Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis and crystal structure determination of aluminium hydroxide methanesulfonate, $Al(OH)(CH_3SO_3)_2$

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Received 1 May 2026
Accepted 26 May 2026

Edited by T. Akitsu, Tokyo University of Science, Japan

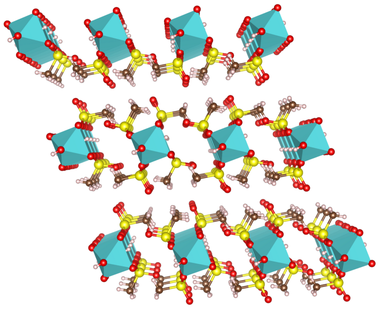
This article is part of the collection *Early Career Scientists in Structural Science*.

Keywords: crystal structure; methanesulfonic acid; aluminium; hydroxide; crystal growth.

CCDC reference: 2541524

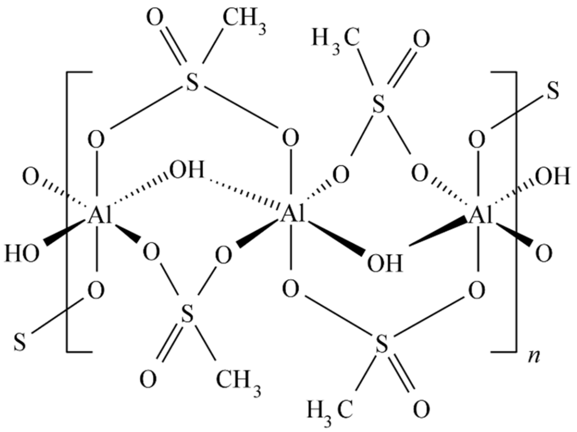
Supporting information: this article has supporting information at journals.iucr.org/e

catena-Poly[aluminium(III)-μ-hydroxido-$\kappa^2 O$:O-di-μ-methanesulfonato-$\kappa^4 O$:O'], $[Al(OH)(CH_3SO_3)_2]_n$, was prepared by mild hydrothermal synthesis at 523 K and crystallizes as millimetre-sized clear and colourless needles. The asymmetric unit contains half of the repeating structure, one-dimensional $(AlO_6)_\infty$ chains corner sharing through the axial hydroxyl group with a bend of $\sim 137^o$. The extended structure shows the chains are connected through weak methyl–hydrogen bonding in the [001] direction and strong hydroxyl–hydrogen bonding in the [100] direction. This is the second aluminium-based methanesulfonate salt reported to date.



1. Chemical context

Crystals containing the methanesulfonate anion, $CH_3SO_3^-$, have attracted interest as potential linear and non-linear optical crystals (Tian *et al.*, 2023; Gabilondo & Halasyamani, 2025). However, there are relatively few crystal structures reported compared to other anionic groups such as Cl^-, F^-, SO_4^{2-}, or PO_4^{3-}, to name a few, rendering structure prediction a challenge. Herein, we report an aluminium-based methanesulfonate salt, $Al(OH)(CH_3SO_3)_2$ (**I**). The title compound is the second Al-based methanesulfonate to be discovered alongside $Al(CH_3SO_3)_3(H_2O)_6$, (**II;** Trella & Frank, 2012).



2. Structural commentary

Compound **I** crystallizes in the triclinic space group $P\bar{1}$. The asymmetric unit, shown in Fig. 1, contains half of the two repeating AlO_6 octahedra, which are corner sharing at the axial positions through a hydroxyl bridge (O3—H3). Each

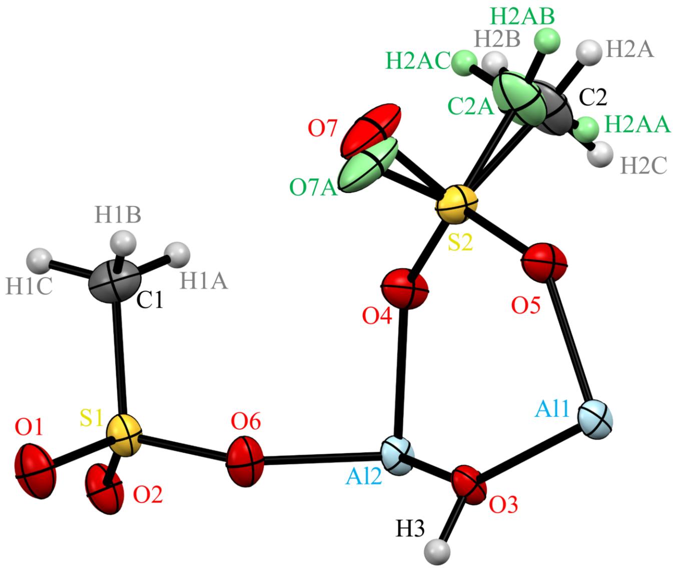


Figure 1
The asymmetric unit of **I** with displacement ellipsoids shown at the 50% probability level. The terminal oxygen (O7) and methyl (C2, H2*A*, H2*B*, H2*C*) groups are disordered with refined occupancies of 0.68 (3)/0.32 (3). The minor residue is shown in green.

Table 1
Hydrogen-bond geometry (Å, °).

Hydrogen-bonding distances refer to the major residue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O7^{i}	0.96	2.62	3.304 (15)	129
C2—H2*B*···O7	0.96	2.72	3.641 (16)	162
O3—H3···O1^{ii}	0.94 (1)	1.87 (1)	2.802 (3)	171 (2)

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x, -y+1, -z+1$.

octahedron is additionally bridged at the equatorial positions by two methanesulfonate anion groups (O6/S1/O2 and O5/S2/O4). The two Al atoms differ by Wyckoff position 1*f* and 1*h*, for Al1 and Al2, respectively. The AlO_6 octahedra have a small axial compression (~4%) with an average bond length of (axial) 1.8394 (14) Å and (equatorial) 1.9165 (15) Å. There is little angular distortion from the ideal values of 90 (1) and 180°. The methanesulfonate groups are largely undistorted and have similar geometries to those in previous reports (Wei & Hingerty, 1981). For example, the average S—O single bond length is 1.473 (1) Å, S═O is 1.439 (3) Å, and S—C is 1.734 (2) Å, compared to literature values of 1.461 (1), 1.452 (1) and 1.754 (2) Å, respectively. One methanesulfonate group (S2) is disordered with refined occupancies of 0.68 (3)/0.32 (3). There is a minor rotation of the O7—S2—C2 angle of 11.7 (12)° between the two residues with S2 unaffected. The cause is likely weak interlayer hydrogen bonding, discussed below and not uncommon in metal methanesulfonates (Singh *et al.*, 2020; Wickleder & Müller, 2004). The structure of **I** is in contrast to the known **II** that has isolated $Al(OH_2)_6$ octahedra bridged via hydrogen bonding to $CH_3SO_3^-$ anions, with no direct coordination of the octahedra nor the $CH_3SO_3^-$ groups. The bond-valence sum for each atom (Brown 2009) is consistent with the expected oxidation states of Al^{III}, S^{VI}, O^{2-}, and C^{IV}, with average experimental values of 3.155 (5), 5.83 (4), 2.0 (1), and 4.136 (3), respectively, and supports reasonable hydrogen-atom assignments.

3. Supramolecular features

The unit cell and packing diagram of **I** is shown in Fig. 2*a* with primary supramolecular structural motifs in Fig. 2*b*–*d*. As shown in Fig. 2*a*, the unit cell contains two asymmetric units to complete a one-dimensional chain of AlO_6 octahedra. The chains are corner-sharing through the OH group at the axial positions and rotate by an Al—O—Al angle of 134.57 (7)°. Fig. 2*b* highlights the extended structure as isolated one-dimensional chains connected *via* hydrogen bonding (Table 1). The chains are connected weakly in the [001] direction through hydrogen bonding (Fig. 2*c*) between the terminal S2═O7 group and the methyl group on C2. The weak hydrogen bonding is likely responsible for the disorder of C2,

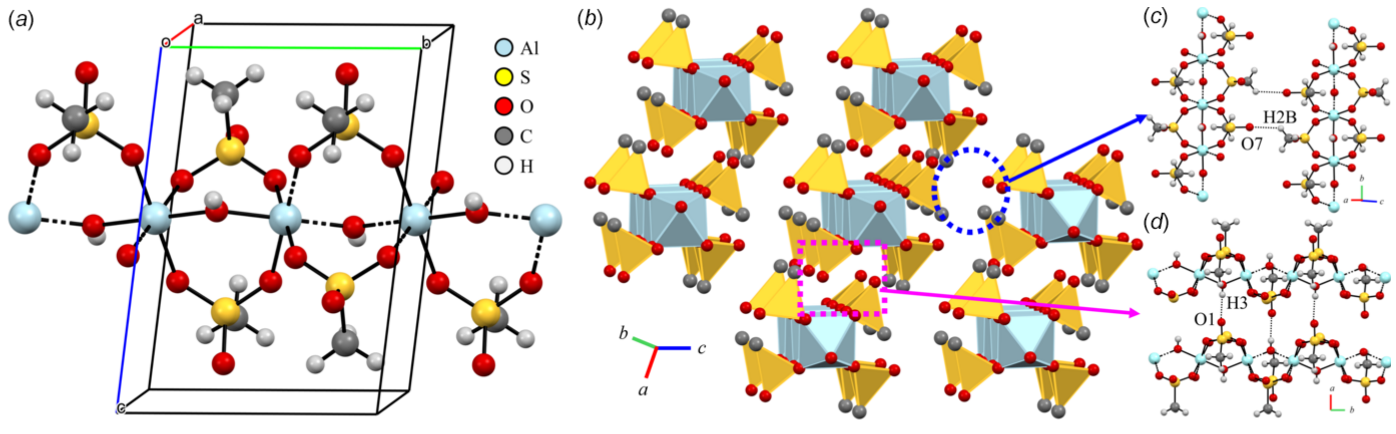


Figure 2
(*a*) Packing diagram and unit cell for **I** and (*b*) polyhedral extended structure of one-dimensional chains. AlO_6 chains are connected via (*c*) weak hydrogen bonding (C2—H2*B*···O7) bonding in the [001] direction and (*d*) with traditional hydrogen bonding (O3—H3···O1) in the [100] direction. Disorder is removed for clarity.

S2, and O7, with weak interactions not 'locking' the terminal groups in place. Meanwhile, stronger and more traditional hydrogen bonding connects the chains in the [100] direction through the hydroxyl group from O3—H3···O1 (Fig. 2*d*). The relative strength of the interchain hydrogen bonding is exemplified by the Al···Al distances of 9.7677 (15) Å in the [001] direction and 6.5099 (11) Å in the [100] direction, corresponding to the unit-cell parameters *c* and *a*, respectively. The extended structure of **I** again contrasts with the structure of **II** by having direct connectivity through one-dimensional chains of AlO_6 octahedra rather than the 0D structure of **II** held together by a hydrogen-bonding network.

4. Database survey

The Cambridge Structural Database (CSD, accessed May 2026; Groom *et al.*, 2016) contains 54 metal–methanesulfonates and the Inorganic Crystalline Structure Database (ICSD; Zagorac *et al.*, 2019) contains 21. Only one of these contains Al, as highlighted earlier: **II** $Al(CH_3SO_3)_3(H_2O)_6$ (LEHREX; Trella & Frank, 2012). Compound **I** is the first reported hydroxide-bridged aluminium methanesulfonate containing one-dimensional, corner-sharing AlO_6 chains. Compound **I** is not isostructural with other reported metal–methanesulfonate hydroxides, even the empirically similar $Sc(OH)(CH_3SO_3)_2$ (ESARAR; Wickleder & Müller, 2004).

5. Synthesis and crystallization

Compound **I** was synthesized by a hydrothermal route. 1.322 g (3.5 mmol) of aluminium nitrate nonahydrate [$Al(NO_3)_3(H_2O)_9$, Alfa Aesar, 98%] were added to 1 mL of methanesulfonic acid (4.9 mmol, 70 *w*/*w*% in H_2O, Thermo Fisher) inside a Teflon-lined autoclave prior to sealing and placing in a muffle furnace. The furnace was heated to 523 K at a rate of 1 K min^{-1}, held for 72 h, then radiatively cooled to room temperature. Solid products were collected via vacuum filtration followed by rinsing with acetonitrile to remove solvent. Millimetre-sized, clear and colourless needle-shaped crystals were separated mechanically from the other insoluble and amorphous solid products. Crystals were dried overnight in a vacuum desiccator prior to further analysis. Yield was ~56% with respect to Al. The crystals are slightly hygroscopic and slowly decompose to **II** in air over the course of several weeks or rapidly upon grinding.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Methyl-H atoms were refined using a riding model with ideal tetrahedral angles once identified using difference maps. The hydroxyl-H atom (H3) was similarly identified by both difference maps and a low bond-valence sum around O3 of 1.2 v.u. (Brown 2009). The O3—H3 bond was restrained to 0.97 (1) Å [$U_{iso}(H) = 1.5U_{eq}(O)$] and restrained to be equidistant from Al1 and Al2 to maintain the ideal OH geometry. Restraints were adopted because the O3—H3 bond became unusually short unrestrained (~0.73 Å). The terminal methanesulfonate unit was treated as a disordered residue due to unusually large anisotropic displacement parameters on C2 and O7, with refined occupancies of 0.68 (3)/0.32 (3).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Al(OH)(CH_3SO_3)_2]$
M_r	234.18
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	301
a, b, c (Å)	6.5099 (10), 6.7869 (10), 9.7677 (15)
α, β, γ (°)	94.712 (6), 109.253 (6), 90.177 (6)
V (Å^3)	405.83 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.76
Crystal size (mm)	0.25 × 0.03 × 0.03
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.674, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15679, 2007, 1707
R_{int}	0.050
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.034, 0.087, 1.07
No. of reflections	2007
No. of parameters	125
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.43, −0.41

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2008), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

Funding information

EAG and PSH thank the Welch Foundation (grant E-1457) for their support.

References

Brown, I. D. (2009). *Chem. Rev.* **109**, 6858–6919.
Bruker (2008). *SAINT* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2023). *APEX5*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gabilondo, E. A. & Halasyamani, P. S. (2025). *Inorg. Chem.* **64**, 19036–19043.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Singh, R., Kociok-Köhn, G., Kaur Jassal, A. & Singh, L. (2020). *Polyhedron* **175**, 114200.

Tian, H., Lin, C., Zhao, X., Xu, F., Wang, C., Ye, N. & Luo, M. (2023). *CCS Chem.* **5**(11), 2497-2505.

Trella, T. & Frank, W. (2012). *Acta Cryst.* E**68**, m1136–m1137.

Wei, C. H. & Hingerty, B. E. (1981). *Acta Cryst.* B**37**, 1992–1997.

Wickleder, M. S. & Müller, I. (2004). *Z. Naturforsch.* **59b**, 33-36.

Zagorac, D., Müller, H., Ruehl, S., Zagorac, J. & Rehme, S. (2019). *J. Appl. Cryst.* **52**, 918–925.

supporting information

Acta Cryst. (2026). E**82** [https://doi.org/10.1107/S2056989026005578]

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Computing details

catena-Poly[aluminium(III)-μ-hydroxido-κ^2O:O-di-μ-methanesulfonato-κ^4O:O']

Crystal data

$[Al(OH)(CH_3SO_3)_2]$
M_r = 234.18
Triclinic, $P\overline{1}$
a = 6.5099 (10) Å
b = 6.7869 (10) Å
c = 9.7677 (15) Å
α = 94.712 (6)°
β = 109.253 (6)°
γ = 90.177 (6)°
V = 405.83 (11) Å^3

Z = 2
F(000) = 240
D_x = 1.916 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4784 reflections
θ = 2.2–27.8°
μ = 0.76 mm^{-1}
T = 301 K
Needle, colourless
0.25 × 0.03 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.674, T_{max} = 0.746
15679 measured reflections

2007 independent reflections
1707 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 28.3°, θ_{min} = 2.2°
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
S = 1.07
2007 reflections
125 parameters
2 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.2379P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
S1	0.26117 (8)	0.76941 (7)	0.66932 (5)	0.01853 (14)	
S2	0.77597 (9)	0.28304 (7)	0.77275 (5)	0.02129 (15)	
Al1	0.500000	0.000000	0.500000	0.0166 (2)	
Al2	0.500000	0.500000	0.500000	0.0165 (2)	
O1	0.0586 (3)	0.7731 (2)	0.69736 (18)	0.0284 (4)	
O2	0.2868 (3)	0.9380 (2)	0.58889 (17)	0.0235 (3)	
O3	0.3839 (2)	0.24615 (19)	0.47067 (15)	0.0171 (3)	
H3	0.2321 (17)	0.2411 (18)	0.424 (2)	0.026*	
O4	0.7021 (3)	0.4503 (2)	0.68421 (16)	0.0247 (4)	
O5	0.6994 (3)	0.0937 (2)	0.68568 (16)	0.0242 (3)	
O6	0.2883 (2)	0.5812 (2)	0.59119 (16)	0.0229 (3)	
C1	0.4736 (4)	0.7916 (4)	0.8366 (2)	0.0319 (5)	
H1A	0.610534	0.780972	0.819857	0.048*	
H1B	0.457894	0.688125	0.894139	0.048*	
H1C	0.468552	0.917766	0.887359	0.048*	
O7	0.740 (3)	0.3028 (15)	0.9115 (14)	0.0442 (18)	0.68 (3)
C2	1.070 (2)	0.2877 (18)	0.8079 (14)	0.0376 (19)	0.68 (3)
H2A	1.131846	0.175313	0.858649	0.056*	0.68 (3)
H2B	1.134113	0.406980	0.866437	0.056*	0.68 (3)
H2C	1.097876	0.283080	0.717226	0.056*	0.68 (3)
C2A	1.035 (4)	0.287 (4)	0.837 (3)	0.0376 (19)	0.32 (3)
H2AA	1.092830	0.265748	0.758451	0.056*	0.32 (3)
H2AB	1.081138	0.184014	0.901309	0.056*	0.32 (3)
H2AC	1.087015	0.412787	0.889476	0.056*	0.32 (3)
O7A	0.683 (4)	0.294 (4)	0.881 (2)	0.0442 (18)	0.32 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0180 (3)	0.0142 (2)	0.0248 (3)	−0.00089 (18)	0.00896 (19)	0.00137 (19)
S2	0.0278 (3)	0.0128 (2)	0.0201 (3)	−0.0013 (2)	0.0036 (2)	0.00119 (18)
Al1	0.0182 (4)	0.0076 (4)	0.0228 (4)	−0.0012 (3)	0.0052 (3)	0.0016 (3)
Al2	0.0181 (4)	0.0077 (4)	0.0228 (4)	−0.0012 (3)	0.0057 (3)	0.0011 (3)
O1	0.0230 (8)	0.0260 (8)	0.0422 (9)	0.0011 (6)	0.0183 (7)	0.0042 (7)
O2	0.0246 (8)	0.0143 (7)	0.0356 (8)	0.0023 (6)	0.0145 (7)	0.0064 (6)
O3	0.0154 (7)	0.0090 (6)	0.0255 (7)	0.0000 (5)	0.0044 (6)	0.0021 (5)
O4	0.0286 (8)	0.0114 (7)	0.0276 (8)	−0.0017 (6)	0.0002 (6)	0.0026 (6)
O5	0.0277 (8)	0.0116 (7)	0.0266 (7)	−0.0010 (6)	−0.0002 (6)	0.0015 (6)
O6	0.0239 (8)	0.0132 (7)	0.0337 (8)	−0.0031 (6)	0.0132 (6)	−0.0008 (6)

C1	0.0322 (13)	0.0359 (13)	0.0244 (11)	−0.0011 (10)	0.0053 (9)	0.0013 (9)
O7	0.078 (6)	0.0363 (14)	0.018 (4)	−0.010 (3)	0.017 (3)	−0.003 (2)
C2	0.017 (4)	0.0316 (15)	0.060 (5)	−0.003 (2)	0.007 (2)	0.002 (3)
C2A	0.017 (4)	0.0316 (15)	0.060 (5)	−0.003 (2)	0.007 (2)	0.002 (3)
O7A	0.078 (6)	0.0363 (14)	0.018 (4)	−0.010 (3)	0.017 (3)	−0.003 (2)

Geometric parameters (Å, º)

S1—O1	1.4324 (16)	Al2—O3	1.8411 (13)
S1—O6	1.4749 (15)	Al2—O3^{ii}	1.8411 (13)
S1—O2	1.4790 (15)	Al2—O4^{ii}	1.9037 (14)
S1—C1	1.753 (2)	Al2—O4	1.9037 (14)
S2—O7A	1.38 (3)	Al2—O6	1.9315 (15)
S2—O7	1.444 (10)	Al2—O6^{ii}	1.9315 (15)
S2—O4	1.4691 (15)	O3—H3	0.941 (10)
S2—O5	1.4696 (15)	C1—H1A	0.9600
S2—C2A	1.59 (2)	C1—H1B	0.9600
S2—C2	1.828 (14)	C1—H1C	0.9600
Al1—O3	1.8407 (13)	C2—H2A	0.9600
Al1—O3^{i}	1.8407 (13)	C2—H2B	0.9600
Al1—O5	1.9056 (14)	C2—H2C	0.9600
Al1—O5^{i}	1.9056 (14)	C2A—H2AA	0.9600
Al1—O2^{ii}	1.9259 (15)	C2A—H2AB	0.9600
Al1—O2^{iii}	1.9259 (15)	C2A—H2AC	0.9600
O1—S1—O6	112.13 (9)	O3^{ii}—Al2—O4	88.31 (6)
O1—S1—O2	111.68 (10)	O4^{ii}—Al2—O4	180.0
O6—S1—O2	110.27 (9)	O3—Al2—O6	88.99 (6)
O1—S1—C1	108.41 (11)	O3^{ii}—Al2—O6	91.01 (6)
O6—S1—C1	107.00 (11)	O4^{ii}—Al2—O6	89.59 (7)
O2—S1—C1	107.08 (11)	O4—Al2—O6	90.41 (7)
O7A—S2—O4	108.2 (11)	O3—Al2—O6^{ii}	91.01 (6)
O7—S2—O4	114.4 (5)	O3^{ii}—Al2—O6^{ii}	88.99 (6)
O7A—S2—O5	106.5 (9)	O4^{ii}—Al2—O6^{ii}	90.41 (7)
O7—S2—O5	115.1 (5)	O4—Al2—O6^{ii}	89.59 (7)
O4—S2—O5	110.97 (9)	O6—Al2—O6^{ii}	180.0
O7A—S2—C2A	112.1 (11)	S1—O2—Al1^{iv}	132.00 (10)
O4—S2—C2A	110.1 (11)	Al1—O3—Al2	134.34 (8)
O5—S2—C2A	108.8 (10)	Al1—O3—H3	113.1 (8)
O7—S2—C2	107.9 (5)	Al2—O3—H3	112.3 (8)
O4—S2—C2	103.3 (4)	S2—O4—Al2	138.91 (9)
O5—S2—C2	103.9 (4)	S2—O5—Al1	138.67 (9)
O3—Al1—O3^{i}	180.0	S1—O6—Al2	131.92 (9)
O3—Al1—O5	91.67 (6)	S1—C1—H1A	109.5
O3^{i}—Al1—O5	88.33 (6)	S1—C1—H1B	109.5
O3—Al1—O5^{i}	88.33 (6)	H1A—C1—H1B	109.5
O3^{i}—Al1—O5^{i}	91.67 (6)	S1—C1—H1C	109.5
O5—Al1—O5^{i}	180.0	H1A—C1—H1C	109.5

O3—Al1—O2^{ii}	90.97 (6)	H1B—C1—H1C	109.5
O3^{i}—Al1—O2^{ii}	89.03 (6)	S2—C2—H2A	109.5
O5—Al1—O2^{ii}	89.78 (7)	S2—C2—H2B	109.5
O5^{i}—Al1—O2^{ii}	90.22 (7)	H2A—C2—H2B	109.5
O3—Al1—O2^{iii}	89.03 (6)	S2—C2—H2C	109.5
O3^{i}—Al1—O2^{iii}	90.98 (6)	H2A—C2—H2C	109.5
O5—Al1—O2^{iii}	90.22 (7)	H2B—C2—H2C	109.5
O5^{i}—Al1—O2^{iii}	89.78 (7)	S2—C2A—H2AA	109.5
O2^{ii}—Al1—O2^{iii}	180.0	S2—C2A—H2AB	109.5
O3—Al2—O3^{ii}	180.0	H2AA—C2A—H2AB	109.5
O3—Al2—O4^{ii}	88.31 (6)	S2—C2A—H2AC	109.5
O3^{ii}—Al2—O4^{ii}	91.69 (6)	H2AA—C2A—H2AC	109.5
O3—Al2—O4	91.69 (6)	H2AB—C2A—H2AC	109.5

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) *x*, *y*+1, *z*.

Hydrogen-bond geometry (Å, º)

H-bonding distances refer to the major residue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···O7^{v}	0.96	2.62	3.304 (15)	129
C2—H2*B*···O7	0.96	2.72	3.641 (16)	162
O3—H3···O1^{vi}	0.94 (1)	1.87 (1)	2.802 (3)	171 (2)

Symmetry codes: (v) −*x*+1, −*y*+1, −*z*+2; (vi) −*x*, −*y*+1, −*z*+1.