



Redetermination of $K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$ from single-crystal X-ray data revealing the correct hydrogen-atom positions

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In comparison with the previous structure determination of $K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$, dipotassium trimagnesium dihydroxide tris(sulfate) dihydrate, from laboratory powder X-ray diffraction data [Kubel & Cabaret-Lampin (2013). *Z. Anorg. Allg. Chem.* **639**, 1782–1786], the present redetermination against CCD single-crystal data has allowed for the modelling of all non-H atoms with anisotropic displacement parameters. As well as higher accuracy and precision in terms of bond lengths and angles, the clear localization of the H-atom positions leads also to a reasonable hydrogen-bonding scheme for this hydroxy hydrate. The structure consists of (100) sheets composed of corner- and edge-sharing $[MgO_6]$ octahedra and sulfate tetrahedra. Adjacent sheets are linked by the potassium cations and a hydrogen bond of medium strength involving the water molecule. The title compound is isotypic with its Co^{II} and Mn^{II} analogues: the three $K_2M_3(OH)_2(SO_4)_3(H_2O)_2$ ($M = Mg, Co, Mn$) structures are quantitatively compared.

1. Chemical context

In our recent projects focused on hydrothermal phase-formation studies in the systems $M/X^{VI}/Te^{IV}/O/H$ ($X = S, Se$), it was tested whether tetrahedral sulfate or selenate anions can be incorporated into oxidotellurates(IV) of different divalent metals M . So far, this concept proved to be successful for $M = Hg$ (Weil & Shir Khanlou, 2015), $M = Ca, Cd, Sr$ (Weil & Shir Khanlou, 2017a), $M = Pb$ (Weil & Shir Khanlou, 2017b) as well as for $M = Zn, Mg$ (Weil & Shir Khanlou, 2017c). However, in nearly all cases multi-phase formation was observed under the given hydrothermal conditions, and the target compounds, *i.e.* metal oxidochalcogenates(IV,VI) with both oxidosulfate(VI) or oxidoselenate(VI) and oxidotellurate(IV) building units, appeared only as minority phases next to other different phases. The same holds for the $Mg/S/Te/O/H$ system when working at pH ~ 10 by using potassium hydroxide as a base. From one of the reaction batches, high-quality single crystals of the title compound, $K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$, could be isolated as one of the products. A crystal-structure refinement of this phase has already been performed by Rietveld refinement against laboratory powder X-ray diffraction data (Kubel & Cabaret-Lampin, 2013). In the corresponding structure model, H-atom positions were estimated and optimized by energy minimization, but the resulting hydrogen-bonding pattern was not discussed in detail. A close check of this model revealed chemically implausible O–H bond lengths and O–H \cdots O angles (Table 1). For example, H1 is more tightly bonded to O7 than

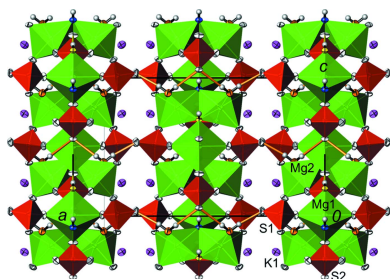


Table 1

Hydrogen-bond geometry (Å, °) from the previous model based on powder X-ray diffraction data and geometry-optimized H-atom positions (Kubel & Cabaret-Lampin, 2013).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O7—H1 \cdots O8 ⁱ	0.82	2.54	3.258 (14)	147
O9—H2 \cdots O8	1.13	2.18	2.901 (14)	119
O9—H2 \cdots O6 ⁱⁱ	1.13	2.52	3.506 (13)	145
O9—H2 \cdots O6 ⁱⁱⁱ	1.13	2.52	3.506 (13)	145
O10—H3 \cdots O5 ^{iv}	0.85	2.41	3.066 (9)	134
O10—H3 \cdots O6 ^{iv}	0.85	2.55	3.038 (13)	118
O10—H3 \cdots O1	0.85	2.52	3.229 (9)	142
O10—H4 \cdots O2 ⁱⁱⁱ	0.97	2.39	2.812 (8)	106
O10—H4 \cdots O3 ^v	0.97	1.77	2.698 (9)	158

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

to the actual hydroxide O atom (O8); the second hydroxyl group (O9) shows a too large O—H distance accompanied with large $D\cdots A$ distances or a too small O9—H2 \cdots O8 angle; the water molecule (O10) shows likewise either unreasonable $H\cdots A$ distances or $D-H\cdots A$ angles. Hence a redetermination of the crystal structure of $K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$ to establish a more reasonable hydrogen-bonding pattern by using single crystal X-ray diffraction CCD data seemed appropriate and is reported here.

2. Structural commentary

Of the 19 atoms in the asymmetric unit (1 K, 2 Mg, 2 S, 10 O, 4 H), eight (Mg1, S2, O5, O7, O8, O9, H1 and H2) are located on a crystallographic mirror plane at $x = 0$ (Wyckoff position 4 *a*); all other atoms in the asymmetric unit are on general sites (8 *b*). Both Mg^{II} atoms are octahedrally coordinated by oxygen atoms. Mg1 is bonded to four O atoms belonging to

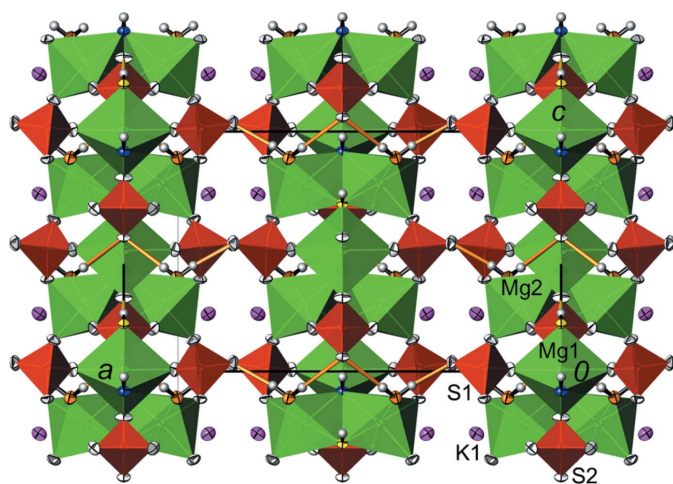


Figure 1

The crystal structure of $K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$ in a projection along $[0\bar{1}0]$. Displacement ellipsoids are drawn at the 98% probability level for non-H atoms, and H atoms are given as spheres of arbitrary radius. Colour code: $[MgO_6]$ octahedra are green, SO_4 tetrahedra are red; sulfate O atoms are white, O atoms of OH are yellow (O8) and blue (O9), and O atoms of water molecules are orange (O10). Hydrogen bonds involving the hydroxy group O8 are indicated by yellow lines and those involving the water molecule by orange lines.

Table 2

Comparison of bond lengths (Å) from the current single-crystal X-ray study and the previous powder X-ray diffraction study (Kubel & Cabaret-Lampin, 2013).

Bond	single-crystal study	powder study
K1—O4 ⁱ	2.8323 (15)	2.902 (7)
K1—O3 ⁱ	2.8594 (15)	2.877 (8)
K1—O10 ⁱⁱ	2.8704 (15)	2.874 (9)
K1—O2 ⁱⁱⁱ	2.9436 (14)	2.948 (8)
K1—O6	2.9743 (15)	2.945 (8)
K1—O3 ⁱⁱ	2.9915 (15)	3.016 (9)
K1—O2	3.0532 (15)	3.116 (9)
K1—O1 ⁱⁱ	3.0740 (15)	3.118 (10)
K1—O1	3.0780 (15)	3.128 (11)
K1—O3	3.3068 (15)	3.311 (10)
Mg1—O9	2.067 (2)	2.139 (11)
Mg1—O8	2.071 (2)	2.104 (10)
Mg1—O5 ^{iv}	2.081 (2)	1.989 (10)
Mg1—O1 ^v	2.0976 (13)	2.049 (5)
Mg1—O1	2.0977 (13)	2.049 (5)
Mg1—O7	2.160 (2)	2.139 (11)
Mg2—O4	2.0220 (15)	2.012 (9)
Mg2—O6 ^{vi}	2.0796 (14)	2.099 (8)
Mg2—O2 ^{vi}	2.0924 (15)	2.117 (8)
Mg2—O8	2.0952 (14)	2.036 (7)
Mg2—O9 ^{vii}	2.1026 (14)	2.045 (9)
Mg2—O10	2.1064 (15)	2.163 (8)
S1—O4	1.4657 (14)	1.487 (10)
S1—O3	1.4659 (14)	1.463 (6)
S1—O2	1.4818 (14)	1.500 (10)
S1—O1	1.4818 (13)	1.476 (6)
S2—O7	1.469 (2)	1.483 (13)
S2—O6	1.4751 (14)	1.468 (8)
S2—O6 ^v	1.4751 (14)	1.468 (8)
S2—O5	1.4779 (19)	1.530 (12)

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

sulfate groups (O5, O1 and its symmetry-related counterpart, O7) and to O atoms of two OH groups (O8, O9), whereas Mg2 is bonded to three sulfate O atoms (O4, O6, O2), two OH groups (O8, O9) and an O atom belonging to a water molecule (O10). Two $[Mg_2(H_2O)(OH)_2O_3]$ octahedra build up a $\{Mg_2(H_2O)_{1/1}O_{3/1}(OH)_{2/2}\}_2$ dimer by edge-sharing the two OH groups. These dimers are linked to the $[Mg_1(OH)_2O_4]$ octahedra by corner-sharing the two OH groups, which leads to the formation of zigzag chains running parallel to $[001]$. Sulfate tetrahedra join neighbouring chains into sheets extending parallel to (100) . Adjacent sheets are linked into a three-dimensional network by potassium cations (irregular nine-coordination), together with a hydrogen bond involving the water molecule (O10) and a sulfate O atom (O3) (Fig. 1).

The bond lengths for the two octahedral $[MgO_6]$ groups, the tetrahedral sulfate groups and the nine-coordinate potassium cations, with mean values of 2.089, 1.474 and 2.964 Å, respectively, are in very good agreement with the expected values of 2.089 (59), 1.473 (7) and 2.955 (214) Å, provided recently by Gagné & Hawthorne (2016, 2018). In terms of a comparison between the current single-crystal study and the previous powder study by Kubel & Cabaret-Lampin (2013), individual bond lengths as obtained from the single crystal study are, as expected, more precise and accurate, with the largest deviation of $\Delta = 0.092$ Å for the Mg1—O5^{iv} bond (Table 2).

Table 3
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H1 \cdots O7 ⁱ	0.86 (4)	2.22 (4)	3.068 (2)	168 (3)
O9—H2	0.73 (5)	?	?	?
O10—H3 \cdots O5 ⁱⁱ	0.79 (4)	2.22 (4)	3.009 (2)	171 (3)
O10—H3 \cdots O6 ⁱⁱ	0.79 (4)	2.59 (3)	3.023 (2)	116 (3)
O10—H4 \cdots O3 ⁱⁱⁱ	0.83 (4)	1.90 (4)	2.722 (2)	171 (4)

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

The hydrogen-bonding pattern derived from the single crystal study is chemically plausible (Table 3, Fig. 1). The water molecule (O10) participates in two nearly linear O—H \cdots O hydrogen bonds to two sulfate O atoms. One is of weak nature to O5 as the acceptor atom [$D\cdots A = 3.009$ (2) Å] within a sheet, the other of medium strength to O3 [$D\cdots A = 2.722$ (2) Å] between adjacent layers. The hydroxy group involving O8 exhibits a weak hydrogen bond to a neighbouring sulfate O atom [O7; $D\cdots A = 3.068$ (2) Å]. The other hydroxy group involving O9 appears not to be involved in hydrogen bonding: the next nearest O atoms that could act as acceptor atoms are two symmetry-related O6 atoms ($-x, -y + 1, z + \frac{1}{2}; x, -y + 1, z + \frac{1}{2}$), both at a distance of 3.405 (2) Å from O9. Such a long $D\cdots A$ distance is usually not considered as relevant for hydrogen bonding but was discussed for the $K_2Co_3(OH)_2(SO_4)_3(H_2O)_2$ structure as part of a bifurcated O—H \cdots (O,O) hydrogen bond of very weak nature, here with $D\cdots A = 3.370$ (9) Å (Effenberger & Langhof, 1984).

$K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$ is isotopic with its Co (Effenberger & Langhof, 1984) and Mn (Yu *et al.*, 2007) analogues. The three isotopic $K_2M_3(OH)_2(SO_4)_3(H_2O)_2$ ($M = Mg, Co, Mn$) structures were quantitatively compared using the *compstru* program (de la Flor *et al.*, 2016), available at the Bilbao Crystallographic Server (Aroyo *et al.*, 2006). For this purpose, the hydrogen atoms were not taken into account. In relation to the title Mg structure, the Co and Mn structures show the following values for evaluation of the structural similarity. Co: the degree of lattice distortion is 0.0034, the maximum displacement between atomic positions of paired atoms is 0.0553 Å for the pair O9, the arithmetic mean of the distance between paired atoms is 0.0295 Å, and the measure of similarity is 0.010. Corresponding values for the Mn structure are: 0.0126, 0.1343 Å for pair O2, 0.0768 Å and 0.013, respectively. The two value sets indicate a higher similarity between the Mg and Co structures compared to the Mn structure. This is most probably related to the ionic radii (Shannon, 1976) of the six-coordinate metal cations that differ only marginally for Mg (0.72 Å) and Co (0.745 Å, assuming a high-spin $3d^7$ configuration), whereas Mn (0.83 Å for a high-spin $3d^5$ state) is considerably greater.

3. Synthesis and crystallization

A mixture of 380 mg of $MgSO_4 \cdot 7H_2O$, 100 mg of TeO_2 and 70 mg of KOH was placed in a 5 ml Teflon container that was subsequently filled with 2 ml of water and sealed with a Teflon lid. The closed container was placed in a steel autoclave and

Table 4
Experimental details.

Crystal data	
Chemical formula	$K_2Mg_3(OH)_2(SO_4)_3(H_2O)_2$
M_r	509.36
Crystal system, space group	Orthorhombic, $Cmc2_1$
Temperature (K)	100
a, b, c (Å)	17.8228 (19), 7.4879 (8), 9.7686 (10)
V (Å ³)	1303.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.45
Crystal size (mm)	0.10 × 0.08 × 0.01
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{min}, T_{max}	0.668, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31799, 2535, 2430
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.768
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.017, 0.039, 1.07
No. of reflections	2535
No. of parameters	132
No. of restraints	1
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.30, -0.38
Absolute structure	Flack x determined using 1125 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	-0.010 (13)

Coordinates taken from previous refinement. Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXL2014/7* (Sheldrick, 2015), *ATOMS for Windows* (Dowty, 2006) and *PUBLICIF* (Westrip, 2010).

was heated at 413 K for one week at autogenous pressure and then cooled down to room temperature within 5 h. The recovered solids consisted of $Mg_2Te_3O_8$ (Lin *et al.*, 2013) as the main product (checked by powder X-ray diffraction of the bulk), besides minor amounts of caminite, $Mg_2(SO_4)(OH)_2$ (Keefer *et al.*, 1981), the sulfate tellurite $Mg_3(SO_4)(TeO_3)(OH)_2(H_2O)_2$ (Weil & Shir Khanlou, 2017c) and the title compound (the latter phases determined by single-crystal X-ray diffraction).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. Atomic coordinates and labelling for the non-H atoms were adapted from the previous refinement from powder X-ray diffraction data (Kubel & Cabaret-Lampin, 2013). H atoms were clearly discernible in difference-Fourier maps and were refined freely. The Flack parameter (Table 4) indicates that the absolute structure has been determined correctly.

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Redetermination of $\text{K}_2\text{Mg}_3(\text{OH})_2(\text{SO}_4)_3(\text{H}_2\text{O})_2$ from single-crystal X-ray data revealing the correct hydrogen-atom positions

Matthias Weil

Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINTE* (Bruker, 2015); data reduction: *SAINTE* (Bruker, 2015); program(s) used to solve structure: coordinates taken from previous refinement; program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: Atoms for Windows (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dipotassium trimagnesium dihydroxide tris(sulfate) dihydrate

Crystal data

$\text{K}_2\text{Mg}_3(\text{OH})_2(\text{SO}_4)_3(\text{H}_2\text{O})_2$

$M_r = 509.36$

Orthorhombic, *Cmc*₂₁

$a = 17.8228$ (19) Å

$b = 7.4879$ (8) Å

$c = 9.7686$ (10) Å

$V = 1303.7$ (2) Å³

$Z = 4$

$F(000) = 1024$

$D_x = 2.595$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9959 reflections

$\theta = 2.8\text{--}33.0^\circ$

$\mu = 1.45$ mm⁻¹

$T = 100$ K

Plate, colourless

0.10 × 0.08 × 0.01 mm

Data collection

Bruker APEXII CCD
diffractometer

ω - and φ -scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.668$, $T_{\max} = 0.747$

31799 measured reflections

2535 independent reflections

2430 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 33.1^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -27 \rightarrow 27$

$k = -11 \rightarrow 11$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.017$

$wR(F^2) = 0.039$

$S = 1.07$

2535 reflections

132 parameters

1 restraint

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0167P)^2 + 0.9127P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.30$ e Å⁻³

$\Delta\rho_{\min} = -0.38$ e Å⁻³

Absolute structure: Flack x determined using

1125 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: -0.010 (13)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
K1	0.19321 (2)	0.04648 (5)	-0.26016 (4)	0.00947 (7)
Mg1	0.0000	0.19893 (11)	0.00487 (10)	0.00514 (15)
Mg2	0.08605 (4)	0.46648 (8)	0.28489 (7)	0.00532 (11)
S1	0.17492 (2)	0.30375 (5)	0.01513 (5)	0.00452 (7)
S2	0.0000	0.18319 (8)	-0.31682 (6)	0.00448 (10)
O1	0.11670 (7)	0.16279 (16)	0.00789 (16)	0.0074 (2)
O2	0.17476 (8)	0.40504 (19)	-0.11519 (14)	0.0075 (2)
O3	0.24837 (8)	0.21941 (17)	0.03462 (15)	0.0091 (2)
O4	0.15996 (8)	0.42187 (18)	0.13162 (14)	0.0079 (2)
O5	0.0000	0.0697 (2)	-0.44063 (19)	0.0067 (3)
O6	0.06775 (8)	0.29624 (17)	-0.32058 (15)	0.0086 (2)
O7	0.0000	0.0711 (2)	-0.1934 (2)	0.0087 (4)
O8	0.0000	0.3133 (2)	0.1979 (2)	0.0055 (3)
O9	0.0000	0.4505 (2)	-0.0823 (2)	0.0062 (3)
O10	0.12236 (8)	0.23658 (19)	0.39003 (15)	0.0084 (2)
H1	0.0000	0.213 (6)	0.241 (5)	0.023 (11)*
H2	0.0000	0.509 (7)	-0.023 (5)	0.031 (13)*
H3	0.092 (2)	0.182 (5)	0.433 (3)	0.030 (9)*
H4	0.159 (2)	0.246 (6)	0.441 (4)	0.046 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.01028 (16)	0.00894 (14)	0.00920 (15)	-0.00051 (13)	0.00151 (15)	-0.00034 (14)
Mg1	0.0061 (4)	0.0045 (3)	0.0048 (4)	0.000	0.000	0.0002 (3)
Mg2	0.0054 (3)	0.0052 (3)	0.0053 (2)	0.00037 (19)	0.0001 (2)	-0.0003 (2)
S1	0.00477 (16)	0.00458 (15)	0.00422 (16)	0.00040 (13)	-0.00005 (15)	0.00002 (15)
S2	0.0054 (2)	0.0040 (2)	0.0041 (2)	0.000	0.000	-0.00057 (19)
O1	0.0063 (5)	0.0060 (5)	0.0101 (6)	-0.0022 (4)	0.0003 (5)	-0.0007 (5)
O2	0.0087 (6)	0.0093 (6)	0.0044 (6)	-0.0004 (5)	-0.0007 (4)	0.0021 (4)
O3	0.0057 (5)	0.0100 (6)	0.0114 (6)	0.0025 (4)	0.0006 (5)	0.0013 (5)
O4	0.0092 (6)	0.0084 (6)	0.0061 (6)	-0.0016 (5)	0.0022 (5)	-0.0028 (4)
O5	0.0087 (8)	0.0062 (8)	0.0053 (8)	0.000	0.000	-0.0021 (6)
O6	0.0082 (6)	0.0082 (5)	0.0096 (6)	-0.0037 (4)	0.0018 (5)	-0.0028 (5)
O7	0.0144 (9)	0.0055 (8)	0.0061 (8)	0.000	0.000	0.0009 (6)
O8	0.0059 (8)	0.0048 (7)	0.0056 (8)	0.000	0.000	0.0006 (6)
O9	0.0081 (8)	0.0049 (7)	0.0056 (8)	0.000	0.000	-0.0005 (6)
O10	0.0077 (6)	0.0084 (6)	0.0093 (6)	-0.0006 (5)	-0.0008 (5)	0.0020 (5)

Geometric parameters (\AA , $^\circ$)

K1—O4 ⁱ	2.8323 (15)	Mg2—O4	2.0220 (15)
K1—O3 ⁱ	2.8594 (15)	Mg2—O6 ^{vi}	2.0796 (14)
K1—O10 ⁱⁱ	2.8704 (15)	Mg2—O2 ^{vi}	2.0924 (15)
K1—O2 ⁱⁱⁱ	2.9436 (14)	Mg2—O8	2.0952 (14)
K1—O6	2.9743 (15)	Mg2—O9 ^{vii}	2.1026 (14)
K1—O3 ⁱⁱ	2.9915 (15)	Mg2—O10	2.1064 (15)
K1—O2	3.0532 (15)	S1—O4	1.4657 (14)
K1—O1 ⁱⁱ	3.0740 (15)	S1—O3	1.4659 (14)
K1—O1	3.0780 (15)	S1—O2	1.4818 (14)
K1—O3	3.3068 (15)	S1—O1	1.4818 (13)
Mg1—O9	2.067 (2)	S2—O7	1.469 (2)
Mg1—O8	2.071 (2)	S2—O6	1.4751 (14)
Mg1—O5 ^{iv}	2.081 (2)	S2—O6 ^v	1.4751 (14)
Mg1—O1 ^v	2.0976 (13)	S2—O5	1.4779 (19)
Mg1—O1	2.0977 (13)	O10—H3	0.79 (4)
Mg1—O7	2.160 (2)	O10—H4	0.83 (4)
O4 ⁱ —K1—O3 ⁱ	49.50 (4)	O4—Mg2—O9 ^{vii}	168.75 (7)
O4 ⁱ —K1—O10 ⁱⁱ	131.23 (4)	O6 ^{vi} —Mg2—O9 ^{vii}	86.48 (7)
O3 ⁱ —K1—O10 ⁱⁱ	166.22 (4)	O2 ^{vi} —Mg2—O9 ^{vii}	97.32 (6)
O4 ⁱ —K1—O2 ⁱⁱⁱ	58.07 (4)	O8—Mg2—O9 ^{vii}	83.00 (6)
O3 ⁱ —K1—O2 ⁱⁱⁱ	105.47 (4)	O4—Mg2—O10	91.48 (6)
O10 ⁱⁱ —K1—O2 ⁱⁱⁱ	80.80 (4)	O6 ^{vi} —Mg2—O10	171.10 (7)
O4 ⁱ —K1—O6	124.61 (4)	O2 ^{vi} —Mg2—O10	85.19 (6)
O3 ⁱ —K1—O6	75.47 (4)	O8—Mg2—O10	88.59 (7)
O10 ⁱⁱ —K1—O6	103.59 (4)	O9 ^{vii} —Mg2—O10	99.50 (7)
O2 ⁱⁱⁱ —K1—O6	157.33 (4)	O4—S1—O3	108.76 (8)
O4 ⁱ —K1—O3 ⁱⁱ	60.13 (4)	O4—S1—O2	110.97 (8)
O3 ⁱ —K1—O3 ⁱⁱ	79.54 (4)	O3—S1—O2	109.50 (8)
O10 ⁱⁱ —K1—O3 ⁱⁱ	89.75 (4)	O4—S1—O1	109.84 (8)
O2 ⁱⁱⁱ —K1—O3 ⁱⁱ	79.64 (4)	O3—S1—O1	108.94 (8)
O6—K1—O3 ⁱⁱ	122.18 (4)	O2—S1—O1	108.80 (8)
O4 ⁱ —K1—O2	101.48 (4)	O7—S2—O6	110.39 (7)
O3 ⁱ —K1—O2	79.94 (4)	O7—S2—O6 ^v	110.39 (7)
O10 ⁱⁱ —K1—O2	111.40 (4)	O6—S2—O6 ^v	109.88 (11)
O2 ⁱⁱⁱ —K1—O2	100.33 (4)	O7—S2—O5	110.07 (11)
O6—K1—O2	57.19 (4)	O6—S2—O5	108.03 (7)
O3 ⁱⁱ —K1—O2	158.66 (4)	O6 ^v —S2—O5	108.03 (7)
O4 ⁱ —K1—O1 ⁱⁱ	100.22 (4)	S1—O1—Mg1	127.09 (8)
O3 ⁱ —K1—O1 ⁱⁱ	87.55 (4)	S1—O1—K1 ^{viii}	90.99 (6)
O10 ⁱⁱ —K1—O1 ⁱⁱ	78.76 (4)	Mg1—O1—K1 ^{viii}	121.06 (6)
O2 ⁱⁱⁱ —K1—O1 ⁱⁱ	121.72 (4)	S1—O1—K1	86.09 (6)
O6—K1—O1 ⁱⁱ	80.84 (4)	Mg1—O1—K1	117.63 (7)
O3 ⁱⁱ —K1—O1 ⁱⁱ	46.57 (4)	K1 ^{viii} —O1—K1	106.63 (4)
O2—K1—O1 ⁱⁱ	137.93 (4)	S1—O2—Mg2 ^{ix}	129.61 (8)
O4 ⁱ —K1—O1	134.68 (4)	S1—O2—K1 ^x	126.58 (7)

O3 ⁱ —K1—O1	125.75 (4)	Mg2 ^{ix} —O2—K1 ^x	102.37 (5)
O10 ⁱⁱ —K1—O1	65.12 (4)	S1—O2—K1	87.03 (6)
O2 ⁱⁱⁱ —K1—O1	92.68 (4)	Mg2 ^{ix} —O2—K1	105.63 (5)
O6—K1—O1	69.99 (4)	K1 ^x —O2—K1	90.41 (4)
O3 ⁱⁱ —K1—O1	154.68 (4)	S1—O3—K1 ^{xi}	98.75 (7)
O2—K1—O1	46.28 (3)	S1—O3—K1 ^{viii}	94.61 (7)
O1 ⁱⁱ —K1—O1	125.08 (4)	K1 ^{xi} —O3—K1 ^{viii}	93.32 (4)
O4 ⁱ —K1—O3	91.01 (4)	S1—O3—K1	77.88 (6)
O3 ⁱ —K1—O3	105.201 (16)	K1 ^{xi} —O3—K1	163.50 (5)
O10 ⁱⁱ —K1—O3	88.56 (4)	K1 ^{viii} —O3—K1	103.02 (4)
O2 ⁱⁱⁱ —K1—O3	58.95 (4)	S1—O4—Mg2	142.48 (9)
O6—K1—O3	98.63 (4)	S1—O4—K1 ^{xi}	99.91 (7)
O3 ⁱⁱ —K1—O3	138.28 (5)	Mg2—O4—K1 ^{xi}	108.16 (6)
O2—K1—O3	44.26 (3)	S2—O5—Mg1 ^{xii}	139.91 (12)
O1 ⁱⁱ —K1—O3	166.75 (4)	S2—O6—Mg2 ^{ix}	127.33 (9)
O1—K1—O3	43.96 (4)	S2—O6—K1	104.45 (7)
O9—Mg1—O8	89.91 (8)	Mg2 ^{ix} —O6—K1	108.72 (6)
O9—Mg1—O5 ^{iv}	170.48 (9)	S2—O7—Mg1	118.84 (11)
O8—Mg1—O5 ^{iv}	99.61 (8)	Mg1—O8—Mg2	126.57 (6)
O9—Mg1—O1 ^v	97.08 (4)	Mg1—O8—Mg2 ^v	126.57 (6)
O8—Mg1—O1 ^v	92.32 (5)	Mg2—O8—Mg2 ^v	94.11 (8)
O5 ^{iv} —Mg1—O1 ^v	82.63 (4)	Mg1—O8—H1	95 (3)
O9—Mg1—O1	97.08 (4)	Mg2—O8—H1	106.4 (19)
O8—Mg1—O1	92.32 (5)	Mg2 ^v —O8—H1	106.4 (19)
O5 ^{iv} —Mg1—O1	82.63 (4)	Mg1—O9—Mg2 ^{xiii}	121.58 (6)
O1 ^v —Mg1—O1	165.09 (8)	Mg1—O9—Mg2 ^{ix}	121.58 (6)
O9—Mg1—O7	91.97 (8)	Mg2 ^{xiii} —O9—Mg2 ^{ix}	93.68 (8)
O8—Mg1—O7	178.12 (9)	Mg1—O9—H2	103 (4)
O5 ^{iv} —Mg1—O7	78.51 (8)	Mg2 ^{xiii} —O9—H2	108 (3)
O1 ^v —Mg1—O7	87.44 (5)	Mg2 ^{ix} —O9—H2	108 (3)
O1—Mg1—O7	87.44 (5)	Mg2—O10—K1 ^{viii}	119.30 (6)
O4—Mg2—O6 ^{vi}	82.90 (6)	Mg2—O10—H3	118 (3)
O4—Mg2—O2 ^{vi}	85.94 (6)	K1 ^{viii} —O10—H3	101 (2)
O6 ^{vi} —Mg2—O2 ^{vi}	87.52 (6)	Mg2—O10—H4	118 (3)
O4—Mg2—O8	94.94 (6)	K1 ^{viii} —O10—H4	92 (3)
O6 ^{vi} —Mg2—O8	98.73 (7)	H3—O10—H4	105 (4)
O2 ^{vi} —Mg2—O8	173.74 (7)		

Symmetry codes: (i) $-x+1/2, -y+1/2, z-1/2$; (ii) $x, -y, z-1/2$; (iii) $-x+1/2, y-1/2, z$; (iv) $-x, -y, z+1/2$; (v) $-x, y, z$; (vi) $x, -y+1, z+1/2$; (vii) $-x, -y+1, z+1/2$; (viii) $x, -y, z+1/2$; (ix) $x, -y+1, z-1/2$; (x) $-x+1/2, y+1/2, z$; (xi) $-x+1/2, -y+1/2, z+1/2$; (xii) $-x, -y, z-1/2$; (xiii) $-x, -y+1, z-1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H1 \cdots O7 ^{iv}	0.86 (4)	2.22 (4)	3.068 (2)	168 (3)
O9—H2	0.73 (5)	?	?	?
O10—H3 \cdots O5 ^{xiv}	0.79 (4)	2.22 (4)	3.009 (2)	171 (3)

O10—H3...O6 ^{xiv}	0.79 (4)	2.59 (3)	3.023 (2)	116 (3)
O10—H4...O3 ^{xi}	0.83 (4)	1.90 (4)	2.722 (2)	171 (4)

Symmetry codes: (iv) $-x, -y, z+1/2$; (xi) $-x+1/2, -y+1/2, z+1/2$; (xiv) $x, y, z+1$.