

The crystal structure of gatehouseite

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ABSTRACT

The crystal structure of the manganese phosphate mineral gatehouseite, ideally $\text{Mn}_5^{2+}(\text{PO}_4)_2(\text{OH})_4$, space group $P2_12_12_1$, $a = 17.9733(18)$, $b = 5.6916(11)$, $c = 9.130(4)$ Å, $V = 933.9(4)$ Å³, $Z = 4$, has been solved by direct methods and refined from single-crystal X-ray diffraction data ($T = 293$ K) to an R index of 3.76%. Gatehouseite is isostructural with arsenoclasite and with synthetic $\text{Mn}_5^{2+}(\text{PO}_4)_2(\text{OH})_4$. The structure contains five octahedrally coordinated Mn sites, occupied by Mn plus very minor Mg with observed $\langle\text{Mn}-\text{O}\rangle$ distances from 2.163 to 2.239 Å. Two tetrahedrally coordinated P sites, occupied by P, Si and As, have $\langle\text{P}-\text{O}\rangle$ distances of 1.559 and 1.558 Å. The structure comprises two types of building unit. A strip of edge-sharing $\text{Mn}(\text{O},\text{OH})_6$ octahedra, alternately one and two octahedra wide, extends along [010]. Chains of edge- and corner-shared $\text{Mn}(\text{O},\text{OH})_6$ octahedra coupled by PO_4 tetrahedra extend along [010]. By sharing octahedron and tetrahedron corners, these two units form a dense three-dimensional framework, which is further strengthened by weak hydrogen bonding. Chemical analyses by electron microprobe gave a unit formula of $(\text{Mn}_{4.99}\text{Mg}_{0.02})_{\Sigma 5.01}(\text{P}_{1.76}\text{Si}_{0.20}\text{As}_{0.07})_{\Sigma 2.03}\text{O}_8(\text{OH})_{3.97}$.

KEYWORDS: gatehouseite, manganese, phosphate, crystal structure.

Introduction

THE manganese phosphate mineral gatehouseite was described as a new mineral from the Iron Monarch quarry, a Precambrian sedimentary iron ore deposit at Iron Knob, South Australia, by Pring and Birch (1993). The mineral forms pale yellow to pale brownish orange bladed crystals and orange equant crystals up to ~100 µm in size as part of an assemblage of phosphate, arsenate and vanadate minerals in a matrix consisting of hematite, hausmannite, baryte, Mn-bearing calcite and rhodochrosite, which was mined from RL130 in the north eastern end of the quarry (Pring *et al.*, 1989, 1992, 2000; Francis, 2010). The secondary minerals at Iron Monarch formed during Tertiary and post-Tertiary weathering of the deposit at low

temperature due to the interaction of basic fluids with hausmannite under changing pH conditions (Pring and Birch, 1993).

The tiny size and intergrowth of crystals has previously prevented easy isolation of a suitable crystal and no single-crystal X-ray investigation of gatehouseite has previously been performed. Pring and Birch (1993) showed, by chemical analysis, powder X-ray diffraction and electron diffraction, that gatehouseite is isostructural with synthetic $\text{Mn}_5^{2+}(\text{PO}_4)_2(\text{OH})_4$ (Ruszala *et al.*, 1977) and is the phosphorus analogue of arsenoclasite (Moore and Molin-Case, 1971), and that, by analogy, the space group is most likely to be $P2_12_12_1$.

Chemical composition

A crystal aggregate of gatehouseite (South Australian Museum specimen G19666) was split into two; one section was used for chemical analysis and the other for X-ray data collection.

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Chemical analyses were carried out using a Cameca SX51 electron microprobe operating under the following conditions in wavelength-dispersive mode: operating voltage 20 kV, specimen current 20 nA and beam size 5 μm . The following standards and X-ray lines were used for calibration: almandine (Mg- $K\alpha$, Si- $K\alpha$), rhodonite (Mn- $K\alpha$), gallium arsenide (As- $K\alpha$) and hydroxylapatite (P- $K\alpha$). No additional element with atomic number ≥ 9 was detected in amounts >0.05 wt.% oxide. Data were reduced using the $\phi(\rho Z)$ method of Pouchou and Pichoir (1985). Ten points were analysed; the chemical composition and unit formula are given in Table 1. The mineral was stable under the electron beam, the analytical totals are, however, slightly low (see below). Low analytical totals for their microprobe data for type gatehouseite were also noted by Pring and Birch (1993).

Structure determination

Single-crystal X-ray data collection

A crystal $0.10 \times 0.08 \times 0.05$ mm in size was attached to a glass fibre and mounted on an Oxford Diffraction Xcalibur E diffractometer equipped with an Eos CCD detector. Intensity data were collected at room temperature using Mo- $K\alpha$ X-radiation ($\lambda = 0.71073$ Å) and a detector distance of 45.53 mm. Data collection conditions are given in Table 2. The data were processed using the *CrysAlisPro* program (Oxford Diffraction, 2009) and corrected for Lorentz and polarization effects. An empirical (multi-scan) absorption correction was applied using the *SCALE3 ABSPACK* algorithm, as implemented

in *CrysAlisPro*. The refined unit-cell parameters are $a = 17.9733(18)$, $b = 5.6916(11)$, $c = 9.130(4)$ Å, $V = 933.9(3)$ Å³, which are close to those of Pring and Birch (1993) [$a = 9.097(2)$, $b = 5.693(2)$, $c = 18.002(10)$ Å, $V = 932.4(8)$ Å³], refined from powder X-ray diffraction data.

Structure solution and refinement

Scattering curves for neutral atoms were taken from the *International Tables for Crystallography* (Wilson, 1992). Systematic absences and reflection statistics confirmed that the space group for gatehouseite is $P2_12_12_1$, as reported by Pring and Birch (1993). The structure was solved by direct methods using the *SHELXS-97* program (Sheldrick, 2008) and refined by full-matrix least squares on F^2 , using *SHELXL-97* (Sheldrick, 2008). At the final stages of refinement, four H (hydrogen) sites were identified in difference-Fourier maps and were included into the refinement with constrained isotropic-displacement parameters and restraints on the O–H distances (~ 0.98 Å). The scattering from each P site is compatible with full occupancy of both by P [occupancy factors 1.007(7) and 0.998(7) for P1 and P2 respectively] and occupancies were fixed to $\text{P}_{0.88}\text{Si}_{0.09}\text{As}_{0.03}$, in accord with the chemical analysis. The final refinement, using the atomic coordinates for arsenoclasite (Moore and Molin-Case, 1971) converged to an R_1 index of 3.76% for a model with anisotropic-displacement parameters for all non-H atoms. The final atomic parameters and anisotropic-displacement parameters are listed in Table 3, selected interatomic-distances and angles are given in Table 4 and a bond-valence analysis (Brown and Altermatt, 1985; Brown, 1996) is presented in Table 5.

TABLE 1. Chemical composition (wt.%) and unit formula (a.p.f.u.)* of gatehouseite.

MnO	63.80	Mn	4.99
MgO	0.18	Mg	0.02
P ₂ O ₅	22.58	Σ	5.01
As ₂ O ₅	1.54	P	1.76
SiO ₂	2.22	As	0.07
H ₂ O (calc.)**	6.45	Si	0.20
Sum	96.77	Σ	2.03
		OH	3.97

* Calculation based on 12 oxygen atoms p.f.u.

** The H₂O content is calculated to obtain charge balance.

Structure description

The structure of gatehouseite contains five symmetrically distinct Mn positions, each of which is surrounded by six anions in an octahedral arrangement. All Mn(O,OH)₆ octahedra are distorted; the maximum distortion is shown by the Mn1 and Mn5 octahedra, with intra-octahedral angles deviating up to 26.19 and 28.37° from ideal angles respectively, a result of the octahedra sharing an edge with a PO₄ tetrahedron.

Based on the low total of their electron microprobe analyses, Pring and Birch (1993) suggested that one of the five Mn cations may

TABLE 2. Crystal data, data collection and refinement details for gatehouseite.

Crystal data	
Formula	(Mn _{4.99} Mg _{0.02}) _{5.01} [(P _{1.76} Si _{0.20} As _{0.07})O ₄] ₂ (OH) _{3.97}
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> , <i>b</i> , <i>c</i> (Å)	17.9733(18), 5.6916(11), 9.130(4)
<i>V</i> (Å ³), <i>Z</i>	933.9(4), 4
<i>F</i> (000)	1024.0
Crystal dimensions (mm)	0.10 × 0.08 × 0.05
Absorption correction; multi-scan	$\mu = 7.180 \text{ (mm}^{-1}\text{)}$, $T_{\min} = 0.62$, $T_{\max} = 1.19$
Data collection	
Diffractometer	Oxford Diffraction Xcalibur E
Temperature (K)	293
Wavelength	Mo- <i>K</i> α , $\lambda = 0.71073 \text{ \AA}$
θ range (°)	2.50–27.87
Detector distance (mm)	45.53
Rotation axes	ω
Rotation width (°)	1.0
Total no. of frames	343
Collection time per frame (s)	20
<i>h</i> , <i>k</i> , <i>l</i> ranges	−23→22, −7→7, −11→12
Total reflections measured	6284
Data completeness (%)	98.3
Unique reflections	2124 ($R_{\text{int}} = 0.0506$)
Refinement	
Refinement on	F^2
Flack parameter <i>x</i>	0.00(4)
$R1^*$ for $F_o > 4\sigma(F_o)$	3.76%
$wR2^\dagger$ for all F_o^2	8.74%
Reflections used $F_o > 4\sigma(F_o)$	1945
Number of parameters refined	191
Extinction factor	0.0000(4)
$(\Delta/\sigma)_{\max}$	0.000
$\Delta\rho_{\min}$, $\Delta\rho_{\max}$ (e/Å ³)	0.86, −0.58
Goof	0.937

* $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$;† $wR2 = \sum w(|F_o|^2 - |F_c|^2)^2 / \sum w|F_o|^2$; $w = 1/[\sigma^2(F_o) + (0.042 P)^2 + 12.60 P]$; $P = ([\max \text{ of } (0 \text{ or } F_o^2)] + 2F_c^2) / 3$.

by trivalent rather than divalent, but concluded that there is no independent evidence for this suggestion. Bond-valence sums (Table 5) and <Mn–O> distances (Table 4) for the Mn1, Mn2, Mn3 and Mn5 sites indicate that Mn is present as Mn²⁺. The <Mn4–O> distance of 2.163 Å is less than that for the remaining Mn(O,OH) octahedra and the bond-valence sum is 2.20 v.u., which may suggest the presence of some Mn³⁺. However, this short <Mn–O> distance is also present in the structures of synthetic Mn₅²⁺(PO₄)₂(OH)₄ (Ruszala *et al.*, 1977) and arsenoclasite (Moore and Molin-Case, 1971) which indicates that it is a character

of the structural arrangement. Ruszala *et al.*, (1977) noted that the short <Mn–O> distance is most probably due to the position of the Mn-centred octahedron in the structure. In addition, although distorted, the Mn4 site does not show a Jahn-Teller [4+2]-distortion characteristic of trivalent Mn (Burns *et al.*, 1994; Foley *et al.*, 1997), typically four short Mn³⁺–O distances (~1.93 Å) and two long Mn³⁺–O distances (~2.24 Å). The site occupancies for the Mn1, Mn2 and Mn3 sites refined to 100%. Occupancy factors of 0.959(5) and 0.952(5) were obtained for the Mn4 and Mn5 sites respectively, which is

TABLE 3. Fractional atomic coordinates, isotropic displacement parameters (in Å²) and site occupancy factors for gatehouseite.

Atom	x	y	z	U _{eq}	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Mn1	0.43287(6)	0.26702(17)	0.75423(12)	0.0127(3)	0.0142(6)	0.0136(5)	0.0105(5)	0.0000(4)	0.0001(4)	-0.0003(4)
Mn2	0.02916(6)	0.05350(17)	0.89058(11)	0.0136(3)	0.0142(6)	0.0128(5)	0.0136(5)	0.0013(4)	-0.0014(4)	-0.0002(4)
Mn3	0.22447(5)	0.06464(17)	0.85360(11)	0.0127(3)	0.0148(6)	0.0120(5)	0.0112(5)	0.0007(4)	-0.0015(4)	-0.0002(4)
Mn4	0.12506(6)	0.55556(16)	0.87768(11)	0.0108(3)	0.0128(5)	0.0098(4)	0.0098(5)	-0.0001(4)	0.0004(4)	-0.0003(4)
Mn5	0.32013(6)	0.58215(17)	-0.00286(12)	0.0137(3)	0.0159(6)	0.0128(5)	0.0125(6)	-0.0001(4)	-0.0017(4)	0.0003(4)
P1*	0.37369(10)	0.11163(3)	0.07189(18)	0.0132(4)	0.0165(8)	0.0141(7)	0.0089(8)	-0.0001(6)	0.0000(6)	-0.0003(7)
P2*	0.12297(9)	0.1934(2)	0.17988(16)	0.0087(4)	0.0111(8)	0.0094(6)	0.0055(7)	0.0005(6)	-0.0017(6)	0.0001(6)
OH1	0.0486(3)	0.7275(8)	0.0169(5)	0.0173(10)	0.019(2)	0.019(2)	0.014(2)	0.001(2)	-0.001(2)	-0.005(2)
OH2	0.2042(3)	0.3842(7)	0.7371(5)	0.0155(10)	0.014(2)	0.015(2)	0.017(2)	0.001(2)	0.001(2)	0.0004(19)
OH3	0.0440(2)	0.3658(8)	0.7560(5)	0.0174(10)	0.021(3)	0.019(2)	0.013(2)	0.002(2)	0.001(2)	0.0035(19)
OH4	0.2165(3)	0.7409(8)	-0.0300(5)	0.0176(10)	0.021(3)	0.022(2)	0.010(2)	-0.0032(19)	-0.0019(19)	0.001(2)
O5	0.1437(2)	0.4287(7)	0.2575(5)	0.0157(9)	0.024(2)	0.0133(19)	0.010(2)	0.000(2)	-0.003(2)	-0.0017(19)
O6	0.1273(3)	0.2246(7)	0.0091(5)	0.0148(9)	0.017(2)	0.0154(19)	0.012(2)	0.0030(19)	-0.003(2)	0.002(2)
O7	0.1732(2)	-0.0138(7)	0.2280(5)	0.0167(10)	0.019(2)	0.014(2)	0.017(3)	-0.0013(18)	-0.001(2)	0.0029(19)
O8	0.0427(2)	0.1159(9)	0.2190(5)	0.0187(11)	0.017(2)	0.019(2)	0.020(3)	-0.005(2)	0.002(2)	0.001(2)
O9	0.3760(3)	0.1170(7)	0.2434(5)	0.0141(9)	0.018(2)	0.0165(19)	0.008(2)	-0.0007(18)	-0.0011(19)	0.000(2)
O10	0.2969(3)	0.2115(8)	0.0201(6)	0.0183(10)	0.016(2)	0.019(2)	0.020(3)	-0.001(2)	-0.002(2)	0.001(2)
O11	0.4311(2)	0.2926(8)	0.0037(5)	0.0179(10)	0.021(3)	0.021(2)	0.012(2)	0.002(2)	-0.002(2)	-0.005(2)
O12	0.3909(3)	0.8645(8)	0.0188(5)	0.0176(10)	0.018(3)	0.022(2)	0.013(2)	-0.002(2)	-0.0023(19)	-0.0020(19)
H1	0.002(2)	0.649(10)	0.017(9)	0.05						
H2	0.245(3)	0.487(11)	0.761(9)	0.05						
H3	0.074(4)	0.330(13)	0.672(5)	0.05						
H4	0.212(4)	0.785(13)	0.072(3)	0.05						

* occupancies fixed to P_{0.88}Si_{0.09}As_{0.03}.

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TABLE 4. Selected interatomic distances (Å) and angles (°) for gatehouseite.

Mn1	O8	2.098(5)	Mn2	OH3	2.159(5)
	OH1	2.193(5)		OH3	2.178(5)
	O5	2.212(4)		O11	2.192(5)
	O8	2.246(5)		OH1	2.212(5)
	O11	2.283(5)		O6	2.286(5)
	O7	2.402(5)		O9	2.378(4)
<Mn–O>		2.239	<Mn–O>		2.234
Mn3	OH4	2.132(5)	Mn4	OH1	2.112(5)
	OH2	2.138(4)		OH4	2.126(5)
	O10	2.169(5)		OH3	2.127(5)
	O7	2.187(5)		OH2	2.149(5)
	O9	2.311(5)		O9	2.231(4)
	O6	2.428(5)		O6	2.233(4)
<Mn–O>		2.228	<Mn–O>		2.163
Mn5	O12	2.060(5)			
	OH4	2.085(5)			
	O10	2.161(5)			
	OH2	2.242(5)			
	O5	2.283(5)			
	O11	2.588(5)			
<Mn–O>		2.237			
P1	O12	1.544(5)	P2	O7	1.548(5)
	O10	1.556(5)		O8	1.551(5)
	O9	1.567(5)		O5	1.561(4)
	O11	1.568(5)		O6	1.572(5)
<P–O>		1.559	<P–O>		1.558
O12–P1–O10		113.9(3)	O7–P2–O8		105.1(3)
O12–P1–O9		108.0(3)	O7–P2–O5		112.7(3)
O10–P1–O9		109.0(3)	O8–P2–O5		111.2(3)
O12–P1–O11		109.7(3)	O7–P2–O6		109.8(3)
O10–P1–O11		103.9(3)	O8–P2–O6		107.9(3)
O9–P1–O11		112.2(3)	O5–P2–O6		110.0(2)
<O–P1–O>		109.47	<O–P2–O>		109.45

consistent with the presence of minor Mg but would not account for the discrepancy in the chemical analysis.

Both of the mean P–O distances (1.559 and 1.558 Å for P1 and P2, respectively) are slightly greater than the average P–O distance (1.537 Å) reported by Huminicki and Hawthorne (2002) for minerals containing PO₄ tetrahedra and are also greater than the equivalent distances in synthetic Mn₅²⁺(PO₄)₂(OH)₄ of 1.542 and 1.538 Å (Ruszala *et al.*, 1977). This suggests that the minor As and Si detected by the chemical analysis are most likely to be evenly distributed over both P sites. The <M–O> distance calculated using a site occupancy of P_{0.88}Si_{0.09}As_{0.03} is 1.548 Å (ionic

radii from Shannon, 1976). The P1O₄ tetrahedron is somewhat more distorted than the P2O₄ tetrahedron, but neither of the distortions is particularly large. The O–P–O angles range from 103.9(3) to 113.9(3)°.

Strips of edge-sharing Mn₂O₃(OH)₃, Mn₃O₄(OH)₂ and Mn₄O₂(OH)₄ octahedra, alternately one and two octahedra wide, and parallel to (010), extend along [010] (Fig. 1). Each strip is linked to an adjacent, but offset strip, via OH3 anions. The Mn1O₅(OH) octahedra share O8 corners to form chains along [010] (Fig. 2). The P2O₄ tetrahedra link to this chain by sharing the O7–O8 edge with one octahedron and the O5 corner with an octahedron adjacent in the

TABLE 5. Bond-valence analysis for gatehouseite.

	Mn1	Mn2	Mn3	Mn4	Mn5	P1	P2	H1	H2	H3	H4	Sum excluding H	Sum including H
OH1	0.34	0.32		0.42				0.85				1.08	1.93
OH2			0.39	0.38	0.29				0.88			1.06	1.94
OH3		0.37 0.35		0.40						0.82		1.12	1.94
OH4			0.40	0.40	0.45						0.83	1.25	2.08
O5	0.32				0.26		1.18		0.12			1.76	1.88
O6		0.26	0.18	0.30			1.15					1.89	1.89
O7	0.19		0.34				1.23				0.17	1.76	1.93
O8	0.43 0.29						1.23					1.95	1.95
O9		0.20	0.25 0.36	0.30		1.16 1.20						1.91	1.91
O10					0.37							1.93	1.93
O11	0.26	0.34			0.12	1.16						1.88	1.88
O12					0.48	1.24		0.15		0.18		1.72	2.05
Sum	1.83	1.84	1.92	2.20	1.97	4.76	4.79	1.00	1.00	1.00	1.00		

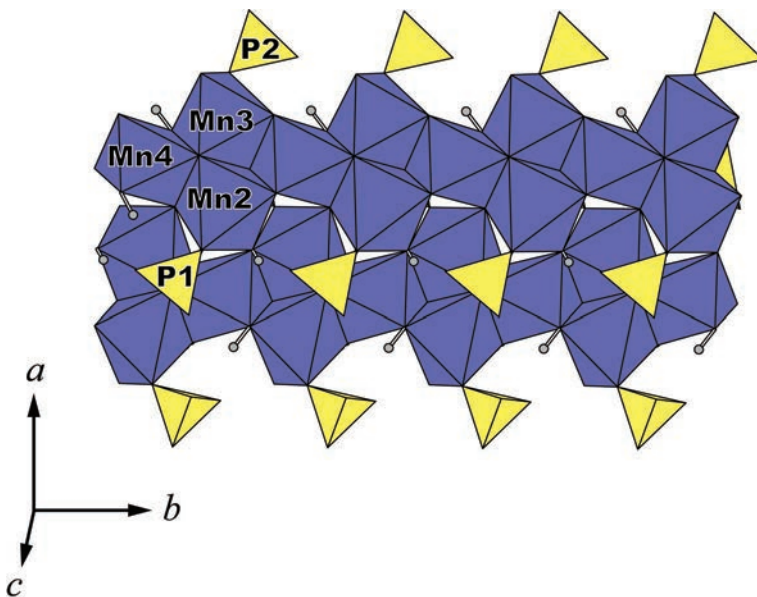


FIG. 1. The crystal structure of gatehouseite viewed in a direction close to $[001]$. The H atoms are shaded grey. The Mn1 and Mn5 polyhedra have been omitted for clarity. All structure drawings were completed using *ATOMS* (Shape Software, 1997).

b direction. The $\text{Mn}_5\text{O}_4(\text{OH})_2$ octahedra share an O10–O11 edge with P1O_4 tetrahedra which in turn shares an O12 corner with a second $\text{Mn}_5\text{O}_4(\text{OH})_2$ octahedron to form chains along $[010]$. These two types of chain link via common O5–O11 edges, and in turn link to the strips of edge-sharing octahedra by extensive polyhedral corner-sharing (Fig. 3).

The bond-valence analysis (Table 5) indicates that there are four (OH) groups in the gate-

houseite structure, in accord with the stereochemistry of the H atoms located during the refinement. Details of the hydrogen bonds are given in Table 6. Each H atom provides a single weak hydrogen bond to an adjacent anion (Fig. 4). Two hydrogen bonds, from the H1 and H3 atoms, are directed toward the O12 anion. The H2 atom hydrogen bonds to the O5 anion and the H4 atom hydrogen bonds to the O7 anion.

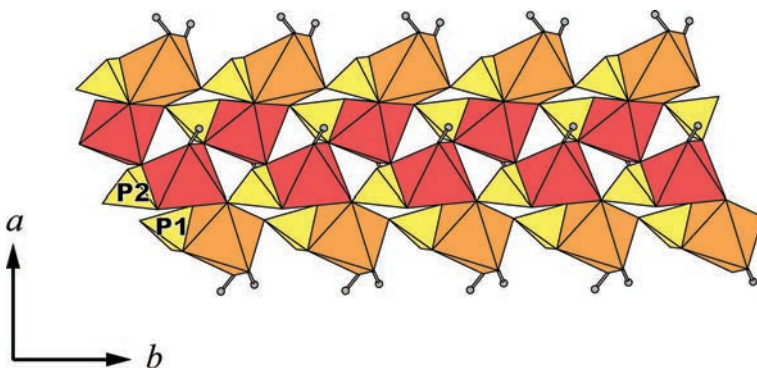


FIG. 2. The crystal structure of gatehouseite viewed in a direction close to $[30\bar{1}]$. The $\text{Mn1}\phi_6$ (ϕ : unspecified ligand) octahedra are red; $\text{Mn5}\phi_6$ octahedra are orange; H atoms are shaded grey. The Mn2, Mn3 and Mn4 polyhedra have been omitted for clarity.

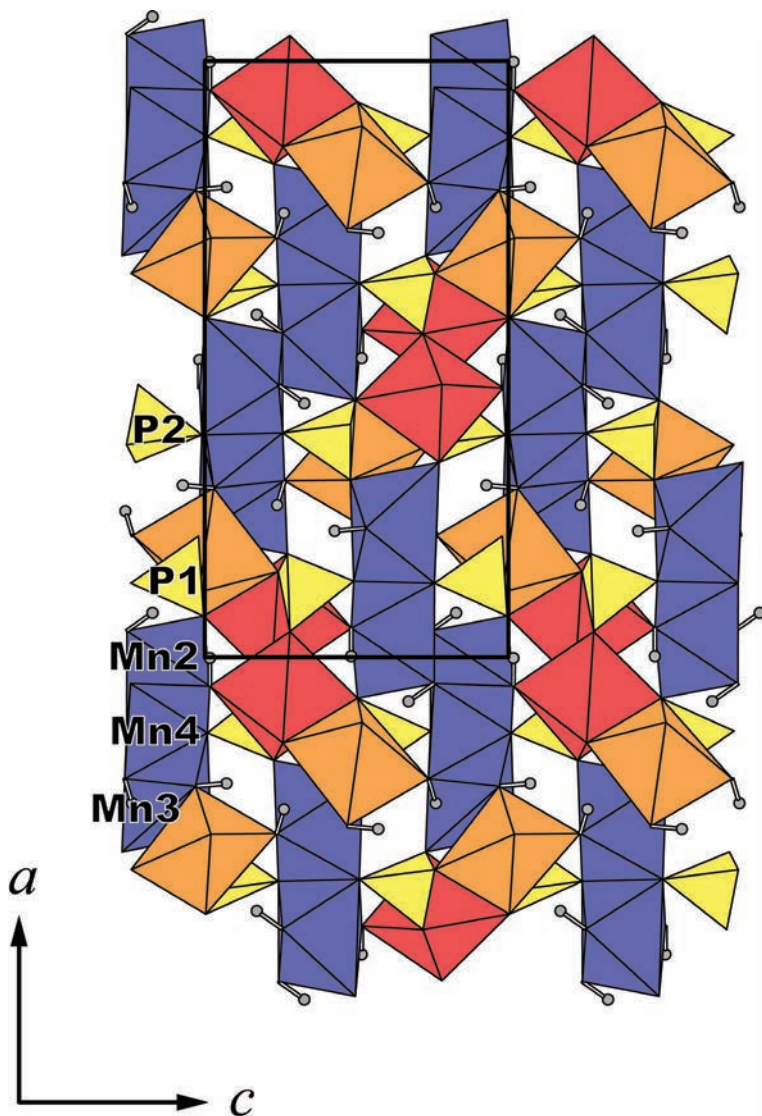


FIG. 3. The crystal structure of gatehouseite viewed along [010] (the unit cell is outlined). Legend as in Fig. 2.

TABLE 6. Details of hydrogen bonding in gatehouseite ($\text{\AA}$, $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$\angle \check{GD}-H\cdots A$
OH1-H1 $\cdots$ O12 ⁱ	0.96(2)	2.02(4)	2.901(7)	153(6)
OH2-H2 $\cdots$ O5 ⁱⁱ	0.96(2)	2.06(5)	2.941(6)	151(7)
OH3-H3 $\cdots$ O12 ⁱⁱ	0.96(2)	1.89(4)	2.788(7)	154(6)
OH4-H4 $\cdots$ O7 ⁱⁱⁱ	0.97(2)	1.96(4)	2.847(7)	152(7)

Symmetry codes: (i) $x-\frac{1}{2}$, $-y+\frac{3}{2}$, $-z$; (ii) $-x+\frac{1}{2}$, $-y+1$, $z+\frac{1}{2}$; (iii) x , $y+1$, z .

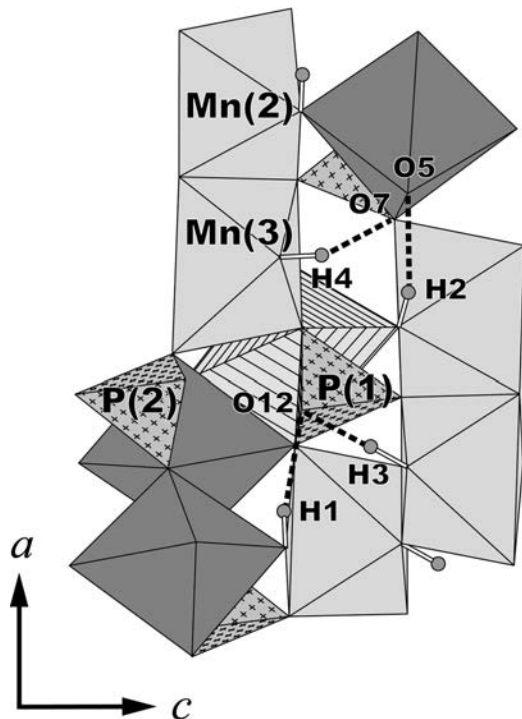


FIG. 4. Hydrogen bonds in gatehouseite. The $\text{Mn}1\phi_6$ octahedra are dark grey; $\text{Mn}5\phi_6$ octahedra are shaded with parallel lines; H atoms are shaded grey.

Structural relations

Gatehouseite is isostructural with arsenoclasite (Moore and Molin-Case, 1971) and belongs to a family of compounds with the general formula $M_5(XO_4)_2(OH)_4$ in which M is divalent Mn, Co, Ni or Cu and X is P, As or V; examples include $\text{Mn}_5^{2+}(\text{PO}_4)_2(\text{OH})_4$ (Ruszala *et al.*, 1977), $\text{Co}_5(\text{AsO}_4)_2(\text{OH})_4$ (Ruszala *et al.*, 1977), $\text{Ni}_5(\text{AsO}_4)_2(\text{OH})_4$ (Barbier, 1996), reppiaite, $\text{Mn}_5(\text{VO}_4)_2(\text{OH})_4$ (Basso *et al.*, 1992), cornubite, $\text{Cu}_5(\text{AsO}_4)_2(\text{OH})_4$ (Sieber *et al.*, 1984) and the $\text{Cu}_5(\text{PO}_4)_2(\text{OH})_4$ polymorphs pseudomalachite (Ghose, 1963; Shoemaker *et al.*, 1977), reichenbachite (Anderson *et al.*, 1977; Sieber *et al.*, 1987) and ludjibaite (Shoemaker *et al.*, 1981). The structural relationships between these compounds has been described by Barbier (1996). Gatehouseite and arsenoclasite are not closely related structurally to these compounds, although the structures of the $M_5(XO_4)_2(\text{OH})_4$ compounds are each based on fragments of brucite-type sheets of octahedra, which differ by

the distribution of vacant octahedral sites in the sheets. Strips of edge-sharing octahedra, topologically identical to those in the gatehouseite and arsenoclasite structures, are found in the structure of waterhouseite (Pring *et al.*, 2005). Strips of edge-sharing octahedra, two octahedra wide, occur in the structures of the isotypic minerals allactite, $\text{Mn}_7(\text{AsO}_4)_2(\text{OH})_8$, (Moore, 1968), raadeite, $\text{Mg}_7(\text{PO}_4)_2(\text{OH})_8$, (Chopin *et al.*, 2001) and argandite, $\text{Mg}_7(\text{VO}_4)_2(\text{OH})_8$, (Brugger *et al.*, 2011).

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