–O4	1.6879(14)	OW1–H1b···O2	0.78(2)	2.27(2)	2.995(2)
As2–O7	1.6931(14)	OW2–H2a···O7	0.78(2)	2.00(2)	2.756(2)
<As2–O>	1.686	OW2–H2b···OH	0.77(2)	2.04(2)	2.804(2)
					<DHA
					179(3)
					163(3)
					155(2)
					163(3)
					172(3)

TABLE 6. Bond-valence analysis for chongite. Values are expressed in valence units.

	O1	O2	O3	O4	O5	O6	O7	OH	OW1	OW2	Σ _c
M1	0.43 ^{×2→}		0.36 ^{×2→}				0.33 ^{×2→}				2.24
M2		0.33		0.37	0.36	0.35			0.22	0.39	2.02
M3	0.36		0.35	0.35	0.35	0.35			0.26		2.02
As1	1.34	1.27	1.29					1.13			5.03
As2				1.24	1.27	1.25	1.22				4.98
H							0.23	0.77			1.00
H1a		0.20							0.80		1.00
H1b		0.10							0.90		1.00
H2a							0.19			0.81	1.00
H2b								0.18		0.82	1.00
Σ _a	2.13	1.90	2.00	1.96	1.98	1.95	1.97	2.08	2.18	2.02	

Multiplicities indicated by ×2→; bond valence parameters from Brown and Altermatt (1985); hydrogen-bond strengths based on O···O bond lengths also from Brown and Altermatt (1985).

TABLE 7. Arsenate members of the hureaulite group.

	M1 (1 apfu)	M2 (2 apfu)	M3 (2 apfu)	Structure reference
chongite	Ca	Mg	Ca	This study
sainfeldite	Ca	Ca	Ca	Ferraris and Abbona, 1972
villyaellenite	Mn	Mn	Ca	Kampf <i>et al.</i> , 2009
miguelromeroite	Mn	Mn	Mn	Kampf <i>et al.</i> , 2009
nyholmite	Cd	Zn	Cd	Elliott <i>et al.</i> , 2009

matched one another in their labelling of the O atom sites, but neither included determinations of the H atom sites. Although the hydrogen bonding schemes

proposed for hureaulite and nyholmite by Moore and Araki (1973) and Elliott *et al.* (2009), respectively, differ in some respects from the above, it appears

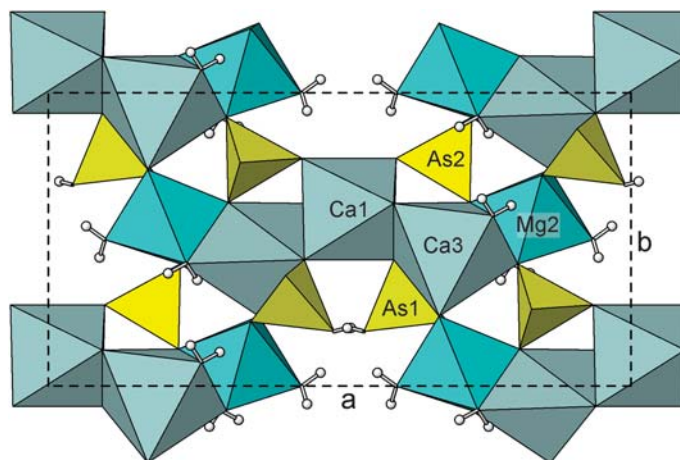


FIG. 3. The crystal structure of chongite viewed perpendicular to $\{001\}$. The unit cell is shown by dashed lines. For clarity, only half of the cell contents along c are shown.

certain that the structures of all members of the hureaulite group have the same hydrogen bonding. For example, Elliot *et al.* (2009) proposed that the OH group (OH2) donates a hydrogen bond to one of the H₂O groups, H₂O(9) [= OW2 in the chongite structure], while our assignment of this hydrogen bond is to O(6) [= O7 in the chongite structure]. The assignment of this hydrogen bond in the nyholmite structure by Elliot *et al.* (2009) is almost certainly incorrect as it results in a bond-valence sum (BVS) of 2.28 vu for the H₂O(9) site and 1.76 vu for the O(6) site, as opposed to 2.09 and 1.98 vu, respectively, using the same hydrogen bond assignment as in the chongite structure.

Chongite can be considered an Mg analogue of sainfeldite, Ca₅(AsO₄)₂(AsO₃OH)₂·4H₂O, in which Mg replaces Ca in the M2 site in the structure. The M2 site is clearly the preferred site in the structure for the smallest octahedrally coordinated cation, as is also seen for nyholmite (Table 7). In the structure of villyaellenite, Mn dominates both the M1 and M2 sites, with Ca occupying the M3 site, so it can be assumed that, after the M2 site, the small cation is accommodated in the M1 site. By analogy with villyaellenite and miguelromeroite, it appears possible to have two additional Mg analogues of sainfeldite, one with Mg dominating the M1 and M2 sites and one with Mg dominating the M1, M2 and M3 sites.

Valid unnamed mineral UM1997-09-AsO: CaH₂MgZn (Smith and Nickel, 2007) was reported from Jáchymov, Czech Republic, by Ondrus *et al.* (1997), who referred to it as “Mg-villyaellenite”

and gave its formula as (Mg,Ca,Zn)₅(AsO₄)₂(AsO₃OH)₂·4H₂O. A chemical analysis is not provided; however, they list the major elements determined by “EDX, WDX” as “Ca, As, Mg”. If that order reflects the relative abundances of these elements, this phase could be the same as chongite, or perhaps simply an Mg-rich sainfeldite. The cell parameters that they determined from a Rietveld refinement, $a = 18.588(2)$, $b = 9.4130(9)$, $c = 9.9762(8)$ Å and $\beta = 96.907(6)^\circ$, give a cell volume of 1732.9(3) Å³, which is much closer to the cell volume of chongite, 1721.75(14), than it is to that of sainfeldite, 1868.9(16) Å³, and strongly suggests that the “Mg-villyaellenite” of Ondrus *et al.* (1997) is chongite.

Finally, it is worth noting that irthemite, Ca₄MgH₂(AsO₄)₄·4H₂O (Pierrot and Schubnel, 1972), has a composition that is intermediate between sainfeldite and chongite. Pierrot and Schubnel (1972) suggested a possible relationship with sainfeldite; however, their material did not provide crystals of sufficient quality for single-crystal study. Their powder diffraction data for irthemite do not match those of chongite and, even so, their chemical analysis provides a composition closer to sainfeldite than to chongite, so clearly irthemite and chongite are different phases.

Acknowledgements

Reviewers Peter Elliot and Henrik Friis and Structures Editor Peter Leverett 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.

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