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Crystal structure of bis(propane-1,3-diammonium) hexafluoridoaluminate fluoride trihydrate

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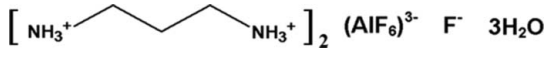
The title compound, $(C_3H_{10}N_2)_2[AlF_6]F{\cdot}3H_2O$, was obtained using the solvothermal method with aluminium hydroxide, HF and propane-1,3-diamine as precursors in ethanol as solvent. The structure consists of isolated $[AlF_6]^{3-}$ octahedra, diprotonated propane-1,3-diamine cations $[(H_2dap)^{2+}]$, free fluoride ions and water molecules of solvation. The Al—F bond lengths in the octahedral $[AlF_6]^{3-}$ anions range from 1.7690 (19) to 1.8130 (19) Å, with an average value of 1.794 Å. Each $[AlF_6]^{3-}$ anion is surrounded by three water molecules and by six diprotonated amine cations. The 'free' fluoride ion is hydrogen bonded to four H atoms belonging to four dications and has a distorted tetrahedral geometry. The three water molecules are connected by hydrogen bonds, forming trimers that connect the AlF_6 octahedra and dications into a three-dimensional framework.

Keywords: crystal structure; hexafluoridoaluminate; hybrid aluminates; hydrogen bonding.

CCDC reference: 1012356

1. Related literature

For general background to hybrid aluminates, their syntheses and applications, see: Ben Ali *et al.* (2007, 2009); Lhoste *et al.* (2009); Adil *et al.* (2010); Martineau *et al.* (2012); Cadiau *et al.* (2013). For a review of hydrogen-bonding interactions, see: Steiner (1998).



2. Experimental

2.1. Crystal data

$(C_3H_{10}N_2)_2[AlF_6]F{\cdot}3H_2O$
M_r = 366.31
Triclinic, $P\overline{1}$
a = 9.825 (2) Å
b = 9.974 (3) Å
c = 10.697 (2) Å
α = 70.01 (2)°
β = 67.89 (2)°
γ = 59.77 (1)°
V = 823.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 K
0.61 × 0.13 × 0.08 mm

2.2. Data collection

Siemens AED2 diffractometer
Absorption correction: gaussian (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.985
3411 measured reflections
3411 independent reflections
3046 reflections with $I > 2\sigma(I)$
3 standard reflections every 120 min
intensity decay: 4%

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.183
S = 1.05
3411 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···F7	0.89	1.81	2.696 (3)	171
N1—H1B···F3^{i}	0.89	1.79	2.663 (3)	166
N1—H1C···F2^{ii}	0.89	2.08	2.826 (3)	141
N1—H1C···F3^{ii}	0.89	2.09	2.796 (3)	136
N2—H2A···F4^{iii}	0.89	2.08	2.657 (3)	122
N2—H2B···OW2^{iv}	0.89	2.11	2.804 (3)	134
N2—H2C···F7^{v}	0.89	2.04	2.724 (3)	132
N3—H3A···F7	0.89	1.79	2.677 (3)	176
N3—H3B···F5	0.89	2.00	2.792 (3)	148
N3—H3C···F5^{iii}	0.89	1.89	2.753 (4)	162
N4—H4A···F2^{ii}	0.89	1.90	2.757 (3)	161
N4—H4B···F1^{vi}	0.89	1.92	2.776 (4)	162
N4—H4C···F7^{ii}	0.89	1.84	2.724 (3)	169
OW1—H11···F5	0.92	1.85	2.743 (3)	161
OW1—H12···OW3^{vii}	0.95	1.85	2.789 (5)	173
OW2—H21···F1	0.74	2.27 (5)	2.943 (3)	152 (5)
OW2—H22···OW1^{viii}	0.82 (7)	1.98	2.785 (5)	170
OW3—H31···F6^{vi}	0.82 (4)	1.79 (4)	2.612 (4)	176
OW3—H32···F1^{ii}	0.81 (7)	1.99 (7)	2.783 (4)	167

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

Data collection: *STADI4* (Stoe, 1998); cell refinement: *STADI4*; data reduction: *X-RED* (Stoe, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 2001) and *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: CQ2011).

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supporting information

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Crystal structure of bis(propane-1,3-diammonium) hexafluoridoaluminate fluoride trihydrate

I. Abdi, K. A. Al-Sadhan and A. Ben Ali

S1. Comment

Hybrid solids, containing both organic and inorganic entities, have diverse crystal structures which can influence their physicochemical properties. In type I solid hybrids, interactions between organic and inorganic networks are generally weak (*e.g.* hydrogen bonds or van der Waals′ interactions), whilst in type II hybrids, covalent bonds are generally established between the metal of the inorganic moiety and the organic moiety. Type II hybrid materials usually exhibit better thermal stability than those of type I. Many chemical systems have been explored by conventional hydro-solvothermal synthesis or microwave heating. This work deals with a new aluminium fluoride salt of hybrid type I prepared under solvothermal conditions. Its structure contains isolated AlF_6 distorted octahedra hydrogen bonded to propane-1,3-diamine dications and water molecules, together with fluoride ions which are also hydrogen bonded to the organic dications (Figures 2-4).

S2. Experimental

The title compound was prepared from a starting mixture of $Al(OH)_3$ (0.75 g) in 40% HF (0.8 ml) and ethanol (5 ml). 1,3-diaminopropane (1 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 colorless single crystals of the title compound.

S3. Refinement

All non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms of the water molecules were located using difference Fourier methods and their positional and isotropic displacement parameters refined. The H atoms of the organic dications were included in the refinement at calculated positions and refined with a common isotropic thermal parameter.

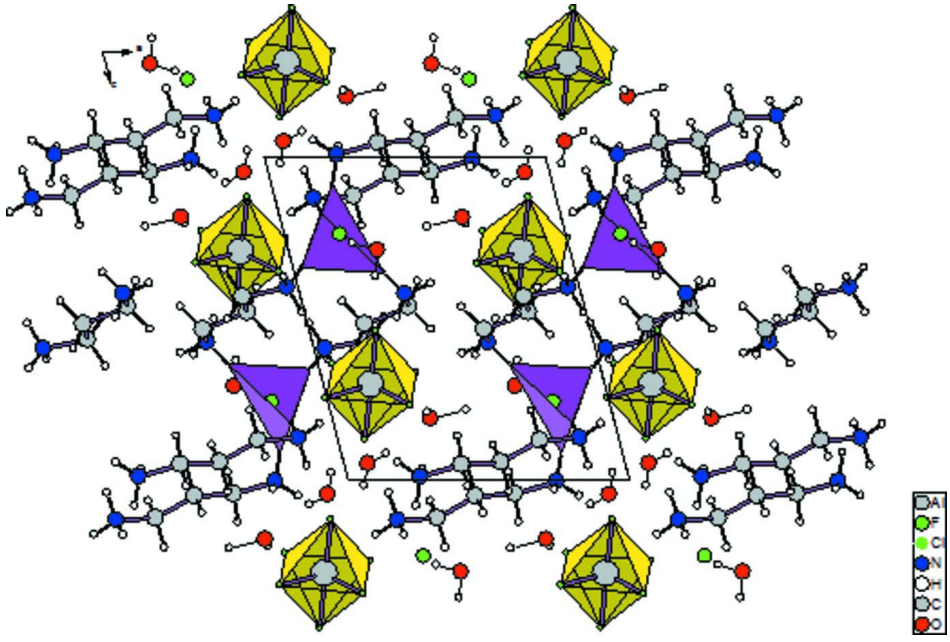

Figure 1

View of the structure of (I) along the [010] axis.

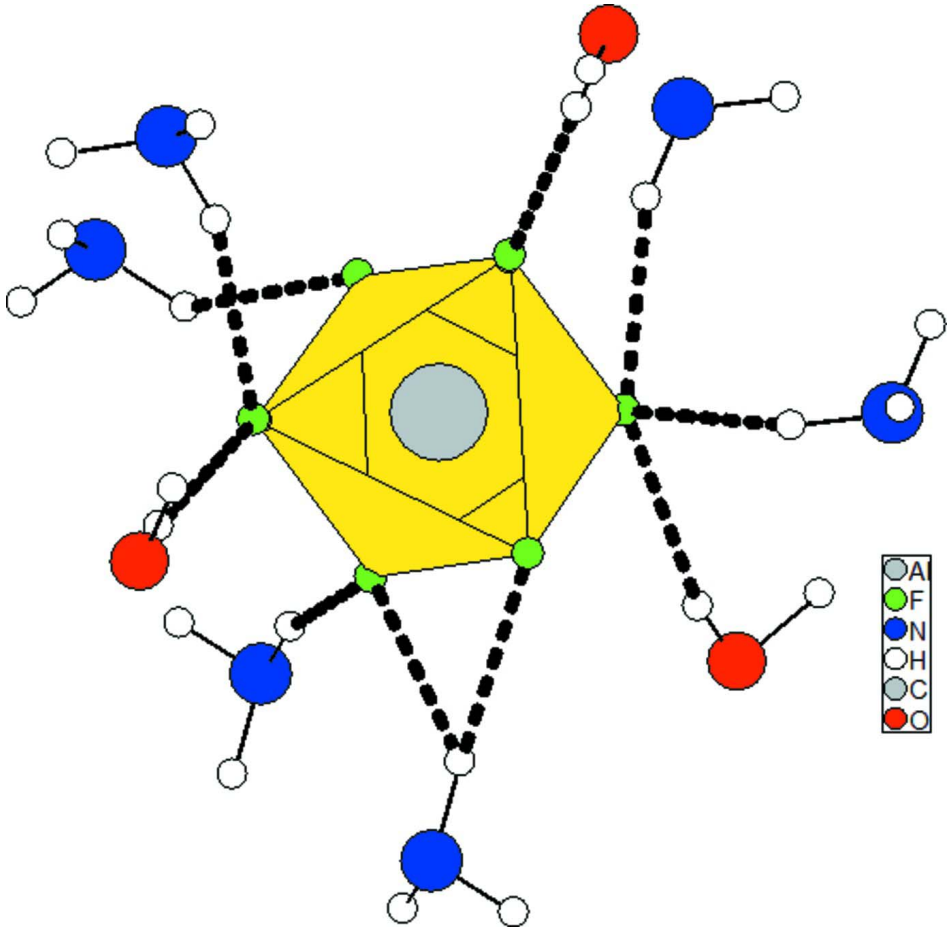

Figure 2

The environment of the AlF_6 octahedron.

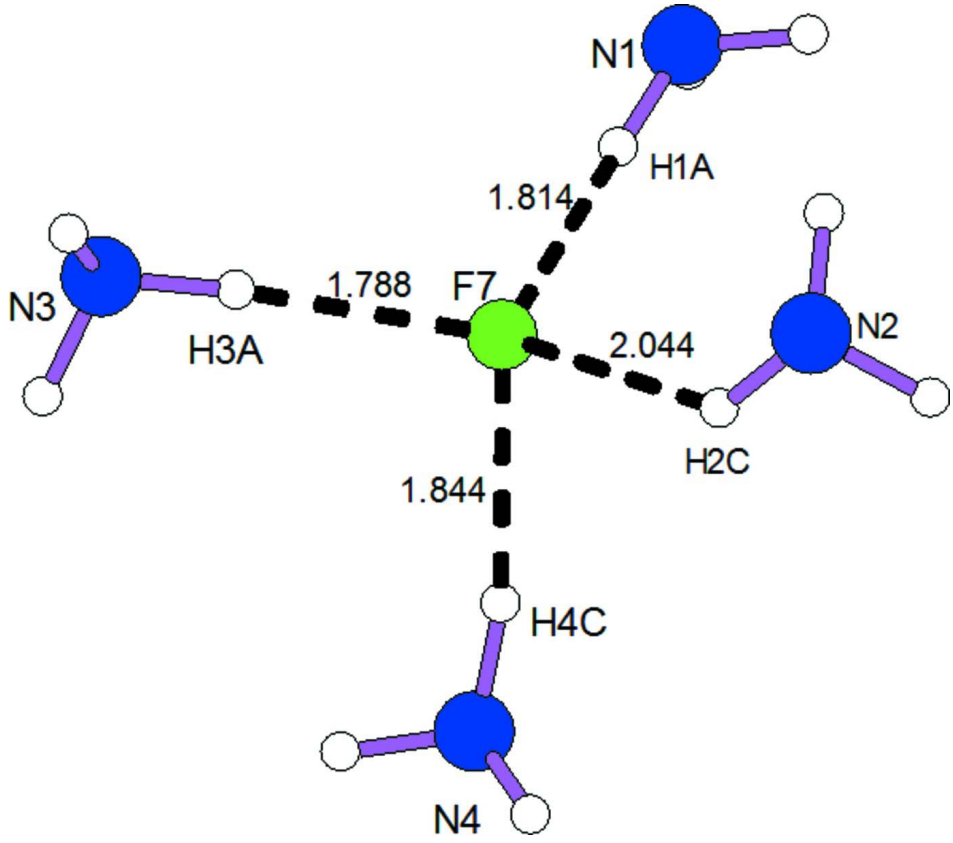

Figure 3

The environment of the isolated fluoride anion.

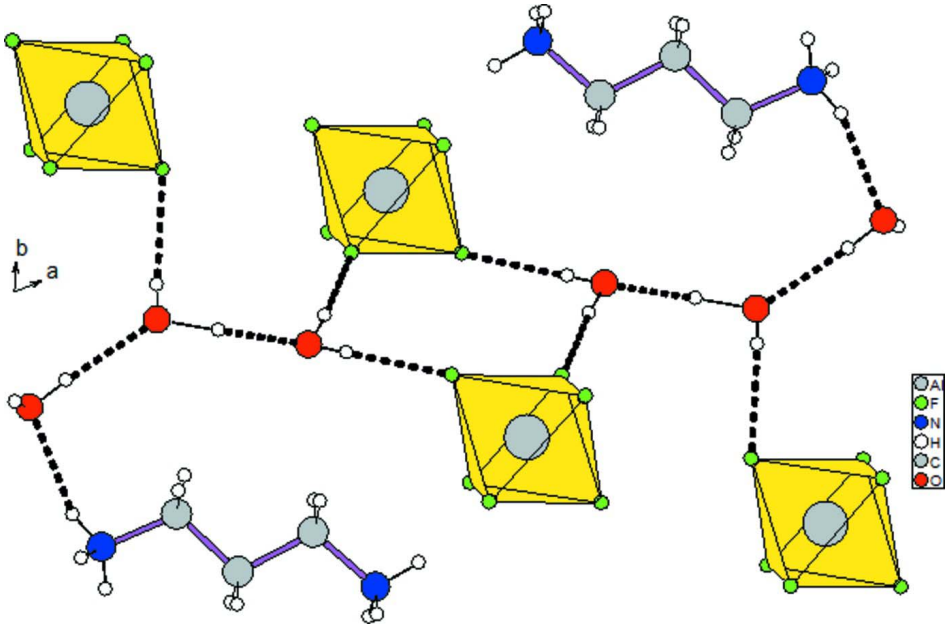

Figure 4

The environment of water molecules

Bis(propane-1,3-diammonium) hexafluoridoaluminate fluoride trihydrate

Crystal data

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Hall symbol: -P 1
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b = 9.974 (3) Å
c = 10.697 (2) Å
α = 70.01 (2)°
β = 67.89 (2)°
γ = 59.77 (1)°
V = 823.8 (3) Å^3
Z = 2
$F(000)$ = 388
D_x = 1.477 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 32 reflections
θ = 5.0–20.0°
μ = 0.21 mm^{-1}
T = 298 K
Platelet, colorless
0.61 × 0.13 × 0.08 mm

Data collection

Siemens AED2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$2\theta/\omega$ scan
Absorption correction: gaussian (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.985
3411 measured reflections
3411 independent reflections
3046 reflections with $I > 2\sigma(I)$
R_{int} = 0.000
θ_{max} = 27.6°, θ_{min} = 2.1°
h = −11→12
k = −11→12
l = 0→13
3 standard reflections every 120 min
intensity decay: 4%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.183
S = 1.05
3411 reflections
215 parameters
0 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
′ $w = 1/[\sigma^2(F_o^2) + (0.1177P)^2 + 0.6344P]$ where $P = (F_o^2 + 2F_c^2)/3$′
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 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.

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 $F^2 > 2$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}
Al1	0.83033 (8)	−0.20234 (8)	0.29308 (6)	0.0238 (2)
F1	1.0025 (2)	−0.3849 (2)	0.2527 (3)	0.0678 (6)

F2	0.9474 (2)	−0.1577 (3)	0.35631 (17)	0.0496 (5)
F3	0.9030 (2)	−0.1056 (3)	0.12502 (16)	0.0518 (5)
F4	0.7092 (2)	−0.2378 (3)	0.2304 (2)	0.0575 (5)
F5	0.6596 (2)	−0.0158 (2)	0.3295 (2)	0.0546 (5)
F6	0.7625 (3)	−0.2962 (3)	0.4612 (2)	0.0747 (8)
F7	0.80224 (19)	−0.13548 (18)	0.76019 (15)	0.0357 (4)
N1	0.86118 (18)	0.02879 (18)	0.8720 (2)	0.0295 (4)
H1A	0.8503	−0.0243	0.8272	0.054 (2)*
H1B	0.8678	−0.0258	0.9567	0.054 (2)*
H1C	0.9513	0.0429	0.8278	0.054 (2)*
N2	0.26017 (18)	0.32258 (18)	0.9923 (2)	0.0333 (4)
H2A	0.2747	0.2379	0.9690	0.054 (2)*
H2B	0.1927	0.4094	0.9480	0.054 (2)*
H2C	0.2178	0.3171	1.0825	0.054 (2)*
N3	0.6255 (3)	0.0499 (3)	0.5761 (2)	0.0348 (5)
H3A	0.6799	−0.0092	0.6407	0.054 (2)*
H3B	0.6738	0.0038	0.5032	0.054 (2)*
H3C	0.5238	0.0599	0.6089	0.054 (2)*
N4	0.9607 (3)	0.3445 (2)	0.4048 (2)	0.0326 (5)
H4A	0.9932	0.3030	0.4823	0.054 (2)*
H4B	0.9584	0.4403	0.3719	0.054 (2)*
H4C	1.0296	0.2828	0.3433	0.054 (2)*
C1	0.7954 (3)	0.3567 (3)	0.4329 (3)	0.0355 (5)
H1D	0.7567	0.4093	0.3501	0.054 (2)*
H1E	0.7214	0.4199	0.5031	0.054 (2)*
C2	0.7184 (3)	0.1845 (3)	0.8795 (3)	0.0308 (5)
H2D	0.7159	0.2468	0.7874	0.054 (2)*
H2E	0.7284	0.2406	0.9314	0.054 (2)*
C3	0.6240 (3)	0.2082 (3)	0.5355 (3)	0.0334 (5)
H3D	0.5688	0.2597	0.6144	0.054 (2)*
H3E	0.5646	0.2727	0.4652	0.054 (2)*
C4	0.5606 (3)	0.1665 (3)	0.9473 (3)	0.0312 (5)
H4D	0.5485	0.1128	0.8945	0.054 (2)*
H4E	0.5628	0.1034	1.0391	0.054 (2)*
C5	0.7966 (3)	0.1947 (3)	0.4807 (3)	0.0312 (5)
H5D	0.8544	0.1343	0.5524	0.054 (2)*
H5E	0.8535	0.1387	0.4046	0.054 (2)*
C6	0.4188 (3)	0.3281 (3)	0.9548 (3)	0.0351 (5)
H6D	0.4199	0.3720	1.0223	0.054 (2)*
H6E	0.4313	0.3976	0.8663	0.054 (2)*
OW1	0.6507 (3)	0.2741 (3)	0.1872 (3)	0.0543 (6)
H11	0.658 (7)	0.173 (3)	0.216 (5)	0.096 (17)*
H12	0.536 (3)	0.334 (6)	0.214 (6)	0.12 (2)*
OW2	1.0850 (3)	−0.3475 (3)	−0.0480 (3)	0.0480 (5)
OW3	0.6830 (3)	0.5567 (4)	0.7114 (3)	0.0670 (8)
H21	1.053 (6)	−0.325 (5)	0.020 (5)	0.063 (14)*
H22	1.160 (6)	−0.322 (6)	−0.080 (5)	0.073 (14)*
H31	0.712 (5)	0.602 (5)	0.633 (4)	0.052 (10)*

H32	0.767 (7)	0.507 (6)	0.735 (6)	0.090 (17)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0238 (3)	0.0282 (4)	0.0245 (3)	−0.0153 (3)	−0.0087 (2)	−0.0013 (2)
F1	0.0399 (10)	0.0365 (9)	0.1124 (18)	−0.0088 (8)	−0.0130 (11)	−0.0167 (10)
F2	0.0553 (10)	0.0851 (13)	0.0371 (8)	−0.0519 (10)	−0.0159 (7)	−0.0044 (8)
F3	0.0537 (10)	0.0853 (14)	0.0284 (8)	−0.0501 (10)	−0.0160 (7)	0.0141 (8)
F4	0.0516 (11)	0.0991 (16)	0.0566 (11)	−0.0513 (11)	−0.0063 (8)	−0.0322 (10)
F5	0.0335 (9)	0.0417 (9)	0.0857 (14)	−0.0117 (7)	−0.0063 (9)	−0.0258 (9)
F6	0.0929 (17)	0.117 (2)	0.0379 (9)	−0.0847 (17)	−0.0185 (10)	0.0246 (11)
F7	0.0399 (8)	0.0398 (8)	0.0357 (8)	−0.0209 (7)	−0.0141 (6)	−0.0054 (6)
N1	0.0270 (9)	0.0363 (10)	0.0326 (10)	−0.0193 (8)	−0.0110 (8)	−0.0020 (8)
N2	0.0315 (10)	0.0368 (11)	0.0344 (10)	−0.0175 (9)	−0.0079 (8)	−0.0058 (8)
N3	0.0325 (10)	0.0493 (12)	0.0352 (10)	−0.0257 (10)	−0.0110 (8)	−0.0065 (9)
N4	0.0341 (11)	0.0329 (10)	0.0366 (10)	−0.0194 (9)	−0.0113 (8)	−0.0027 (8)
C1	0.0297 (11)	0.0318 (12)	0.0465 (14)	−0.0128 (10)	−0.0151 (10)	−0.0035 (10)
C2	0.0329 (12)	0.0322 (12)	0.0343 (11)	−0.0206 (10)	−0.0095 (9)	−0.0027 (9)
C3	0.0271 (11)	0.0391 (13)	0.0379 (12)	−0.0158 (10)	−0.0099 (9)	−0.0071 (10)
C4	0.0307 (11)	0.0317 (11)	0.0367 (12)	−0.0184 (10)	−0.0101 (9)	−0.0031 (9)
C5	0.0249 (10)	0.0349 (12)	0.0374 (12)	−0.0144 (9)	−0.0082 (9)	−0.0082 (9)
C6	0.0303 (12)	0.0337 (12)	0.0475 (14)	−0.0162 (10)	−0.0118 (10)	−0.0086 (10)
OW1	0.0534 (13)	0.0473 (12)	0.0579 (13)	−0.0279 (11)	−0.0084 (11)	−0.0017 (10)
OW2	0.0400 (11)	0.0468 (12)	0.0585 (14)	−0.0144 (10)	−0.0093 (10)	−0.0217 (10)
OW3	0.0425 (13)	0.0716 (17)	0.0512 (14)	−0.0207 (12)	−0.0061 (11)	0.0162 (12)

Geometric parameters (Å, º)

Al1—F6	1.7690 (19)	N3—H3B	0.8900
Al1—F4	1.7832 (17)	N3—H3C	0.8900
Al1—F3	1.7929 (16)	N4—C1	1.483 (3)
Al1—F1	1.803 (2)	N4—H4A	0.8900
Al1—F2	1.8126 (16)	N4—H4B	0.8900
Al1—F5	1.8130 (19)	N4—H4C	0.8900
F1—F3	2.499 (3)	C1—C5	1.514 (3)
F1—F4	2.556 (3)	C1—H1D	0.9700
F1—F6	2.570 (4)	C1—H1E	0.9700
F1—F2	2.586 (3)	C2—C4	1.518 (3)
F2—F3	2.507 (2)	C2—H2D	0.9700
F2—F5	2.527 (3)	C2—H2E	0.9700
F2—F6	2.529 (3)	C3—C5	1.521 (3)
F3—F4	2.556 (2)	C3—H3D	0.9700
F3—F5	2.559 (3)	C3—H3E	0.9700
F4—F5	2.529 (3)	C4—C6	1.513 (3)
F4—F6	2.529 (3)	C4—H4D	0.9700
F5—F6	2.522 (3)	C4—H4E	0.9700
F5—H11	1.85 (3)	C5—H5D	0.9700

N1—C2	1.481 (3)	C5—H5E	0.9700
N1—H1A	0.8900	C6—H6D	0.9700
N1—H1B	0.8900	C6—H6E	0.9700
N1—H1C	0.8900	OW1—H11	0.925 (19)
N2—C6	1.481 (3)	OW1—H12	0.95 (2)
N2—H2A	0.8900	OW2—H21	0.74 (5)
N2—H2B	0.8900	OW2—H22	0.82 (5)
N2—H2C	0.8900	OW3—H31	0.83 (4)
N3—C3	1.482 (3)	OW3—H32	0.81 (6)
N3—H3A	0.8900		

F6—Al1—F4	90.79 (10)	H1A—N1—H1C	109.5
F6—Al1—F3	177.96 (9)	H1B—N1—H1C	109.5
F4—Al1—F3	91.25 (9)	C6—N2—H2A	109.5
F6—Al1—F1	92.04 (13)	C6—N2—H2B	109.5
F4—Al1—F1	90.93 (11)	H2A—N2—H2B	109.5
F3—Al1—F1	88.04 (11)	C6—N2—H2C	109.5
F6—Al1—F2	89.84 (9)	H2A—N2—H2C	109.5
F4—Al1—F2	177.63 (11)	H2B—N2—H2C	109.5
F3—Al1—F2	88.11 (8)	C3—N3—H3A	109.5
F1—Al1—F2	91.33 (11)	C3—N3—H3B	109.5
F6—Al1—F5	89.49 (12)	H3A—N3—H3B	109.5
F4—Al1—F5	89.36 (10)	C3—N3—H3C	109.5
F3—Al1—F5	90.41 (11)	H3A—N3—H3C	109.5
F1—Al1—F5	178.44 (10)	H3B—N3—H3C	109.5
F2—Al1—F5	88.36 (10)	C1—N4—H4A	109.5
F3—F1—F4	60.73 (8)	C1—N4—H4B	109.5
F3—F1—F6	89.25 (9)	H4A—N4—H4B	109.5
F4—F1—F6	59.11 (8)	C1—N4—H4C	109.5
F3—F1—F2	59.05 (7)	H4A—N4—H4C	109.5
F4—F1—F2	88.70 (8)	H4B—N4—H4C	109.5
F6—F1—F2	58.74 (8)	N4—C1—C5	111.0 (2)
F3—F2—F5	61.11 (8)	N4—C1—H1D	109.4
F3—F2—F6	90.00 (8)	C5—C1—H1D	109.4
F5—F2—F6	59.83 (8)	N4—C1—H1E	109.4
F3—F2—F1	58.74 (8)	C5—C1—H1E	109.4
F5—F2—F1	90.00 (8)	H1D—C1—H1E	108.0
F6—F2—F1	60.32 (9)	N1—C2—C4	111.36 (18)
F1—F3—F2	62.21 (9)	N1—C2—H2D	109.4
F1—F3—F4	60.74 (8)	C4—C2—H2D	109.4
F2—F3—F4	90.47 (7)	N1—C2—H2E	109.4
F1—F3—F5	91.25 (8)	C4—C2—H2E	109.4
F2—F3—F5	59.82 (8)	H2D—C2—H2E	108.0
F4—F3—F5	59.25 (7)	N3—C3—C5	110.7 (2)
F5—F4—F6	59.81 (9)	N3—C3—H3D	109.5
F5—F4—F3	60.43 (8)	C5—C3—H3D	109.5
F6—F4—F3	88.90 (7)	N3—C3—H3E	109.5
F5—F4—F1	90.64 (8)	C5—C3—H3E	109.5

F6—F4—F1	60.72 (10)	H3D—C3—H3E	108.1
F3—F4—F1	58.52 (7)	C6—C4—C2	109.45 (19)
F6—F5—F4	60.10 (9)	C6—C4—H4D	109.8
F6—F5—F2	60.13 (8)	C2—C4—H4D	109.8
F4—F5—F2	90.65 (8)	C6—C4—H4E	109.8
F6—F5—F3	89.00 (9)	C2—C4—H4E	109.8
F4—F5—F3	60.32 (7)	H4D—C4—H4E	108.2
F2—F5—F3	59.07 (7)	C1—C5—C3	110.8 (2)
Al1—F5—H11	120.3 (17)	C1—C5—H5D	109.5
F6—F5—H11	160.8 (17)	C3—C5—H5D	109.5
F4—F5—H11	120.6 (16)	C1—C5—H5E	109.5
F2—F5—H11	101.0 (17)	C3—C5—H5E	109.5
F3—F5—H11	76.8 (17)	H5D—C5—H5E	108.1
F5—F6—F2	60.03 (8)	N2—C6—C4	112.33 (19)
F5—F6—F4	60.09 (9)	N2—C6—H6D	109.1
F2—F6—F4	90.59 (8)	C4—C6—H6D	109.1
F5—F6—F1	90.47 (8)	N2—C6—H6E	109.1
F2—F6—F1	60.94 (8)	C4—C6—H6E	109.1
F4—F6—F1	60.16 (9)	H6D—C6—H6E	107.9
C2—N1—H1A	109.5	H11—OW1—H12	100 (5)
C2—N1—H1B	109.5	H21—OW2—H22	100 (5)
H1A—N1—H1B	109.5	H31—OW3—H32	102 (5)
C2—N1—H1C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···F7	0.89	1.81	2.696 (3)	171
N1—H1*B*···F3^{i}	0.89	1.79	2.663 (3)	166
N1—H1*C*···F2^{ii}	0.89	2.08	2.826 (3)	141
N1—H1*C*···F3^{ii}	0.89	2.09	2.796 (3)	136
N2—H2*A*···F4^{iii}	0.89	2.08	2.657 (3)	122
N2—H2*B*···O*W*2^{iv}	0.89	2.11	2.804 (3)	134
N2—H2*C*···F7^{v}	0.89	2.04	2.724 (3)	132
N3—H3*A*···F7	0.89	1.79	2.677 (3)	176
N3—H3*B*···F5	0.89	2.00	2.792 (3)	148
N3—H3*C*···F5^{iii}	0.89	1.89	2.753 (4)	162
N4—H4*A*···F2^{ii}	0.89	1.90	2.757 (3)	161
N4—H4*B*···F1^{vi}	0.89	1.92	2.776 (4)	162
N4—H4*C*···F7^{ii}	0.89	1.84	2.724 (3)	169
O*W*1—H11···F5	0.92	1.85	2.743 (3)	161
O*W*1—H12···O*W*3^{vii}	0.95	1.85	2.789 (5)	173
O*W*2—H21···F1	0.74	2.27 (5)	2.943 (3)	152 (5)
O*W*2—H22···O*W*1^{viii}	0.82 (7)	1.98	2.785 (5)	170
O*W*3—H31···F6^{vi}	0.82 (4)	1.79 (4)	2.612 (4)	176
O*W*3—H32···F1^{ii}	0.81 (7)	1.99 (7)	2.783 (4)	167

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