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6-Benzyl-2-methyl-1,3-bis(pentafluorophenyl)-1,3,6,2-triazaalumocane

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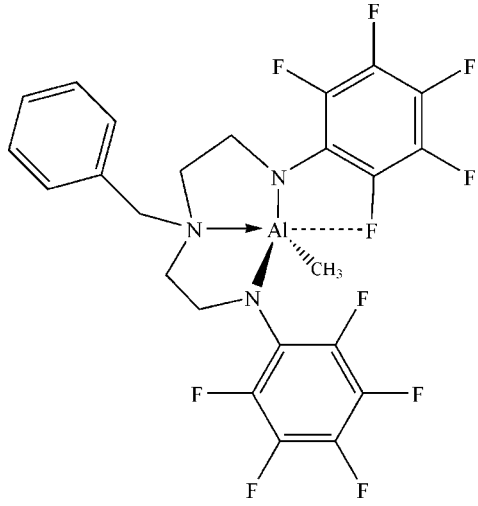
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 12.0.

In the title compound, $[Al(CH_3)(C_{23}H_{15}F_{10}N_3)]$, the Al^{III} atom is coordinated in a distorted tetrahedral geometry by three N atoms from the tridentate amine and by one C atom of the methyl substituent. Further, there is a short intramolecular Al···F contact [2.5717 (11) Å], leading to an overall distorted trigonal–bipyramidal coordination environment around Al^{III}.

Related literature

For general background to the chemistry affording the tridentate ligand *N*-benzyl-*N*′-(pentafluorophenyl)-*N*-{2-[(pentafluorophenyl)amino]ethyl}ethane-1,2-diamine, see: Lermontova *et al.* (2009). Complexes of germanium and tin based on that and the related ligands and their X-ray structures have been described by Huang *et al.* (2011, 2012). For related structures having short Al···F—C contacts, see: Smith *et al.* (2010); Jansen & Mokros (1992). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$[Al(CH_3)(C_{23}H_{15}F_{10}N_3)]$
M_r = 565.39
Monoclinic, $P2_1/c$
a = 7.9530 (14) Å
b = 33.577 (6) Å
c = 8.7247 (15) Å
β = 100.809 (2)°
V = 2288.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 173 K
0.20 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.963, T_{max} = 0.991
19211 measured reflections
4972 independent reflections
4317 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 1.02
4972 reflections
415 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5205).

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supporting information

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6-Benzyl-2-methyl-1,3-bis(pentafluorophenyl)-1,3,6,2-triazaalumocane

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S1. Comment

As a part of our investigation on chemistry of germanium, tin and aluminium complexes based on tridentate ligands (Lermontova *et al.*, 2009; Huang *et al.*, 2011, 2012) we obtained and studied the structure of title compound, [Al[$C_6H_5CH_2N(CH_2CH_2NHC_6F_5)_2$]($CH_3$)].

The aluminium centre and aromatic F18 atom form a short intramolecular contact [2.5717 (11) Å]. Of interest, F18—C18 bond length [1.359 (2) Å] is the longest among ten F—C distances in the structure. Analysis of Cambridge Structural Database (ver. 5.33, August 2012; Allen, 2002) shows that similar but somewhat longer Al···F—C contacts are observed in the structures EKIBIK (2.690 Å, Smith *et al.*, 2010) and YADTEC (2.719 Å, Jansen & Mokros, 1992).

The Al1 atom has trigonal bipyramid coordination environment. Three equatorial positions are occupied by methyl group C10 and trigonal nitrogen atoms N1 and N2. The angles between C10, N1 and N2 atoms range within 112.86 (7)–124.64 (7)°. The aluminium atom is only slightly displaced [0.1937 (9) Å] from the plane of these ligands towards the coordinated tetrahedral donor atom N3. The N3 and F18 atoms lie in the apical positions with an N3—Al1—F18 angle equal to 152.24 (5)°. As expected, the dative N3→Al1 bond length [2.0104 (13) Å] is significantly longer than equatorial nitrogen-aluminium distances [1.8575 (14) and 1.8697 (14) Å].

S2. Experimental

A solution of 0.26 g (0.50 mmol) of $BnN(CH_2CH_2NHC_6F_5)_2$ (Lermontova *et al.*, 2009) in toluene (10 ml) was added dropwise to a solution of 0.25 ml (0.50 mmol) of Me_3Al in toluene (10 ml) under stirring at 243 K. The reaction mixture was allowed to warm to room temperature and stirred overnight. The volatiles were removed under vacuum. The residue was washed by ether (3×5 ml) and dried to give 0.24 g (86%) of $BnN(CH_2CH_2NHC_6F_5)_2AlMe$ as a white solid.

^{1}H NMR ($CDCl_3$): δ -0.56 (br s, 3H, AlMe); 2.88–2.97, 3.00–3.09, 3.57–3.66, 3.67–3.76 (4 m, 8H, NCH_2); 4.03 (s, 2H, NCH_2Ph); 7.29–7.34, 7.42–7.47 (2 m, 5H, Ph). ^{13}C NMR ($CDCl_3$): δ 44.29, 49.94 ($4NCH_2$); 56.01 (NCH_2Ph); 128.77, 129.00, 131.39, 131.55 (Ph). ^{1}H NMR (C_6D_6): δ -0.31 (p, $J_{F—H}$ = 2.4 Hz, 3H, AlMe); 1.95–2.04, 2.10–2.17, 3.08–3.20 (3 m, 8H, NCH_2); 3.34 (s, 2H, NCH_2Ph); 6.53–6.57, 7.00–7.06, 7.07–7.10 (3 m, 5H, Ph). ^{13}C NMR (C_6D_6): δ 49.48, 53.34 ($4NCH_2$); 55.61 (NCH_2Ph); 128.54, 129.24, 129.31, 131.72 (Ph). EI m/*z* 564 (*M*, 5%); 432 (M—Bn, 3%); 91 (Bn, 100%); 42 (AlMe, 78%). Anal. Calcd. for $C_{24}H_{18}AlN_3F_{10}$: C 50.98, H 3.21, N 7.43. Found: C 50.68, H 3.36, N 7.39.

The crystals were obtained from the concentrated toluene solution under storing at 255 K for several days.

S3. Refinement

All H atoms were located in a difference Fourier map and refined isotropically. [Refined C—H distances: 0.90 (2)–0.97 (3) Å for aromatic CH, 0.931 (19)–1.004 (19) Å for CH_2 and 0.92 (3)–0.98 (2) Å for CH_3.]

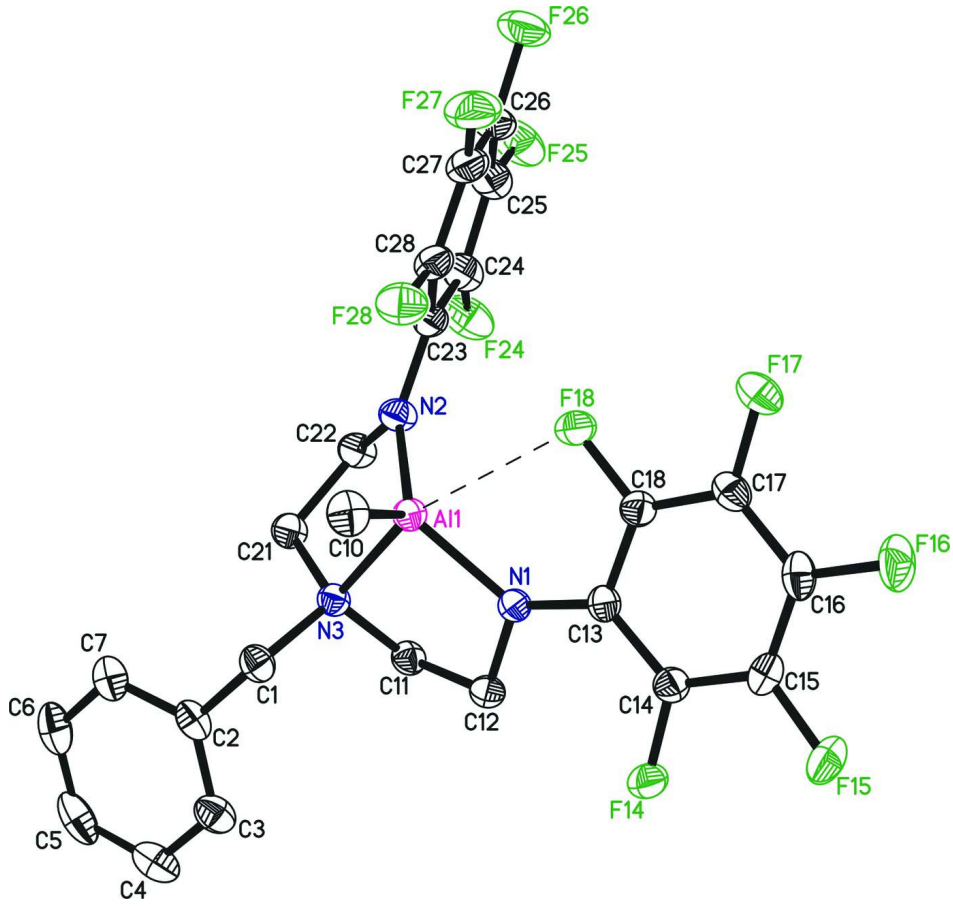

Figure 1

The molecular structure of the title compound, showing the numbering scheme adopted. Displacement ellipsoids are shown at the 50% probability level. The short intramolecular contact Al···F—C is drawn by dashed line. Hydrogen atoms are omitted for clarity.

[*N*-Benzyl-*N*,*N*-bis(pentafluorophenylanide)ethyl]amine -methylaluminium(III)

Crystal data

$[Al(CH_3)(C_{23}H_{15}F_{10}N_3)]$
$M_r = 565.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.9530\ (14)$ Å
$b = 33.577\ (6)$ Å
$c = 8.7247\ (15)$ Å
$\beta = 100.809\ (2)°$
$V = 2288.5\ (7)$ Å^3
$Z = 4$
$F(000) = 1144$
$D_x = 1.641$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8521 reflections
$\theta = 2.5–28.1°$
$\mu = 0.19$ mm^{-1}
$T = 173$ K
Plate, colourless
0.20 × 0.20 × 0.05 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.963$, $T_{max} = 0.991$

19211 measured reflections
4972 independent reflections
4317 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -42 \rightarrow 42$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.094$
$S = 1.02$
4972 reflections
415 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 1.3304P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.55982 (6)	0.117782 (13)	0.49859 (5)	0.02089 (11)
N1	0.60780 (16)	0.16461 (4)	0.39907 (14)	0.0223 (3)
N2	0.68539 (17)	0.07207 (4)	0.47836 (15)	0.0254 (3)
N3	0.74288 (16)	0.13396 (4)	0.67940 (14)	0.0214 (3)
C1	0.6675 (2)	0.15076 (5)	0.81197 (18)	0.0247 (3)
C2	0.7938 (2)	0.16032 (5)	0.95983 (18)	0.0267 (3)
C3	0.8602 (2)	0.19843 (5)	0.9886 (2)	0.0308 (4)
C4	0.9723 (2)	0.20708 (6)	1.1272 (2)	0.0375 (4)
C5	1.0209 (2)	0.17743 (7)	1.2368 (2)	0.0408 (5)
C6	0.9549 (3)	0.13976 (7)	1.2102 (2)	0.0407 (5)
C7	0.8404 (2)	0.13109 (6)	1.0735 (2)	0.0340 (4)
C10	0.3337 (2)	0.11830 (6)	0.5555 (2)	0.0304 (4)
C11	0.84769 (19)	0.16404 (5)	0.61234 (18)	0.0236 (3)
C12	0.7313 (2)	0.19083 (5)	0.49746 (18)	0.0232 (3)
C13	0.51390 (18)	0.17824 (5)	0.26115 (17)	0.0212 (3)
C14	0.4895 (2)	0.21746 (5)	0.20674 (18)	0.0235 (3)
C15	0.3887 (2)	0.22716 (5)	0.06498 (19)	0.0261 (3)
C16	0.3087 (2)	0.19796 (5)	−0.03367 (18)	0.0279 (3)
C17	0.3261 (2)	0.15883 (5)	0.01513 (18)	0.0257 (3)
C18	0.4249 (2)	0.15007 (5)	0.15781 (18)	0.0235 (3)
C21	0.8424 (2)	0.09669 (5)	0.72549 (19)	0.0258 (3)

C22	0.8566 (2)	0.07283 (5)	0.58014 (19)	0.0270 (3)
C23	0.6498 (2)	0.04053 (5)	0.37471 (18)	0.0274 (3)
C24	0.7699 (2)	0.01889 (5)	0.3099 (2)	0.0338 (4)
C25	0.7253 (3)	−0.01322 (6)	0.2104 (2)	0.0405 (5)
C26	0.5577 (3)	−0.02420 (5)	0.1651 (2)	0.0408 (5)
C27	0.4342 (3)	−0.00290 (5)	0.2209 (2)	0.0371 (4)
C28	0.4803 (2)	0.02780 (5)	0.3244 (2)	0.0304 (4)
F14	0.56225 (13)	0.24841 (3)	0.29513 (11)	0.0310 (2)
F15	0.36334 (13)	0.26570 (3)	0.02492 (12)	0.0354 (2)
F16	0.21053 (13)	0.20771 (3)	−0.17192 (11)	0.0392 (3)
F17	0.24581 (13)	0.12973 (3)	−0.07535 (12)	0.0371 (2)
F18	0.43879 (13)	0.11143 (3)	0.20488 (11)	0.0309 (2)
F24	0.93701 (14)	0.02933 (4)	0.34006 (13)	0.0452 (3)
F25	0.84828 (18)	−0.03270 (4)	0.15369 (15)	0.0569 (4)
F26	0.51315 (19)	−0.05520 (3)	0.06690 (14)	0.0553 (4)
F27	0.26773 (16)	−0.01208 (3)	0.17435 (14)	0.0492 (3)
F28	0.35477 (13)	0.04643 (3)	0.37978 (13)	0.0382 (3)
H112	0.917 (2)	0.1790 (5)	0.6947 (19)	0.018 (4)*
H122	0.803 (2)	0.2058 (5)	0.436 (2)	0.020 (4)*
H121	0.675 (2)	0.2111 (5)	0.554 (2)	0.020 (4)*
H222	0.894 (2)	0.0457 (6)	0.615 (2)	0.027 (5)*
H3	0.833 (2)	0.2184 (5)	0.912 (2)	0.025 (4)*
H12	0.605 (2)	0.1750 (6)	0.774 (2)	0.030 (5)*
H111	0.921 (2)	0.1507 (5)	0.558 (2)	0.024 (4)*
H212	0.778 (2)	0.0818 (5)	0.790 (2)	0.028 (5)*
H221	0.950 (2)	0.0841 (6)	0.530 (2)	0.028 (5)*
H11	0.585 (2)	0.1307 (6)	0.834 (2)	0.031 (5)*
H211	0.955 (2)	0.1031 (6)	0.787 (2)	0.029 (5)*
H7	0.792 (2)	0.1051 (6)	1.055 (2)	0.031 (5)*
H103	0.310 (3)	0.1447 (7)	0.596 (3)	0.050 (6)*
H4	1.012 (3)	0.2322 (7)	1.140 (2)	0.036 (5)*
H5	1.097 (3)	0.1834 (6)	1.326 (3)	0.045 (6)*
H102	0.322 (3)	0.0973 (7)	0.630 (3)	0.048 (6)*
H6	0.982 (3)	0.1182 (7)	1.285 (3)	0.060 (7)*
H101	0.255 (3)	0.1136 (8)	0.465 (3)	0.064 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0208 (2)	0.0198 (2)	0.0209 (2)	0.00011 (17)	0.00084 (17)	0.00025 (17)
N1	0.0248 (6)	0.0209 (6)	0.0193 (6)	−0.0020 (5)	−0.0004 (5)	0.0001 (5)
N2	0.0265 (7)	0.0217 (6)	0.0254 (7)	0.0034 (5)	−0.0016 (5)	−0.0024 (5)
N3	0.0222 (6)	0.0213 (6)	0.0201 (6)	0.0019 (5)	0.0022 (5)	−0.0006 (5)
C1	0.0233 (7)	0.0286 (8)	0.0216 (7)	0.0019 (6)	0.0028 (6)	−0.0012 (6)
C2	0.0231 (7)	0.0362 (9)	0.0208 (7)	0.0034 (6)	0.0042 (6)	−0.0041 (6)
C3	0.0287 (8)	0.0338 (9)	0.0293 (8)	0.0055 (7)	0.0038 (7)	−0.0060 (7)
C4	0.0307 (9)	0.0450 (11)	0.0368 (10)	−0.0016 (8)	0.0066 (7)	−0.0164 (8)
C5	0.0278 (9)	0.0717 (14)	0.0219 (8)	0.0035 (9)	0.0016 (7)	−0.0107 (9)

C6	0.0403 (10)	0.0600 (13)	0.0212 (8)	0.0057 (9)	0.0042 (7)	0.0045 (8)
C7	0.0361 (9)	0.0418 (10)	0.0242 (8)	0.0004 (8)	0.0059 (7)	0.0013 (7)
C10	0.0238 (8)	0.0363 (10)	0.0303 (9)	0.0002 (7)	0.0031 (7)	0.0010 (8)
C11	0.0217 (7)	0.0258 (8)	0.0223 (7)	−0.0029 (6)	0.0020 (6)	−0.0018 (6)
C12	0.0238 (7)	0.0222 (7)	0.0230 (7)	−0.0033 (6)	0.0024 (6)	−0.0022 (6)
C13	0.0200 (7)	0.0241 (7)	0.0201 (7)	0.0002 (6)	0.0051 (5)	0.0007 (6)
C14	0.0241 (7)	0.0227 (7)	0.0237 (7)	−0.0022 (6)	0.0049 (6)	−0.0006 (6)
C15	0.0261 (8)	0.0254 (8)	0.0273 (8)	0.0012 (6)	0.0065 (6)	0.0075 (6)
C16	0.0229 (7)	0.0391 (9)	0.0205 (7)	0.0007 (7)	0.0007 (6)	0.0063 (7)
C17	0.0232 (7)	0.0313 (8)	0.0223 (7)	−0.0039 (6)	0.0034 (6)	−0.0045 (6)
C18	0.0250 (7)	0.0221 (7)	0.0236 (7)	0.0008 (6)	0.0054 (6)	−0.0003 (6)
C21	0.0262 (8)	0.0249 (8)	0.0237 (8)	0.0044 (6)	−0.0018 (6)	0.0008 (6)
C22	0.0256 (8)	0.0256 (8)	0.0274 (8)	0.0059 (6)	−0.0017 (6)	−0.0017 (6)
C23	0.0370 (9)	0.0188 (7)	0.0238 (8)	0.0026 (6)	−0.0005 (6)	0.0020 (6)
C24	0.0374 (9)	0.0299 (9)	0.0310 (9)	0.0079 (7)	−0.0020 (7)	−0.0021 (7)
C25	0.0567 (12)	0.0293 (9)	0.0326 (9)	0.0163 (8)	0.0013 (8)	−0.0025 (7)
C26	0.0650 (13)	0.0200 (8)	0.0313 (9)	0.0015 (8)	−0.0064 (9)	−0.0029 (7)
C27	0.0492 (11)	0.0227 (8)	0.0343 (9)	−0.0062 (8)	−0.0050 (8)	0.0036 (7)
C28	0.0389 (9)	0.0200 (8)	0.0302 (8)	−0.0011 (7)	0.0008 (7)	0.0029 (6)
F14	0.0387 (5)	0.0212 (5)	0.0299 (5)	−0.0042 (4)	−0.0014 (4)	0.0004 (4)
F15	0.0387 (6)	0.0295 (5)	0.0362 (5)	0.0026 (4)	0.0024 (4)	0.0130 (4)
F16	0.0365 (6)	0.0502 (7)	0.0257 (5)	−0.0025 (5)	−0.0074 (4)	0.0107 (5)
F17	0.0392 (6)	0.0393 (6)	0.0286 (5)	−0.0072 (4)	−0.0045 (4)	−0.0082 (4)
F18	0.0384 (5)	0.0214 (5)	0.0300 (5)	−0.0022 (4)	−0.0009 (4)	−0.0010 (4)
F24	0.0363 (6)	0.0525 (7)	0.0453 (6)	0.0106 (5)	0.0041 (5)	−0.0165 (5)
F25	0.0693 (8)	0.0504 (7)	0.0465 (7)	0.0275 (6)	−0.0010 (6)	−0.0186 (6)
F26	0.0880 (10)	0.0271 (6)	0.0431 (7)	0.0011 (6)	−0.0074 (6)	−0.0131 (5)
F27	0.0533 (7)	0.0347 (6)	0.0531 (7)	−0.0174 (5)	−0.0067 (6)	−0.0040 (5)
F28	0.0328 (5)	0.0360 (6)	0.0452 (6)	−0.0056 (4)	0.0054 (5)	−0.0057 (5)

Geometric parameters (Å, º)

Al1—N2	1.8575 (14)	C11—H111	0.931 (19)
Al1—N1	1.8697 (14)	C12—H122	0.990 (17)
Al1—C10	1.9536 (18)	C12—H121	0.995 (17)
Al1—N3	2.0104 (13)	C13—C14	1.401 (2)
Al1—F18	2.5717 (11)	C13—C18	1.403 (2)
N1—C13	1.3704 (19)	C14—F14	1.3573 (17)
N1—C12	1.4700 (19)	C14—C15	1.381 (2)
N2—C23	1.387 (2)	C15—F15	1.3457 (18)
N2—C22	1.480 (2)	C15—C16	1.379 (2)
N3—C21	1.4947 (19)	C16—F16	1.3486 (18)
N3—C11	1.497 (2)	C16—C17	1.380 (2)
N3—C1	1.5086 (19)	C17—F17	1.3404 (18)
C1—C2	1.514 (2)	C17—C18	1.373 (2)
C1—H12	0.976 (19)	C18—F18	1.3591 (18)
C1—H11	0.99 (2)	C21—C22	1.522 (2)
C2—C3	1.389 (2)	C21—H212	0.972 (19)

C2—C7	1.395 (2)	C21—H211	0.980 (19)
C3—C4	1.392 (2)	C22—H222	0.987 (19)
C3—H3	0.946 (19)	C22—H221	1.004 (19)
C4—C5	1.384 (3)	C23—C24	1.401 (2)
C4—H4	0.90 (2)	C23—C28	1.404 (2)
C5—C6	1.372 (3)	C24—F24	1.352 (2)
C5—H5	0.91 (2)	C24—C25	1.388 (3)
C6—C7	1.390 (3)	C25—F25	1.345 (2)
C6—H6	0.97 (3)	C25—C26	1.368 (3)
C7—H7	0.96 (2)	C26—F26	1.353 (2)
C10—H103	0.98 (2)	C26—C27	1.375 (3)
C10—H102	0.98 (2)	C27—F27	1.346 (2)
C10—H101	0.92 (3)	C27—C28	1.374 (2)
C11—C12	1.524 (2)	C28—F28	1.342 (2)
C11—H112	0.963 (17)		

N2—Al1—N1	119.38 (6)	H112—C11—H111	107.5 (14)
N2—Al1—C10	124.64 (7)	N1—C12—C11	106.70 (12)
N1—Al1—C10	112.86 (7)	N1—C12—H122	112.0 (10)
N2—Al1—N3	88.55 (6)	C11—C12—H122	108.6 (10)
N1—Al1—N3	87.50 (6)	N1—C12—H121	112.8 (10)
C10—Al1—N3	111.33 (7)	C11—C12—H121	110.5 (10)
N2—Al1—F18	86.80 (5)	H122—C12—H121	106.2 (14)
N1—Al1—F18	71.20 (4)	N1—C13—C14	129.02 (14)
C10—Al1—F18	93.65 (6)	N1—C13—C18	117.72 (14)
N3—Al1—F18	152.24 (5)	C14—C13—C18	113.25 (13)
C13—N1—C12	120.47 (12)	F14—C14—C15	116.26 (14)
C13—N1—Al1	124.31 (10)	F14—C14—C13	120.67 (13)
C12—N1—Al1	113.87 (9)	C15—C14—C13	123.05 (14)
C23—N2—C22	117.19 (13)	F15—C15—C16	119.51 (14)
C23—N2—Al1	130.18 (11)	F15—C15—C14	119.53 (14)
C22—N2—Al1	112.29 (10)	C16—C15—C14	120.92 (15)
C21—N3—C11	111.39 (12)	F16—C16—C15	120.50 (15)
C21—N3—C1	111.92 (12)	F16—C16—C17	120.99 (15)
C11—N3—C1	112.20 (12)	C15—C16—C17	118.46 (14)
C21—N3—Al1	104.70 (9)	F17—C17—C18	120.41 (15)
C11—N3—Al1	104.48 (9)	F17—C17—C16	120.21 (14)
C1—N3—Al1	111.67 (9)	C18—C17—C16	119.37 (14)
N3—C1—C2	115.91 (12)	F18—C18—C17	118.59 (13)
N3—C1—H12	107.5 (11)	F18—C18—C13	116.52 (13)
C2—C1—H12	109.0 (11)	C17—C18—C13	124.89 (15)
N3—C1—H11	105.8 (11)	N3—C21—C22	109.57 (12)
C2—C1—H11	109.8 (11)	N3—C21—H212	106.1 (11)
H12—C1—H11	108.7 (15)	C22—C21—H212	110.1 (11)
C3—C2—C7	118.60 (15)	N3—C21—H211	110.3 (11)
C3—C2—C1	121.23 (15)	C22—C21—H211	111.8 (11)
C7—C2—C1	120.12 (16)	H212—C21—H211	108.7 (15)
C2—C3—C4	120.60 (18)	N2—C22—C21	107.78 (13)

C2—C3—H3	119.8 (11)	N2—C22—H222	111.0 (10)
C4—C3—H3	119.5 (11)	C21—C22—H222	107.3 (11)
C5—C4—C3	120.01 (19)	N2—C22—H221	114.4 (10)
C5—C4—H4	122.9 (13)	C21—C22—H221	110.1 (11)
C3—C4—H4	117.1 (13)	H222—C22—H221	106.0 (15)
C6—C5—C4	119.88 (17)	N2—C23—C24	126.01 (16)
C6—C5—H5	121.3 (14)	N2—C23—C28	120.22 (15)
C4—C5—H5	118.9 (14)	C24—C23—C28	113.77 (15)
C5—C6—C7	120.41 (19)	F24—C24—C25	116.72 (16)
C5—C6—H6	123.0 (15)	F24—C24—C23	120.44 (15)
C7—C6—H6	116.6 (15)	C25—C24—C23	122.82 (17)
C6—C7—C2	120.45 (19)	F25—C25—C26	119.94 (17)
C6—C7—H7	121.0 (12)	F25—C25—C24	119.32 (19)
C2—C7—H7	118.6 (12)	C26—C25—C24	120.70 (18)
Al1—C10—H103	109.9 (13)	F26—C26—C25	121.03 (19)
Al1—C10—H102	111.6 (13)	F26—C26—C27	120.31 (18)
H103—C10—H102	111.6 (19)	C25—C26—C27	118.66 (16)
Al1—C10—H101	106.8 (16)	F27—C27—C28	119.72 (18)
H103—C10—H101	108 (2)	F27—C27—C26	120.11 (16)
H102—C10—H101	108 (2)	C28—C27—C26	120.17 (18)
N3—C11—C12	109.96 (12)	F28—C28—C27	117.51 (16)
N3—C11—H112	110.2 (10)	F28—C28—C23	118.72 (14)
C12—C11—H112	112.0 (10)	C27—C28—C23	123.77 (17)
N3—C11—H111	108.8 (11)	C18—F18—Al1	102.48 (8)
C12—C11—H111	108.3 (11)		