Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[propane-1,2-diammonium [μ_2-hydroxido-di-μ_2-phosphonato-aluminium(III)] monohydrate]

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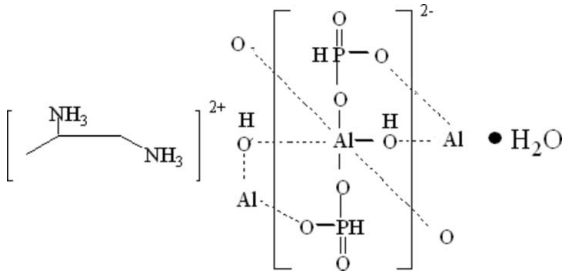
Received 16 July 2007; accepted 15 August 2007

Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.080; data-to-parameter ratio = 15.7.

The title compound, $\{(C_3H_{12}N_2)[Al(OH)(HPO_3)_2]\cdot H_2O\}_n$, has been prepared using a hydrothermal technique and characterized by X-ray diffraction data. The Al atoms are in a distorted octahedral environment. Anions and cations are linked through O—H···O and N—H···O hydrogen bonds.

Related literature

For related literature, see: Cheetham *et al.* (1999); Harrison (2002); Yamase *et al.* (1997).



Experimental

Crystal data

$(C_3H_{12}N_2)[Al(OH)(HPO_3)_2]\cdot H_2O$
M_r = 298.11
Monoclinic, $P2_1/n$
a = 11.059 (2) Å
b = 6.9782 (14) Å
c = 15.319 (3) Å
β = 100.01 (3)°
V = 1164.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 170 (2) K
0.58 × 0.27 × 0.18 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.856, T_{max} = 0.917
10911 measured reflections
2654 independent reflections
2513 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
2 standard reflections
every 150 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.080
S = 1.01
2654 reflections
169 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O6	0.89	1.87	2.7425 (16)	165
N1—H1B···O4^{i}	0.89	2.00	2.8751 (14)	169
N1—H1C···O7^{ii}	0.89	1.98	2.7833 (14)	149
N2—H2A···O1^{iii}	0.89	1.95	2.7295 (15)	145
N2—H2A···O$W1^{iv}$	0.89	2.66	3.2446 (18)	124
N2—H2B···O$W1^{i}$	0.89	1.89	2.7716 (16)	171
N2—H2C···O1	0.89	1.84	2.7218 (16)	172
O$W1$—H$W1B$···O2^{ii}	0.77 (3)	1.98 (3)	2.7363 (16)	167 (3)
O$W1$—H$W1A$···O6	0.83 (3)	1.86 (3)	2.6528 (16)	159 (2)
O5—H1···O$W1^{v}$	0.779 (15)	2.390 (16)	3.1429 (17)	163.0 (18)

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+2, -y, -z+1$; (iii) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

This work was supported by the Science and Technology Development Foundation of Fuzhou University (grant No. 2004-xq-05) and the Scientific Research Foundation of Fujian Education Department (grant No. JB04010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2443).

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 doi:10.1107/S1600536807040512

supplementary materials

Acta Cryst. (2007). E**63**, m2401 [**doi:10.1107/S1600536807040512**]

Poly[propane-1,2-diammonium [μ_2-hydroxido-di-μ_2-phosphonato-aluminium(III)] monohydrate]

W.-H. Chen, Y. Xiang, J.-Z. Chen and Q.-X. Zeng

Comment

At present, it is well known that a remarkable range of compositions and structures of organically templated inorganic framework solids have been synthesized and studied, because of their potential applications in many fields (Cheetham *et al.*, 1999; Harrison, 2002). There are also lots of studies about the synthesis and characterization of metal phosphates containing V, Zn, Co, *etc*. (Yamase *et al.*, 1997) and most of the known metal–phosphite compounds have been prepared by various solvent-volatilizing methods. However, only a few organically templated aluminophosphites have been reported. In our present work, we have hydrothermally synthesized and characterized the title compound (Fig. 1).

As seen in Figs. 2 and 3, its structure consists of aluminophosphite lines constructed from AlO_6 distorted octahedrons and HPO_3 pyramids. Each AlO_6 octahedron shares two opposite hydroxy groups with two adjacent AlO_6 octahedra to construct an infinte Al—O—Al chain running along the [100] direction. Each P atom shares two oxygen atoms with adjacent Al atoms.

The propane-1,2-diammonium cations and water molecules link Al—O—Al chains *via* numerous N—H···O and O—H···O hydrogen bonds (Table 1 and Fig. 4).

Experimental

All reagents were used as purchased without further purification. The synthesis was carried out in a rational way from a mixture of $[(CH_3)_2CHO]_3Al$, $C_3N_2H_{10}$, H_3PO_3 and H_2O in a molar ratio of 1:1:2:250. The mixture was loaded in a Teflon-lined autoclave (23 ml capacity) and was heated at 443k for 4 d under autogenous pressure. The solid product was collected by filtration, washed with water and dried at room temperature. Colorless crystals of the title compound were isolated.

Refinement

All H atoms were located in a difference Fourier map. Those bonded to C and N were refined using a riding model with C—H ranging from 0.96 to 0.97Å and N—H = 0.89Å and U(H)= 1.2 U_{eq}(C,*N*). The other H atoms were isotropically refined. The distance O5—H1 was restrained to 0.82 (2) Å.

Figures

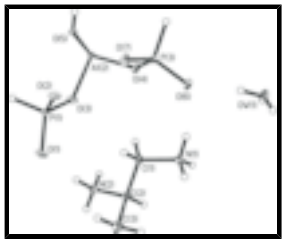

Fig. 1. The structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms shown as arbitrary spheres.

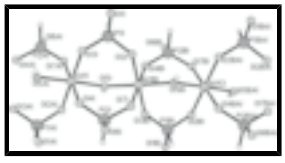

Fig. 2. View of the infinite Al—O—Al chain.

Fig. 3. A polyhedral respresentation of the one-dimensional Al—O—Al chain of the title compound.

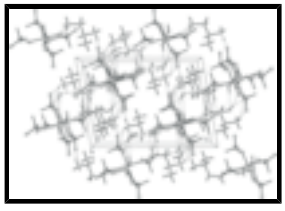

Fig. 4. A packing diagram of the title compound, viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Poly[propane-1,2-diammonium [μ_2-hydroxido-di-μ_2-phosphonato-aluminium(III)] monohydrate]

Crystal data

$(C_3H_{12}N_2)[Al(OH)(HPO_3)_2]\cdot H_2O$	F_{000} = 624
M_r = 298.11	D_x = 1.701 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.059 (2) Å	Cell parameters from 10198 reflections
b = 6.9782 (14) Å	θ = 3.0–27.5º
c = 15.319 (3) Å	μ = 0.48 mm^{-1}
β = 100.01 (3)º	T = 170 (2) K
V = 1164.2 (4) Å^3	Chunk, colorless
Z = 4	0.58 × 0.27 × 0.18 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer	R_{int} = 0.021
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 3.2º
T = 170(2) K	h = −14→14

ω oscillation scans	$k = -9 \rightarrow 8$
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$l = -19 \rightarrow 19$
$T_{min} = 0.856$, $T_{max} = 0.917$	2 standard reflections
10911 measured reflections	every 150 reflections
2654 independent reflections	intensity decay: none
2513 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.080$	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.5902P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
2654 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
169 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.95407 (3)	0.19849 (4)	0.19018 (2)	0.00995 (10)
P2	0.78292 (3)	0.20388 (4)	0.42460 (2)	0.00997 (10)
Al1	0.75189 (3)	0.45005 (4)	0.24929 (2)	0.00802 (10)
O1	1.09179 (9)	0.19119 (13)	0.19924 (8)	0.0202 (2)
O2	0.90558 (8)	0.01902 (12)	0.22963 (6)	0.01556 (19)
O3	0.90834 (8)	0.38056 (12)	0.22784 (6)	0.0160 (2)
O4	0.80156 (8)	0.38466 (12)	0.37257 (6)	0.01461 (19)
O5	0.68994 (8)	0.20026 (11)	0.22253 (6)	0.00947 (18)

O6	0.86642 (9)	0.20370 (13)	0.51352 (6)	0.0186 (2)
O7	0.79587 (9)	0.01972 (12)	0.37372 (6)	0.0165 (2)
C1	1.11228 (12)	0.30966 (18)	0.42461 (9)	0.0162 (3)
H1D	1.0536	0.4074	0.4003	0.019*
H1E	1.0867	0.1898	0.3950	0.019*
C2	1.23836 (11)	0.36369 (19)	0.40522 (9)	0.0159 (3)
C3	1.32693 (15)	0.1959 (2)	0.41037 (11)	0.0267 (3)
H3A	1.4043	0.2397	0.3977	0.040*
H3B	1.2937	0.1002	0.3679	0.040*
H3C	1.3387	0.1417	0.4689	0.040*
N1	1.11006 (11)	0.28876 (14)	0.52071 (7)	0.0143 (2)
H1A	1.0348	0.2565	0.5284	0.022*
H1B	1.1313	0.3994	0.5481	0.022*
H1C	1.1628	0.1979	0.5433	0.022*
N2	1.21957 (10)	0.44677 (16)	0.31407 (7)	0.0163 (2)
H2A	1.2918	0.4807	0.3007	0.024*
H2B	1.1713	0.5494	0.3118	0.024*
H2C	1.1844	0.3598	0.2753	0.024*
OW1	0.90717 (12)	0.20990 (16)	0.68934 (8)	0.0274 (3)
HW1B	0.951 (2)	0.136 (4)	0.7146 (17)	0.049 (7)*
HW1A	0.887 (2)	0.181 (3)	0.6364 (19)	0.049 (7)*
H1	0.6189 (14)	0.201 (3)	0.2196 (14)	0.026 (5)*
H2	1.2722 (16)	0.463 (3)	0.4441 (12)	0.026 (4)*
H3	0.6632 (16)	0.207 (2)	0.4384 (11)	0.015 (4)*
H4	0.9074 (16)	0.193 (2)	0.1039 (12)	0.019 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.00979 (17)	0.00724 (17)	0.01291 (17)	0.00029 (10)	0.00221 (12)	0.00012 (10)
P2	0.01221 (17)	0.00701 (17)	0.01020 (17)	−0.00064 (10)	0.00061 (12)	0.00013 (10)
Al1	0.00911 (18)	0.00394 (17)	0.01038 (18)	0.00018 (12)	−0.00004 (13)	−0.00020 (12)
O1	0.0118 (4)	0.0137 (5)	0.0367 (6)	0.0001 (3)	0.0089 (4)	−0.0039 (4)
O2	0.0106 (4)	0.0076 (4)	0.0287 (5)	0.0002 (3)	0.0038 (3)	0.0037 (3)
O3	0.0126 (4)	0.0070 (4)	0.0292 (5)	−0.0002 (3)	0.0063 (4)	−0.0025 (3)
O4	0.0233 (5)	0.0067 (4)	0.0120 (4)	−0.0028 (3)	−0.0021 (3)	0.0005 (3)
O5	0.0082 (4)	0.0048 (4)	0.0146 (4)	−0.0001 (3)	−0.0003 (3)	−0.0002 (3)
O6	0.0250 (5)	0.0188 (5)	0.0101 (4)	−0.0025 (4)	−0.0021 (4)	0.0008 (3)
O7	0.0287 (5)	0.0066 (4)	0.0121 (4)	0.0021 (4)	−0.0028 (3)	−0.0005 (3)
C1	0.0159 (6)	0.0196 (6)	0.0128 (6)	−0.0022 (5)	0.0015 (5)	0.0002 (4)
C2	0.0150 (6)	0.0152 (6)	0.0170 (6)	−0.0014 (5)	0.0017 (4)	−0.0012 (5)
C3	0.0242 (7)	0.0284 (8)	0.0271 (8)	0.0112 (6)	0.0036 (6)	0.0038 (6)
N1	0.0180 (5)	0.0113 (5)	0.0132 (5)	−0.0001 (4)	0.0013 (4)	0.0010 (4)
N2	0.0149 (5)	0.0133 (5)	0.0215 (5)	−0.0009 (4)	0.0058 (4)	0.0024 (4)
OW1	0.0371 (6)	0.0265 (6)	0.0164 (5)	0.0170 (5)	−0.0019 (5)	0.0001 (4)

Geometric parameters (Å, °)

P1—O1	1.5060 (10)	C1—N1	1.4837 (17)

P1—O3	1.5179 (9)	C1—C2	1.5226 (18)
P1—O2	1.5276 (9)	C1—H1D	0.9700
P1—H4	1.333 (18)	C1—H1E	0.9700
P2—O6	1.5070 (11)	C2—N2	1.4928 (16)
P2—O7	1.5225 (9)	C2—C3	1.5199 (19)
P2—O4	1.5252 (9)	C2—H2	0.946 (19)
P2—H3	1.376 (17)	C3—H3A	0.9600
Al1—O3	1.8799 (10)	C3—H3B	0.9600
Al1—O5^{i}	1.8847 (9)	C3—H3C	0.9600
Al1—O2^{i}	1.8879 (10)	N1—H1A	0.8900
Al1—O5	1.8916 (9)	N1—H1B	0.8900
Al1—O4	1.9277 (10)	N1—H1C	0.8900
Al1—O7^{i}	1.9288 (10)	N2—H2A	0.8900
O2—Al1^{ii}	1.8879 (10)	N2—H2B	0.8900
O5—Al1^{ii}	1.8847 (9)	N2—H2C	0.8900
O5—H1	0.779 (15)	OW1—HW1B	0.77 (3)
O7—Al1^{ii}	1.9288 (10)	OW1—HW1A	0.83 (3)
O1—P1—O3	113.06 (5)	P2—O7—Al1^{ii}	132.74 (6)
O1—P1—O2	110.78 (5)	N1—C1—C2	113.05 (11)
O3—P1—O2	111.89 (6)	N1—C1—H1D	109.0
O1—P1—H4	107.5 (8)	C2—C1—H1D	109.0
O3—P1—H4	107.8 (7)	N1—C1—H1E	109.0
O2—P1—H4	105.3 (7)	C2—C1—H1E	109.0
O6—P2—O7	111.38 (5)	H1D—C1—H1E	107.8
O6—P2—O4	110.84 (5)	N2—C2—C3	109.36 (11)
O7—P2—O4	113.42 (6)	N2—C2—C1	107.18 (10)
O6—P2—H3	108.4 (7)	C3—C2—C1	113.75 (12)
O7—P2—H3	105.7 (7)	N2—C2—H2	106.4 (11)
O4—P2—H3	106.7 (7)	C3—C2—H2	110.4 (11)
O3—Al1—O5^{i}	89.49 (4)	C1—C2—H2	109.5 (11)
O3—Al1—O2^{i}	179.72 (4)	C2—C3—H3A	109.5
O5^{i}—Al1—O2^{i}	90.74 (4)	C2—C3—H3B	109.5
O3—Al1—O5	91.95 (4)	H3A—C3—H3B	109.5
O5^{i}—Al1—O5	178.48 (2)	C2—C3—H3C	109.5
O2^{i}—Al1—O5	87.82 (4)	H3A—C3—H3C	109.5
O3—Al1—O4	89.77 (5)	H3B—C3—H3C	109.5
O5^{i}—Al1—O4	88.11 (4)	C1—N1—H1A	109.5
O2^{i}—Al1—O4	90.40 (5)	C1—N1—H1B	109.5
O5—Al1—O4	91.43 (4)	H1A—N1—H1B	109.5
O3—Al1—O7^{i}	89.91 (5)	C1—N1—H1C	109.5
O5^{i}—Al1—O7^{i}	90.85 (4)	H1A—N1—H1C	109.5
O2^{i}—Al1—O7^{i}	89.93 (5)	H1B—N1—H1C	109.5
O5—Al1—O7^{i}	89.61 (4)	C2—N2—H2A	109.5
O4—Al1—O7^{i}	178.92 (4)	C2—N2—H2B	109.5
P1—O2—Al1^{ii}	132.40 (6)	H2A—N2—H2B	109.5

P1—O3—Al1	131.29 (6)	C2—N2—H2C	109.5
P2—O4—Al1	131.79 (5)	H2A—N2—H2C	109.5
Al1^{ii}—O5—Al1	135.05 (5)	H2B—N2—H2C	109.5
Al1^{ii}—O5—H1	108.5 (13)	HW1B—OW1—HW1A	111 (2)
Al1—O5—H1	109.5 (13)		
O1—P1—O2—Al1^{ii}	172.54 (7)	O2^{i}—Al1—O4—P2	82.63 (8)
O3—P1—O2—Al1^{ii}	45.39 (10)	O5—Al1—O4—P2	−5.19 (8)
O1—P1—O3—Al1	−170.02 (7)	O7^{i}—Al1—O4—P2	−170 (2)
O2—P1—O3—Al1	−44.11 (10)	O3—Al1—O5—Al1^{ii}	43.65 (7)
O5^{i}—Al1—O3—P1	−172.71 (8)	O5^{i}—Al1—O5—Al1^{ii}	−118.6 (10)
O2^{i}—Al1—O3—P1	−28 (11)	O2^{i}—Al1—O5—Al1^{ii}	−136.52 (7)
O5—Al1—O3—P1	7.75 (8)	O4—Al1—O5—Al1^{ii}	−46.17 (7)
O4—Al1—O3—P1	99.18 (8)	O7^{i}—Al1—O5—Al1^{ii}	133.54 (7)
O7^{i}—Al1—O3—P1	−81.86 (8)	O6—P2—O7—Al1^{ii}	−163.64 (7)
O6—P2—O4—Al1	165.35 (7)	O4—P2—O7—Al1^{ii}	−37.76 (10)
O7—P2—O4—Al1	39.19 (10)	N1—C1—C2—N2	−160.17 (10)
O3—Al1—O4—P2	−97.14 (8)	N1—C1—C2—C3	78.82 (14)
O5^{i}—Al1—O4—P2	173.36 (8)		

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O6	0.89	1.87	2.7425 (16)	165
N1—H1B···O4^{iii}	0.89	2.00	2.8751 (14)	169
N1—H1C···O7^{iv}	0.89	1.98	2.7833 (14)	149
N2—H2A···O1^{v}	0.89	1.95	2.7295 (15)	145
N2—H2A···OW1^{vi}	0.89	2.66	3.2446 (18)	124
N2—H2B···OW1^{iii}	0.89	1.89	2.7716 (16)	171
N2—H2C···O1	0.89	1.84	2.7218 (16)	172
OW1—HW1B···O2^{iv}	0.77 (3)	1.98 (3)	2.7363 (16)	167 (3)
OW1—HW1A···O6	0.83 (3)	1.86 (3)	2.6528 (16)	159 (2)
O5—H1···OW1^{vii}	0.779 (15)	2.390 (16)	3.1429 (17)	163.0 (18)

Symmetry codes: (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+2, −*y*, −*z*+1; (v) −*x*+5/2, *y*+1/2, −*z*+1/2; (vi) *x*+1/2, −*y*+1/2, *z*−1/2; (vii) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1

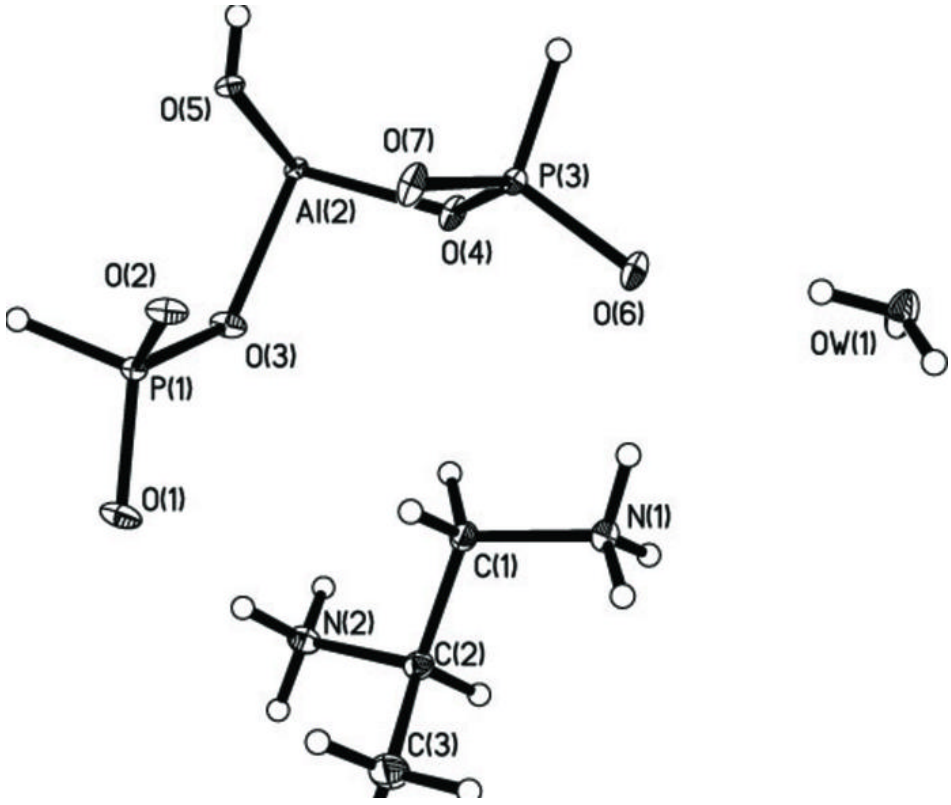

Fig. 2

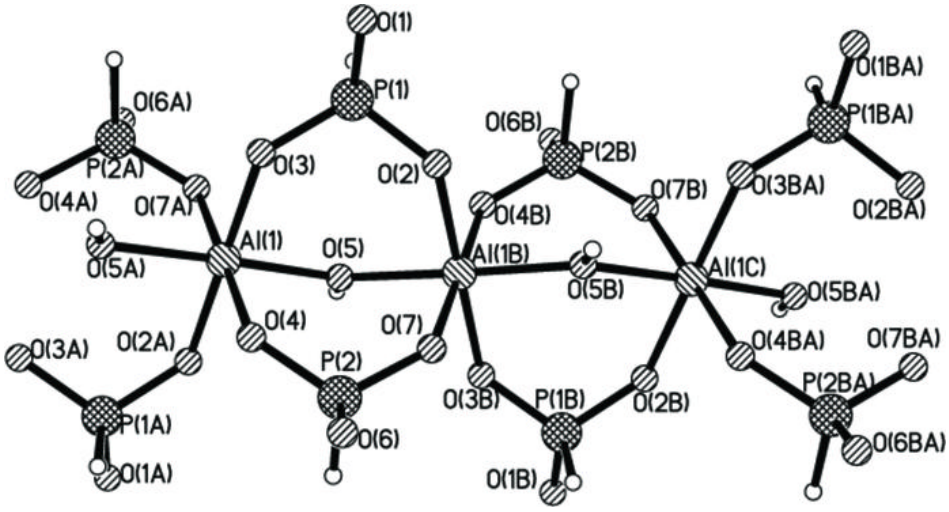
O(1)
P(1)
O(6A)
P(2A)
O(4A)
O(7A)
O(3)
O(2)
O(6B)
P(2B)
O(4B)
O(7B)
O(1BA)
P(1BA)
O(3BA)
O(2BA)
Al(1)
O(5)
Al(1B)
Al(1C)
O(5A)
O(5B)
O(5BA)
O(4)
O(7)
O(3A)
O(2A)
P(2)
O(4BA)
O(7BA)
P(2BA)
O(3B)
P(1B)
O(2B)
P(1A)
O(6)
O(6BA)
O(1A)
O(1B)

Fig. 3

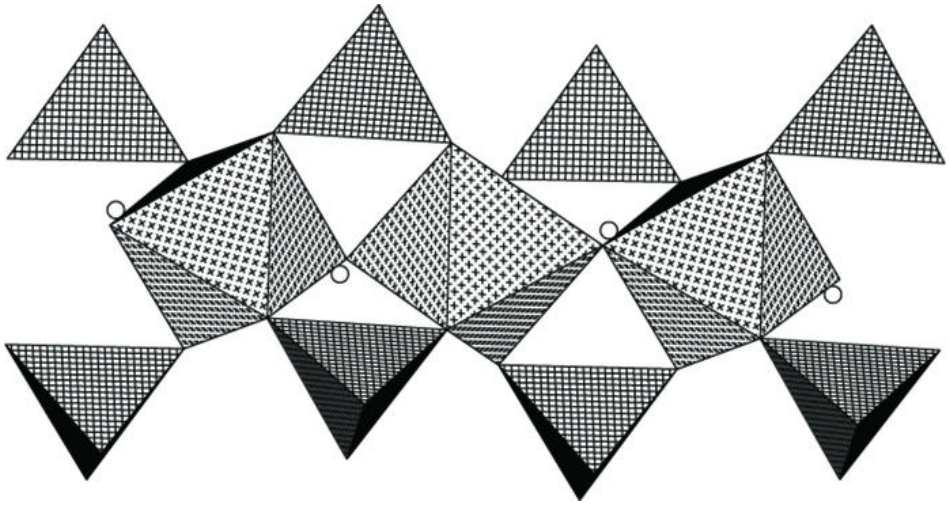

Fig. 4