Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Crystal structure of bis(propane-1,3-diaminium) hexafluoridoaluminate diaquatetrafluoridoaluminate tetrahydrate

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Received 30 August 2014
Accepted 1 November 2014

Edited by V. V. Chernyshev, Moscow State University, Russia

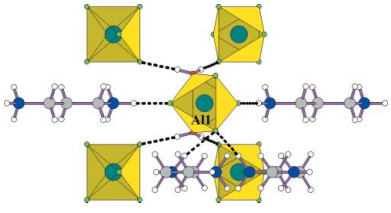
Keywords: crystal structure; hybrid organic–inorganic fluoride compound; fluoridoaluminate; aluminium; hydrothermal synthesis; hydrogen bonding

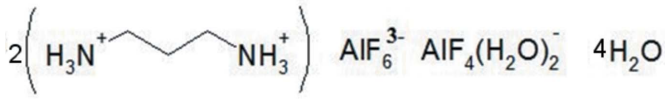
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The title compound, $(C_3H_{12}N_2)_2[AlF_6][AlF_4(H_2O)_2]\cdot 4H_2O$, was obtained by a solvothermal method in ethanol as solvent and with aluminium hydroxide, HF and 1,3-diaminopropane as educts. The asymmetric unit contains a quarter each of two crystallographically independent propane-1,3-diammonium dications, $[AlF_6]^{3-}$ and $[AlF_4(H_2O)_2]^-$ anions and four water molecules. The cations, anions and three of the independent water molecules are situated on special positions *mm*, while the fourth water molecule is disordered about a mirror plane. In the crystal, intermolecular N—H···F and O—H···F hydrogen bonds link the cations and anions into a three-dimensional framework with the voids filled by water molecules, which generate O—H···O hydrogen bonds and further consolidate the packing.

1. Chemical context

Hybrid organic–inorganic fluoride compounds are composed of both organic and inorganic moieties. The search for new compounds in this class of materials is still intense due to their applications in many domains such as gas storage, catalysis, separation, ion-exchange and biomedicine (Horcajada *et al.*, 2012; Stock & Biswas, 2012). Various hybrid materials containing fluorine organic ligands have been described in the literature (Ben Ali *et al.*, 2007). The dimensionality of the metal fluoride entities are 0D (isolated polyanions) (Adil, Ben Ali *et al.*, 2006; Adil, Leblanc & Maisonneuve, 2006; Fourquet *et al.*, 1987) , 1D (chains) or 2D (layers) (Adil *et al.*, 2010). The structural architecture of hybrid materials mainly depends on the metal and an organic part. However, other physical and physicochemical factors affect the resulting products such as the synthesis method (temperature, concentration, time of heating *etc.*) (Su *et al.*, 2010). This work is a continuation of an exploration of chemical systems including metal fluoride and amine, and the study of their structures.





2. Structural commentary

The asymmetric unit of the title compound contains aluminum atoms located in two crystallographically independent sites with different environments, $[Al2F_6]$ and $[Al1F_4(H_2O)_2]$, and two independent 1,3-propane diamine (dap) dications (Fig. 1). The Al—F distances in the two octahedra range from 1.768 (2)

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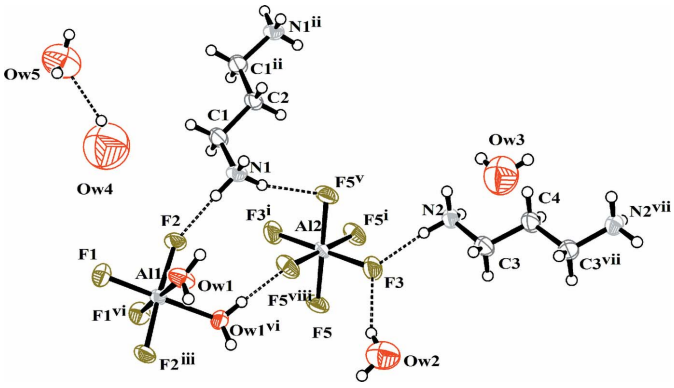


Figure 1
A portion of the crystal structure of the title compound showing the atom labelling and 50% probability displacement ellipsoids. Dashed lines denote hydrogen bonds. [Symmetry codes: (i) $\frac{1}{2}-x,\frac{1}{2}-y,-1-z$; (ii) $1-x,y,z$; (iii) $x,y,-z$; (v) $\frac{1}{2}-x,\frac{1}{2}-y,1+z$; (vi) $-x,y,z$; (vii) $x,-y,-1-z$; (viii) $x,y,1+z$.]

to 1.809 (3) Å while the Al1—O*W*1 distance is longer [1.944 (4) Å]. The [AlF_6] octahedron is regular whereas [$AlF_4(H_2O)_2$] exhibits a pronounced distortion due to the strong influence of the crystal field created by the hetero-ligands (F^-/H_2O). The value of the calculated valences (3.08 for Al1 and 3.01 for Al2) of the individual Al^{3+} cations (Brese & O'Keeffe, 1991) is in good agreement with the theoretical value, whereas those for the F^- anions are equal to 0.5. These anions complete their valence by establishing strong hydrogen bonds.

3. Supramolecular features

Each [$AlF_4(H_2O)_2$] octahedron is linked *via* N—H···F or O—H···F hydrogen bonds (Table 1) to one type of the organic cations (Fig. 2), with the formation of infinite chains parallel to the *a* axis. These chains are linked to each other by the AlF_6^{3-} dications and form infinite (H_2dap)[$AlF_4(H_2O)_2$] layers parallel to the *ac* plane (Fig. 3) . These layers are connected by the second organic cations and form a three-dimensional framework showing cavities, which are filled with the lattice water molecules.

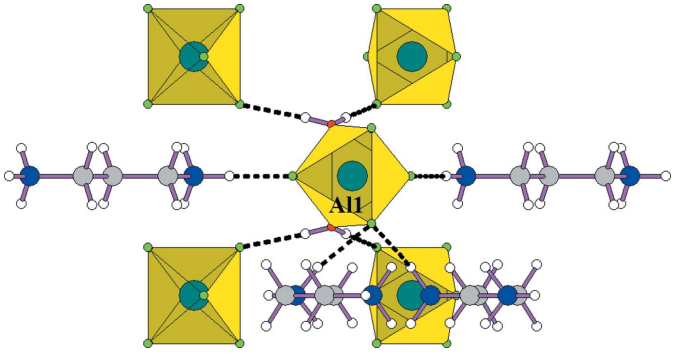


Figure 2
The environment of the $AlF_4(H_2O)_2$ octahedron. Dashed lines denote hydrogen bonds.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F2	0.89	1.79	2.679 (6)	177
N1—H1*B*···F5^{i}	0.89	1.99	2.846 (5)	161
N1—H1*C*···F5^{ii}	0.89	1.99	2.846 (5)	161
N2—H2*A*···F3	0.89	1.84	2.722 (6)	173
N2—H2*B*···F1^{iii}	0.89	2.00	2.841 (5)	158
Ow1—H1···F5^{iv}	0.83 (4)	1.74 (4)	2.569 (5)	178
Ow2—H2···F3	0.84 (4)	2.10 (4)	2.880 (5)	178
Ow4—H4···Ow5^{v}	0.84 (4)	2.13	2.910 (5)	154

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

4. Database survey

In the Cambridge Structural Database (Version 5.35; Groom & Allen, 2014) numerous *Class I* fluoridoaluminates with isolated (poly)anions or extended 1D inorganic chains, 2D inorganic layers or 3D networks are mentioned. Eight compounds with AlF_6^{3-} anions exist (Grottel *et al.*, 1992; Rother *et al.*, 1996, 1998; Touret *et al.*, 2001; Adil *et al.*, 2009; Bentrup *et al.*, 1996) and seven compounds containing the $AlF_5(H_2O)^{2-}$ anion (Cadiau *et al.*, 2008; Petrosyants *et al.*, 1997; Schröder *et al.*, 1993). However, to our knowledge, no fluoridoaluminate hybrid compounds containing both the AlF_6^{3-} and $AlF_5(H_2O)^{2-}$ anions have been reported.

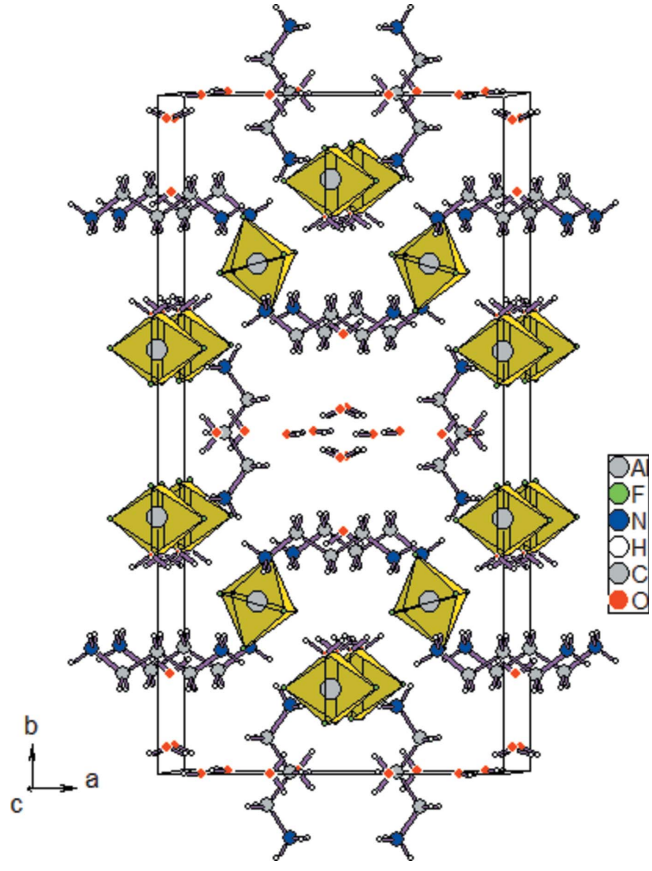


Figure 3
The crystal packing of the title compound, viewed approximately along [001].

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_3H_{12}N_2)_2[AlF_6][AlF_4(H_2O)_2]\cdot 4H_2O$
M_r	504.35
Crystal system, space group	Orthorhombic, *Cmmm*
Temperature (K)	293
a, *b*, *c* (Å)	12.975 (5), 25.115 (9), 6.452 (9)
V (Å^3)	2103 (3)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.26
Crystal size (mm)	0.24 × 0.12 × 0.05
Data collection	
Diffractometer	Siemens AED2
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1371, 1371, 939
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.148, 1.12
No. of reflections	1371
No. of parameters	105
No. of restraints	10
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.48

Computer programs: *STADI4* and *X-RED* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

5. Synthesis and crystallization

The title compound was prepared from a starting mixture of AlF_3 (0.5 g) in 40% HF (1.5 ml) and ethanol (5 ml). 1,3-Diaminopropane (0.54 ml) was added and mild hydrothermal conditions (463 K) were applied in a Teflon-lined autoclave (25 ml). The resulting product was washed with ethanol and dried in air giving colourless single crystals.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms of the NH_3 and CH_2 groups of the organic molecule were fixed geometrically [N—H = 0.89 (1) and C—H = 0.97 (1) Å with U_{iso}(H) = 1.2U_{eq}(N,C)]. All H atoms of the water molecules were located from a Fourier difference map. The O—H distances and H—O—H angles were fixed [O—H = 0.84 (1) and H···H = 1.34 (1) Å with U_{iso}(H) =1.5U_{eq}(O)]. The water molecule O*W*5 is disordered over two positions with the occupanies fixed to 0.5.

Acknowledgements

The authors are indebted to Dr Vincent Maisonneuve (University of Le Mans) for the data collection

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supporting information

Acta Cryst. (2014). E**70**, 471-473 [doi:10.1107/S1600536814024155]

Crystal structure of bis(propane-1,3-diaminium) hexafluoridoaluminate diaqua-tetrafluoridoaluminate tetrahydrate

Insaf Abdi, Khulood Al-Sadhan and Amor Ben Ali

Computing details

Data collection: *STADI4* (Stoe & Cie, 2002); cell refinement: *STADI4* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXS97* (Sheldrick, 2008) within *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Bis(propane-1,3-diaminium) hexafluoridoaluminate diaquatetrafluoridoaluminate tetrahydrate

Crystal data

$(C_3H_{12}N_2)_2[AlF_6][AlF_4(H_2O)_2]\cdot 4H_2O$
$M_r = 504.35$
Orthorhombic, *Cmmm*
Hall symbol: -C 2 2
$a = 12.975$ (5) Å
$b = 25.115$ (9) Å
$c = 6.452$ (9) Å
$V = 2103$ (3) Å^3
$Z = 4$
$F(000) = 1056$
$D_x = 1.593$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 32 reflections
$\theta = 2$–$27.5°$
$\mu = 0.26$ mm^{-1}
$T = 293$ K
Platelets, colourless
0.24 × 0.12 × 0.05 mm

Data collection

Siemens AED2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$2\theta/\omega$ scan
1371 measured reflections
1371 independent reflections
939 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0000$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = 0\rightarrow16$
$k = 0\rightarrow32$
$l = 0\rightarrow8$
3 standard reflections every 120 min
intensity decay: 4%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.148$
$S = 1.12$
1371 reflections
105 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 2.9098P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}

$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Extinction correction: *WinGX* (Farrugia, 2012), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (7)

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}	Occ. (<1)
Al1	0.0000	0.37606 (7)	0.0000	0.0234 (4)	
Al2	0.2500	0.2500	−0.5000	0.0245 (4)	
F1	0.0000	0.42435 (10)	0.2015 (4)	0.0382 (6)	
F2	0.13615 (17)	0.37342 (11)	0.0000	0.0374 (6)	
F3	0.2107 (2)	0.18091 (10)	−0.5000	0.0493 (8)	
F5	0.15743 (14)	0.26362 (8)	−0.7007 (3)	0.0447 (5)	
N1	0.3125 (2)	0.31814 (15)	0.0000	0.0325 (8)	
H1A	0.2551	0.3375	0.0000	0.049*	
H1B	0.3141	0.2977	0.1126	0.049*	0.50
H1C	0.3141	0.2977	−0.1126	0.049*	0.50
N2	0.3447 (3)	0.09755 (14)	−0.5000	0.0331 (8)	
H2A	0.3055	0.1266	−0.5000	0.050*	
H2B	0.3843	0.0974	−0.6126	0.050*	0.50
H2C	0.3843	0.0974	−0.3874	0.050*	0.50
C1	0.4029 (3)	0.35390 (18)	0.0000	0.0375 (11)	
H1D	0.4014	0.3765	0.1219	0.045*	0.50
H1E	0.4014	0.3765	−0.1219	0.045*	0.50
C2	0.5000	0.3205 (2)	0.0000	0.0336 (14)	
H2D	0.5000	0.2977	0.1215	0.040*	0.50
H2E	0.5000	0.2977	−0.1215	0.040*	0.50
C3	0.2784 (3)	0.04975 (18)	−0.5000	0.0415 (11)	
H3A	0.2346	0.0501	−0.6217	0.050*	0.50
H3B	0.2346	0.0501	−0.3783	0.050*	0.50
C4	0.3432 (5)	0.0000	−0.5000	0.0427 (16)	
H4A	0.3872	0.0000	−0.6215	0.051*	0.50
H4B	0.3872	0.0000	−0.3785	0.051*	0.50
OW1	0.0000	0.32173 (12)	0.2146 (6)	0.0400 (8)	
OW2	0.0000	0.1449 (3)	−0.5000	0.080 (2)	
OW3	0.3272 (7)	0.0000	0.0000	0.104 (3)	
OW4	0.3732 (11)	0.5000	0.0000	0.200 (6)	
OW5	0.5000	0.5374 (6)	0.342 (2)	0.110 (4)	0.50
H1	0.0517 (4)	0.3034 (11)	0.241 (9)	0.165*	

H2	0.0517 (4)	0.1650 (8)	−0.5000	0.165*	
H3	0.3669 (15)	0.0267 (2)	0.0000	0.165*	
H4	0.4125 (17)	0.5000	−0.1039 (8)	0.165*	
H5	0.5516 (4)	0.526 (5)	0.408 (12)	0.165*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0187 (8)	0.0233 (8)	0.0282 (9)	0.000	0.000	0.000
Al2	0.0230 (8)	0.0257 (8)	0.0248 (8)	0.0074 (7)	0.000	0.000
F1	0.0469 (14)	0.0332 (13)	0.0346 (13)	0.000	0.000	−0.0076 (11)
F2	0.0190 (11)	0.0373 (14)	0.0560 (16)	−0.0036 (10)	0.000	0.000
F3	0.0445 (16)	0.0282 (14)	0.075 (2)	0.0027 (12)	0.000	0.000
F5	0.0370 (9)	0.0582 (13)	0.0388 (10)	0.0178 (8)	−0.0120 (8)	−0.0007 (9)
N1	0.0211 (16)	0.043 (2)	0.0338 (18)	0.0014 (15)	0.000	0.000
N2	0.0342 (19)	0.0262 (17)	0.039 (2)	0.0023 (15)	0.000	0.000
C1	0.027 (2)	0.030 (2)	0.056 (3)	0.0028 (17)	0.000	0.000
C2	0.020 (3)	0.029 (3)	0.053 (4)	0.000	0.000	0.000
C3	0.027 (2)	0.033 (2)	0.064 (3)	0.0040 (18)	0.000	0.000
C4	0.028 (3)	0.029 (3)	0.071 (5)	0.000	0.000	0.000
OW1	0.0266 (14)	0.0385 (16)	0.055 (2)	0.000	0.000	0.0203 (16)
OW2	0.065 (4)	0.104 (6)	0.070 (4)	0.000	0.000	0.000
OW3	0.121 (7)	0.090 (6)	0.102 (6)	0.000	0.000	0.000
OW4	0.209 (14)	0.204 (17)	0.188 (13)	0.000	0.000	0.000
OW5	0.101 (8)	0.110 (9)	0.119 (10)	0.000	0.000	0.032 (8)

Geometric parameters (Å, º)

Al1—F2^{i}	1.768 (2)	N2—H2C	0.8900
Al1—F2	1.768 (2)	C1—C2	1.514 (5)
Al1—F1	1.778 (3)	C1—H1D	0.9700
Al1—F1^{ii}	1.778 (3)	C1—H1E	0.9700
Al1—OW1	1.944 (4)	C2—C1^{vi}	1.514 (5)
Al1—OW1^{ii}	1.944 (4)	C2—H2D	0.9700
Al2—F5^{iii}	1.799 (2)	C2—H2E	0.9700
Al2—F5	1.799 (2)	C3—C4	1.505 (5)
Al2—F5^{iv}	1.799 (2)	C3—H3A	0.9700
Al2—F5^{v}	1.799 (2)	C3—H3B	0.9700
Al2—F3	1.809 (3)	C4—C3^{vii}	1.505 (5)
Al2—F3^{iii}	1.809 (3)	C4—H4A	0.9700
N1—C1	1.476 (6)	C4—H4B	0.9700
N1—H1A	0.8900	OW1—H1	0.831 (10)
N1—H1B	0.8900	OW2—H2	0.840 (10)
N1—H1C	0.8900	OW3—H3	0.846 (10)
N2—C3	1.477 (6)	OW4—H4	0.842 (10)
N2—H2A	0.8900	OW5—H5	0.840 (10)
N2—H2B	0.8900		

F2^{i}—Al1—F2	175.7 (2)	H1A—N1—H1C	109.5
F2^{i}—Al1—F1	91.47 (7)	H1B—N1—H1C	109.5
F2—Al1—F1	91.47 (7)	C3—N2—H2A	109.5
F2^{i}—Al1—F1^{ii}	91.47 (7)	C3—N2—H2B	109.5
F2—Al1—F1^{ii}	91.47 (7)	H2A—N2—H2B	109.5
F1—Al1—F1^{ii}	94.0 (2)	C3—N2—H2C	109.5
F2^{i}—Al1—OW1	88.49 (7)	H2A—N2—H2C	109.5
F2—Al1—OW1	88.49 (7)	H2B—N2—H2C	109.5
F1—Al1—OW1	87.59 (16)	N1—C1—C2	108.9 (4)
F1^{ii}—Al1—OW1	178.44 (16)	N1—C1—H1D	109.9
F2^{i}—Al1—OW1^{ii}	88.49 (7)	C2—C1—H1D	109.9
F2—Al1—OW1^{ii}	88.49 (7)	N1—C1—H1E	109.9
F1—Al1—OW1^{ii}	178.44 (16)	C2—C1—H1E	109.9
F1^{ii}—Al1—OW1^{ii}	87.60 (16)	H1D—C1—H1E	108.3
OW1—Al1—OW1^{ii}	90.8 (2)	C1^{vi}—C2—C1	112.7 (5)
F5^{iii}—Al2—F5	180.00 (14)	C1^{vi}—C2—H2D	109.1
F5^{iii}—Al2—F5^{iv}	87.92 (14)	C1—C2—H2D	109.1
F5—Al2—F5^{iv}	92.08 (14)	C1^{vi}—C2—H2E	109.1
F5^{iii}—Al2—F5^{v}	92.08 (14)	C1—C2—H2E	109.1
F5—Al2—F5^{v}	87.92 (14)	H2D—C2—H2E	107.8
F5^{iv}—Al2—F5^{v}	180.00 (13)	N2—C3—C4	110.5 (4)
F5^{iii}—Al2—F3	90.34 (9)	N2—C3—H3A	109.6
F5—Al2—F3	89.66 (9)	C4—C3—H3A	109.6
F5^{iv}—Al2—F3	89.66 (9)	N2—C3—H3B	109.6
F5^{v}—Al2—F3	90.34 (9)	C4—C3—H3B	109.6
F5^{iii}—Al2—F3^{iii}	89.66 (9)	H3A—C3—H3B	108.1
F5—Al2—F3^{iii}	90.34 (9)	C3^{vii}—C4—C3	112.2 (5)
F5^{iv}—Al2—F3^{iii}	90.34 (9)	C3^{vii}—C4—H4A	109.2
F5^{v}—Al2—F3^{iii}	89.66 (9)	C3—C4—H4A	109.2
F3—Al2—F3^{iii}	180.0	C3^{vii}—C4—H4B	109.2
C1—N1—H1A	109.5	C3—C4—H4B	109.2
C1—N1—H1B	109.5	H4A—C4—H4B	107.9
H1A—N1—H1B	109.5	Al1—OW1—H1	122 (2)
C1—N1—H1C	109.5		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F2	0.89	1.79	2.679 (6)	177
N1—H1*B*···F5^{viii}	0.89	1.99	2.846 (5)	161
N1—H1*C*···F5^{iii}	0.89	1.99	2.846 (5)	161
N2—H2*A*···F3	0.89	1.84	2.722 (6)	173
N2—H2*B*···F1^{ix}	0.89	2.00	2.841 (5)	158
Ow1—H1···F5^{x}	0.83 (4)	1.74 (4)	2.569 (5)	178

Ow2—H2···F3	0.84 (4)	2.10 (4)	2.880 (5)	178
Ow4—H4···Ow5^{ii}	0.84 (4)	2.13	2.910 (5)	154

Symmetry codes: (ii) x, y, $-z$; (iii) $-x+1/2$, $-y+1/2$, $-z-1$; (viii) $-x+1/2$, $-y+1/2$, $z+1$; (ix) $-x+1/2$, $-y+1/2$, $z-1$; (x) x, y, $z+1$.