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Aluminium(III) amidinates formed from reactions of 'AlCl' with lithium amidinates

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The disproportionation of $AlCl(THF)_n$ (THF is tetrahydrofuran) in the presence of lithium amidinate species gives aluminium(III) amidinate complexes with partial or full chloride substitution. Three aluminium amidinate complexes formed during the reaction between aluminium monochloride and lithium amidinates are presented. The homoleptic complex tris(*N*,*N*′-diisopropylbenzimidamido)aluminium(III), $[Al(C_{13}H_{19}N_2)_3]$ or $Al\{PhC[N(i\text{-}Pr)]_2\}_3$, (I), crystallizes from the same solution as the heteroleptic complex chloridobis(*N*,*N*′-diisopropylbenzimidamido)aluminium(III), $[Al(C_{13}H_{19}N_2)_2Cl]$ or $Al\{PhC[N(i\text{-}Pr)]_2\}_2Cl$, (II). Both have two crystallographically independent molecules per asymmetric unit (Z' = 2) and (I) shows disorder in four of its N(i-Pr) groups. Changing the ligand substituent to the bulkier cyclohexyl allows the isolation of the partial THF solvate chloridobis(*N*,*N*′-dicyclohexylbenzimidamido)aluminium(III) tetrahydrofuran 0.675-solvate, $[Al(C_{19}H_{27}N_2)_2Cl]\cdot0.675C_4H_8O$ or $Al[PhC(NCy)_2]_2Cl\cdot0.675THF$, (III). Despite having a two-fold rotation axis running through its Al and Cl atoms, (III) has a similar molecular structure to that of (II).

Keywords: crystal structure; aluminium(III) amidinates; disorder.

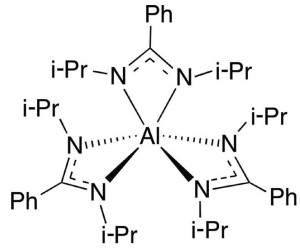
1. Introduction

Metastable aluminium(I) halides are known to undergo disproportionation reactions to form aluminium metal and aluminium trihalides at temperatures above 195 K [equation (1) of Schnoeckel (2010)], *i.e.*

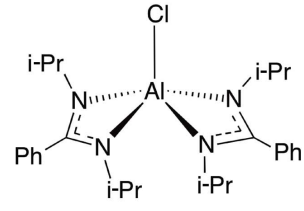
$$3AlCl \rightarrow 2Al + AlCl_3.$$

In order to stabilize metalloid aluminium clusters ($Al_nR_mX_y$ or Al_nR_m, where $n > m + y$), nucleophilic ligand compounds with the potential to undergo ligand metathesis reactions are added. Due to the high reactivity of many aluminium monohalide solutions, these reactions are typically initiated in solution at 195 K and with subsequent warming to room temperature.

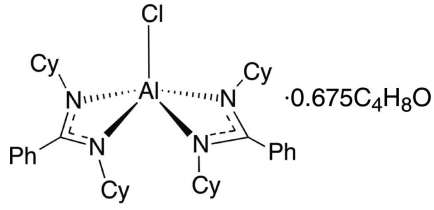
The majority of ligands used in metalloid aluminium cluster chemistry have been monodentate nitrogen- or oxygen-based species. To study the effect of ligand denticity on metalloid aluminium cluster formation, amidinate ligands were selected for use in the present study. Amidinate and guanidate ligands containing bulky alkyl groups have previously been used to stabilize reduced oxidation state alane derivatives and are known to form crystalline aluminium(III) compounds in the presence of aluminium monohalides (Bonyhady *et al.*, 2010; Dange *et al.*, 2012). Nitrogen-bound alkyl groups of varying steric bulk (isopropyl and cyclohexyl) have been selected in the present study in an attempt to probe the effect of ligand sterics on metal-cluster formation. Lithium amidinates were generated *in situ* through reaction of phenyllithium with the corresponding carbodiimide reagent (Luo *et al.*, 2002). The reaction of $AlCl(THF)_n$ (THF is tetrahydrofuran) with lithium amidinates resulted in the formation of three novel aluminium(III) amidinate complexes, (I)–(III) (see Scheme).



(I)



(II)



(III)

2. Experimental

2.1. Synthesis and crystallization

For the preparation of $Al\{PhC[N(i\text{-}Pr)]_2\}_3$, (I), and $Al\{PhC[N(i\text{-}Pr)]_2\}_2Cl$, (II), $Li\{PhC[N(i\text{-}Pr)]_2\}$ (1.45 g, 7.0 mmol) was dissolved in toluene (10 ml) and cooled to 195 K. To this suspension was added cold $AlCl(THF)_n$ (6.6 mmol, 17.6 ml of

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Table 1
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$[Al(C_{13}H_{19}N_2)_3]$	$[Al(C_{13}H_{19}N_2)_2Cl]$	$[Al(C_{19}H_{27}N_2)_2Cl]\cdot0.675C_4H_8O$
M_r	636.88	469.03	677.95
Crystal system, space group	Orthorhombic, *Pccn*	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$
Temperature (K)	150	100	150
a, b, c (Å)	31.286 (3), 33.409 (3), 14.3488 (12)	19.205 (1), 16.4832 (9), 17.8498 (10)	22.042 (4), 16.007 (3), 12.852 (2)
α, β, γ (°)	90, 90, 90	90, 106.287 (1), 90	90, 115.396 (2), 90
V (Å^3)	14998 (2)	5423.8 (5)	4096.6 (12)
Z	16	8	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.09	0.19	0.15
Crystal size (mm)	0.35 × 0.30 × 0.11	0.21 × 0.20 × 0.14	0.40 × 0.34 × 0.12
Data collection			
Diffractometer	Bruker SMART APEXII area-detector diffractometer	Bruker SMART APEXII area-detector diffractometer	Bruker SMART APEXII area-detector diffractometer
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2008)	Multi-scan (*TWINABS*; Sheldrick, 2008)	Multi-scan (*SADABS*; Sheldrick, 2008)
T_{min}, T_{max}	0.930, 0.990	0.858, 0.973	0.872, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	242499, 14753, 10759	100296, 10641, 7375	20863, 4038, 3577
R_{int}	0.086	0.080	0.023
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617	0.617
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.087, 1.03	0.046, 0.090, 1.00	0.037, 0.082, 1.00
No. of reflections	14753	10641	4038
No. of parameters	901	593	200
No. of restraints	58	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.23	0.45, −0.31	0.28, −0.25

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXS97* (Sheldrick, 2008), *XSHELL* (Bruker, 2004) and *SHELXL2012* (Sheldrick, 2012).

a 380 mmol solution in toluene–THF, 3:1 *v*/*v*) *via* syringe. The resultant brown reaction mixture was warmed to room temperature over the course of 2 h and then heated to 333 K for 16 h. The reaction mixture was subsequently cooled to room temperature and the solvent removed *in vacuo*. Extraction of the brown residue into pentane (50 ml) and filtration *via* cannula resulted in a dark-brown solution. This solution was concentrated to approximately 10 ml, from which colourless blocks of (I) were obtained. Further filtration and concentration of the solution resulted in a few pale-yellow crystals of (II).

For the preparation of $Al[PhC(NCy)_2]_2Cl$, (III), dicyclohexylcarbodiimide (1.044 g, 5.06 mmol) was dissolved in toluene (10 ml) at room temperature. To this solution was added phenyllithium (5.06 mmol, 2.5 ml of a 2.0 *M* solution in dibutyl ether) and the reaction mixture stirred for 1 h. The resultant yellow solution was cooled to 195 K and cold $AlCl(THF)_n$ (4.82 mmol, 20 ml of a 240 m*M* solution in toluene–THF, 3:1 *v*/*v*) was added quickly *via* syringe. The resultant brown solution was warmed slowly to room temperature overnight. The reaction mixture was subsequently concentrated to *ca* 10 ml, filtered *via* cannula and stored at 258 K for 10 d, after which a few pale-yellow plates of (III) formed on the glass wall.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were positioned geometrically and refined in riding mode, with C—H = 0.95, 0.98, 0.99, and 1.00 Å for sp^2, CH_3, CH_2, and tertiary C—H, respectively. $U_{iso}(H)$ values were set at $1.5U_{eq}(C)$ for CH_3 groups and at $1.2U_{eq}(C)$ otherwise. Four isopropyl groups in (I) were modelled as disordered over two sites. A total of 58 rigid-bond, equivalent displacement parameter, and distance restraints were required to give a chemically sensible model.

3. Results and discussion

The reaction of $AlCl(THF)_n$ with $Li\{PhC[N(i\text{-}Pr)]_2\}$ gave two separate crystalline products. The initial product formed was the homoleptic aluminium amidinate $Al\{PhC[N(i\text{-}Pr)]_2\}_3$, (I), which crystallized out of the reaction mixture as colourless blocks (Fig. 1). Two crystallographically independent molecules ($Z' = 2$) with similar core coordination geometries are present within the crystal structure. Each has a central six-coordinate Al^{III} cation, which is distorted from octahedral geometry due to the demands of bonding to three chelating ligands. The Al—N bond lengths are in the range 1.9826 (15)–2.0344 (15) Å in one molecule and 2.0156 (15)–2.0382 (15) Å in the other (Table 2). Of these, the Al1—N1*A* bond is noticably shorter than the others. However, as this is one of four N atoms which is bound to a disordered isopropyl group, this may not be chemically significant. The N—C(N) bond lengths in the amidinate ligands are in the ranges 1.320 (2)–1.330 (2) and 1.326 (2)–1.329 (2) Å for the two independent molecules (see *Supplementary materials*). The Al—N metric

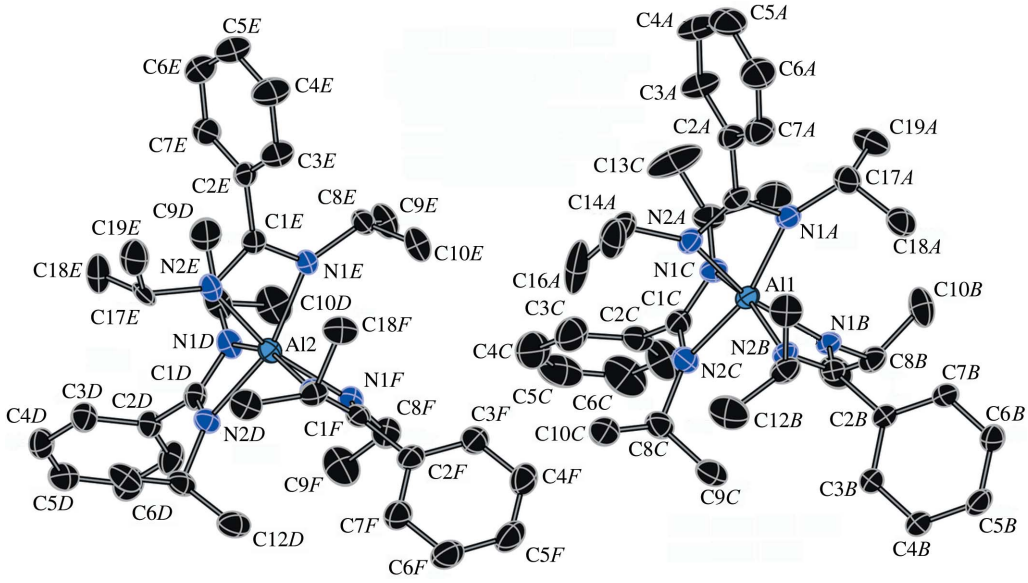

Figure 1
A view of (I), showing the two crystallographically independent molecules and the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms and the isopropyl groups of the minor-disorder components have been omitted for clarity. (Colour key in the electronic version of the paper: aluminium = light blue, carbon = black and nitrogen = blue.)

Table 2
Selected bond lengths (Å) for (I).

Al1—N1*A*	1.9826 (15)	Al2—N2*E*	2.0156 (15)
Al1—N1*C*	2.0168 (15)	Al2—N1*E*	2.0185 (15)
Al1—N2*B*	2.0220 (14)	Al2—N2*D*	2.0267 (15)
Al1—N1*B*	2.0299 (14)	Al2—N2*F*	2.0279 (14)
Al1—N2*C*	2.0310 (16)	Al2—N1*F*	2.0295 (15)
Al1—N2*A*	2.0344 (15)	Al2—N1*D*	2.0382 (15)

parameters are very similar to those of the homoleptic Al^{III} guanidinate complex reported by Kenney *et al.* (2005); indeed, the bond lengths and angles agree to within ±0.02 Å and ±1°, respectively (except for the differing guanidinate C—N connectivity).

From the same reaction mixture that formed (I), yellow plates of the heteroleptic Al{PhC[N(i-Pr)]$_2$}$_2$Cl complex, (II), formed upon further cooling of the solution (Fig. 2). Again, there are two crystallographically independent (Z' = 2) but geometrically similar molecules present. Differences between the two molecules are most pronounced in the orientations of the isopropyl substituents. Both display a five-coordinate Al^{III} centre with slightly wider N—Al—N chelate bite angles than those seen in six-coordinate (I) (all approximately 68°, compared with approximately 65.5°). The Al—N bond lengths in (II) are in the ranges 1.9102 (18)–1.9932 (18) and 1.9046 (18)–2.0076 (18) Å, with Al—Cl bond lengths of 2.2046 (8) and 2.2027 (8) Å for the two molecules (Table 3). As expected, the Al—N distances are thus systematically shorter than those in the higher coordination number complex, (I). The N—C(N) bond lengths are in the range 1.317 (3)–1.346 (3) Å and the N—$C_{i\text{-Pr}}$ bond lengths are in the range 1.464 (3)–1.477 (3) Å. The bond lengths in (II) are in close agreement with those in the heteroleptic aluminium amidinate Al{MeC[N(i-Pr)]$_2$}$_2$Cl reported by Coles *et al.* (1997). Despite the size and electronic differences between Ph and Me, the structural differences between (II) and Al{MeC[N(i-Pr)]$_2$}$_2$Cl are minor, resulting in bond lengths that generally agree to within 0.02 Å.

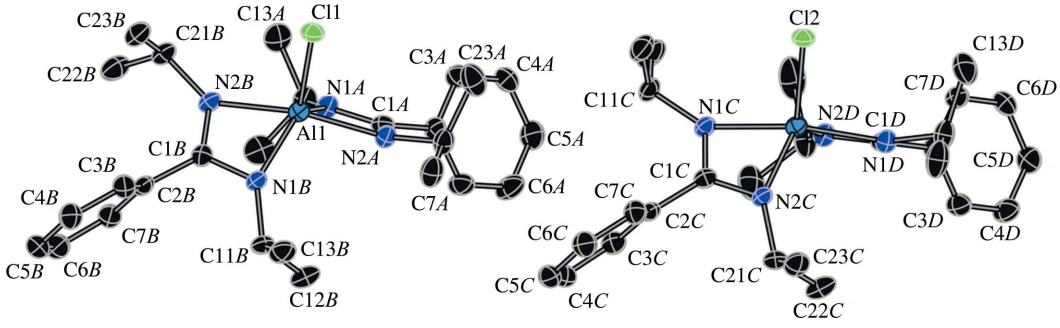

Figure 2
A view of (II), showing the two crystallographically independent molecules and the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. (Colour key in the electronic version of the paper: aluminium = light blue, carbon = black, chlorine = green and nitrogen = blue.)

Table 3
Selected geometric parameters (Å, °) for (II).

Al1—N1*A*	1.9102 (18)	Al2—N2*D*	1.9046 (18)
Al1—N1*B*	1.9157 (18)	Al2—N2*C*	1.9194 (18)
Al1—N2*B*	1.9791 (18)	Al2—N1*D*	2.0039 (18)
Al1—N2*A*	1.9932 (18)	Al2—N1*C*	2.0076 (18)
Al1—Cl1	2.2046 (8)	Al2—Cl2	2.2027 (8)
N1*A*—Al1—N1*B*	122.18 (8)	N2*D*—Al2—N2*C*	117.22 (8)
N1*A*—Al1—N2*B*	103.84 (8)	N2*D*—Al2—N1*D*	68.20 (7)
N1*B*—Al1—N2*B*	68.12 (7)	N2*C*—Al2—N1*D*	105.37 (8)
N1*A*—Al1—N2*A*	68.06 (7)	N2*D*—Al2—N1*C*	106.71 (8)
N1*B*—Al1—N2*A*	106.08 (8)	N2*C*—Al2—N1*C*	67.95 (7)
N2*B*—Al1—N2*A*	166.28 (8)	N1*D*—Al2—N1*C*	169.27 (8)
N1*A*—Al1—Cl1	118.73 (6)	N2*D*—Al2—Cl2	119.70 (6)
N1*B*—Al1—Cl1	119.03 (6)	N2*C*—Al2—Cl2	123.08 (6)
N2*B*—Al1—Cl1	95.62 (6)	N1*D*—Al2—Cl2	95.41 (6)
N2*A*—Al1—Cl1	98.02 (6)	N1*C*—Al2—Cl2	95.31 (6)

Table 4
Selected geometric parameters (Å, °) for (III).

Cl1—Al1	2.1855 (9)	Al1—N1	1.9952 (12)
Al1—N2	1.9260 (12)		
N2—Al1—N2^{i}	112.73 (8)	N1—Al1—N1^{i}	167.92 (8)
N2—Al1—N1	68.04 (5)	N2—Al1—Cl1	123.64 (4)
N2^{i}—Al1—N1	104.92 (5)	N1—Al1—Cl1	96.04 (4)

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

The reaction between $AlCl(THF)_n$ and $Li[PhC(NCy)_2]$ resulted in a dark-brown solution which yielded $Al[PhC(NCy)_2]_2Cl$, (III), as yellow plate crystals (Fig. 3). Each molecule is bisected by a twofold rotation axis that runs through the Al and Cl atoms, and thus the two $PhC(NCy)_2$ ligands are identical and have $Z' = 0.5$. The central Al^{III} cation in (III) has a similar coordination geometry to that of (II), with Al—N bond lengths of 1.9260 (12) and 1.9952 (12) Å, and an Al—Cl bond length of 2.1855 (9) Å (Table 4). The N—C(N) bond lengths are 1.3213 (18) and 1.3407 (18) Å, and the N—$C_{i\text{-Pr}}$ bond lengths are 1.4647 (18) and 1.4680 (18) Å. The bond lengths and angles in (III) are quite similar to those in Al[*t*-BuC(NCy)$_2$]$_2$Cl (Coles *et al.*, 1997). In general, the bond lengths in (III) are within 0.02 Å of those reported in Al[*t*-BuC(NCy)$_2$]$_2$Cl, and the bond angles in (III) are similarly close. The amidinate ligand groups in (II) and (III) are also similar, such that the bond angles and lengths between the ligand and Al^{III} cation generally agree to within 1° and 0.01 Å, respectively. The structure of (III) contains THF solvent, which was found to be both disordered and partially present. As this could not be refined satisfactorily, the SQUEEZE procedure of *PLATON* (Spek, 2009) was used to remove the effects of approximately 2.7 THF molecules from the unit cell. The disorder of these molecules may be related to the channel solvate nature of the packed structure, with the channels running parallel to the crystallographic *c* direction.

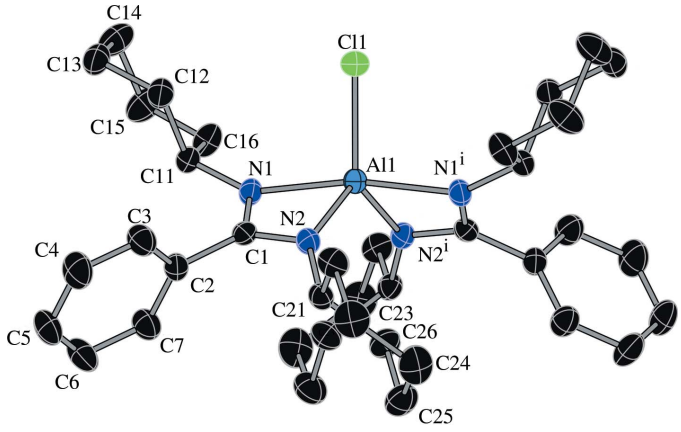

Figure 3
The molecular structure of (III), showing the coordination geometry at the Al^{III} cation and the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. The colour key is as in Fig. 2. [Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.]

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: KY3026). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Computing details

For all compounds, data collection: *APEX2* (Bruker, 2010); cell refinement: *APEX2* (Bruker, 2010); data reduction: *APEX2* and *SAINT* (Bruker, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2012); molecular graphics: XSHEL (Bruker, 2004); software used to prepare material for publication: *APEX2* (Bruker, 2010) and *SHELXL2012* (Sheldrick, 2012).

(AlPhCNiPr23) Tris(*N*,*N*′-diisopropylbenzimidamido)aluminium(III)

Crystal data

$[Al(C_{13}H_{19}N_2)_3]$
M_r = 636.88
Orthorhombic, *Pccn*
a = 31.286 (3) Å
b = 33.409 (3) Å
c = 14.3488 (12) Å
V = 14998 (2) Å^3
Z = 16
$F(000)$ = 5536
D_x = 1.128 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 18169 reflections
θ = 2.3–22.3°
μ = 0.09 mm^{-1}
T = 150 K
Prism, colourless
0.35 × 0.30 × 0.11 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 11.198 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (TWINABS; Sheldrick, 2008)
T_{min} = 0.930, T_{max} = 0.990
242499 measured reflections
14753 independent reflections
10759 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 26.0°, θ_{min} = 1.7°
h = 0→38
k = 0→41
l = 0→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.087
S = 1.03
14753 reflections
901 parameters
58 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 9.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Special details

Experimental. Crystal was split into 2 domains tilted \sim5° from each other. After integration of the twin, reflections were merged into single domain set and used in all further refinements. Using 2 domains reflection set yields worse agreement between calculated and observed intensities.

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. 4 of 12 iso-propyl groups are disordered in 2 alternatiove orientations which geometry was restrained to be similar to each other and anisotropic adp's were retrained to rigid body motions.

H atoms were positioned from geometric consideration and refined as riding on the attached atoms with orientation of CH3 groups optimized. U_{iso} of H atoms were constrained to value 20% larger than Ueqv of attached atoms (50% larger for CH3 groups).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.37698 (2)	0.36642 (2)	0.11857 (4)	0.02437 (12)	
C1A	0.37432 (6)	0.29394 (5)	0.09789 (12)	0.0284 (4)	
C2A	0.37184 (6)	0.24948 (6)	0.08663 (13)	0.0338 (4)	
C3A	0.40335 (7)	0.22501 (6)	0.12315 (15)	0.0489 (6)	
H3A	0.4276	0.2365	0.1528	0.059*	
C4A	0.39974 (9)	0.18382 (6)	0.11669 (17)	0.0598 (7)	
H4A	0.4215	0.1672	0.1420	0.072*	
C5A	0.36490 (8)	0.16680 (6)	0.07382 (17)	0.0568 (7)	
H5A	0.3623	0.1385	0.0706	0.068*	
C6A	0.33390 (8)	0.19065 (6)	0.03580 (16)	0.0527 (6)	
H6A	0.3101	0.1789	0.0052	0.063*	
C7A	0.33738 (7)	0.23199 (6)	0.04205 (14)	0.0417 (5)	
H7A	0.3158	0.2484	0.0154	0.050*	
N1A	0.35255 (5)	0.31477 (4)	0.16089 (10)	0.0285 (3)	
C8A	0.42881 (9)	0.30258 (13)	−0.0230 (2)	0.0388 (6)	0.866 (6)
H8A	0.4263	0.2727	−0.0245	0.047*	0.866 (6)
C9A	0.41914 (8)	0.31832 (12)	−0.11927 (17)	0.0531 (9)	0.866 (6)
H9A1	0.3900	0.3108	−0.1369	0.080*	0.866 (6)
H9A2	0.4394	0.3069	−0.1640	0.080*	0.866 (6)
H9A3	0.4217	0.3476	−0.1194	0.080*	0.866 (6)
C10A	0.47426 (9)	0.31317 (15)	0.0056 (2)	0.0755 (13)	0.866 (6)
H10A	0.4765	0.3422	0.0149	0.113*	0.866 (6)
H10B	0.4942	0.3048	−0.0434	0.113*	0.866 (6)
H10C	0.4814	0.2993	0.0639	0.113*	0.866 (6)
C14A	0.4342 (5)	0.3029 (8)	−0.0110 (12)	0.0388 (6)	0.134 (6)
H14A	0.4466	0.2786	0.0193	0.047*	0.134 (6)
C15A	0.4170 (6)	0.2915 (7)	−0.1056 (12)	0.0531 (9)	0.134 (6)
H15A	0.4002	0.3137	−0.1310	0.080*	0.134 (6)
H15B	0.3988	0.2678	−0.0997	0.080*	0.134 (6)
H15C	0.4409	0.2855	−0.1477	0.080*	0.134 (6)
C16A	0.4692 (7)	0.3341 (8)	−0.0227 (17)	0.0755 (13)	0.134 (6)
H16A	0.4917	0.3235	−0.0631	0.113*	0.134 (6)
H16B	0.4813	0.3407	0.0384	0.113*	0.134 (6)

H16C	0.4571	0.3583	−0.0509	0.113*	0.134 (6)
N2A	0.39878 (5)	0.31796 (4)	0.04708 (10)	0.0295 (3)	
C11A	0.32115 (9)	0.30161 (8)	0.22974 (18)	0.0364 (7)	0.853 (4)
H11A	0.3209	0.3227	0.2791	0.044*	0.853 (4)
C12A	0.27625 (13)	0.30108 (10)	0.1887 (3)	0.0428 (9)	0.853 (4)
H12A	0.2702	0.3270	0.1594	0.064*	0.853 (4)
H12B	0.2554	0.2962	0.2385	0.064*	0.853 (4)
H12C	0.2742	0.2798	0.1420	0.064*	0.853 (4)
C13A	0.33126 (9)	0.26254 (8)	0.27962 (18)	0.0490 (8)	0.853 (4)
H13A	0.3274	0.2401	0.2364	0.073*	0.853 (4)
H13B	0.3120	0.2593	0.3329	0.073*	0.853 (4)
H13C	0.3609	0.2631	0.3017	0.073*	0.853 (4)
C17A	0.3173 (4)	0.2924 (6)	0.2075 (9)	0.0364 (7)	0.147 (4)
H17A	0.3160	0.2652	0.1785	0.044*	0.147 (4)
C18A	0.2738 (8)	0.3122 (8)	0.193 (2)	0.0428 (9)	0.147 (4)
H18A	0.2751	0.3402	0.2132	0.064*	0.147 (4)
H18B	0.2521	0.2979	0.2290	0.064*	0.147 (4)
H18C	0.2663	0.3112	0.1264	0.064*	0.147 (4)
C19A	0.3252 (5)	0.2866 (5)	0.3120 (9)	0.0490 (8)	0.147 (4)
H19A	0.3503	0.2695	0.3211	0.073*	0.147 (4)
H19B	0.3002	0.2740	0.3405	0.073*	0.147 (4)
H19C	0.3303	0.3127	0.3413	0.073*	0.147 (4)
C1B	0.31026 (5)	0.40381 (5)	0.10400 (12)	0.0255 (4)	
C2B	0.26968 (5)	0.42727 (5)	0.09307 (12)	0.0274 (4)	
C3B	0.26978 (6)	0.46290 (6)	0.04392 (14)	0.0385 (5)	
H3B	0.2957	0.4725	0.0175	0.046*	
C4B	0.23256 (6)	0.48476 (6)	0.03284 (15)	0.0433 (5)	
H4B	0.2330	0.5091	−0.0012	0.052*	
C5B	0.19492 (6)	0.47118 (6)	0.07120 (14)	0.0366 (5)	
H5B	0.1694	0.4863	0.0640	0.044*	
C6B	0.19430 (6)	0.43573 (5)	0.11999 (14)	0.0358 (5)	
H6B	0.1683	0.4263	0.1462	0.043*	
C7B	0.23155 (6)	0.41387 (5)	0.13095 (13)	0.0333 (4)	
H7B	0.2310	0.3894	0.1648	0.040*	
N1B	0.33336 (4)	0.40256 (4)	0.18092 (10)	0.0255 (3)	
C8B	0.32265 (6)	0.42696 (5)	0.26272 (13)	0.0327 (4)	
H8B	0.3013	0.4476	0.2432	0.039*	
C9B	0.36203 (7)	0.44842 (6)	0.29873 (14)	0.0460 (5)	
H9B1	0.3830	0.4287	0.3203	0.069*	
H9B2	0.3540	0.4660	0.3506	0.069*	
H9B3	0.3745	0.4645	0.2485	0.069*	
C10B	0.30292 (7)	0.40195 (6)	0.34012 (14)	0.0461 (5)	
H10D	0.2776	0.3881	0.3163	0.069*	
H10E	0.2947	0.4194	0.3919	0.069*	
H10F	0.3238	0.3822	0.3620	0.069*	
C11B	0.30466 (6)	0.37478 (6)	−0.05187 (13)	0.0354 (5)	
H11B	0.2761	0.3881	−0.0475	0.042*	
C12B	0.32803 (8)	0.39243 (7)	−0.13483 (14)	0.0550 (6)	
H12D	0.3274	0.4217	−0.1309	0.082*	

H12E	0.3140	0.3838	−0.1925	0.082*
H12F	0.3578	0.3832	−0.1347	0.082*
N2B	0.32770 (4)	0.38256 (4)	0.03550 (10)	0.0266 (3)
C13B	0.29714 (6)	0.33021 (6)	−0.06506 (14)	0.0419 (5)
H13D	0.3247	0.3163	−0.0674	0.063*
H13E	0.2816	0.3257	−0.1235	0.063*
H13F	0.2802	0.3199	−0.0128	0.063*
C1C	0.44314 (6)	0.40129 (5)	0.15950 (13)	0.0319 (4)
C2C	0.48328 (6)	0.42313 (6)	0.18523 (14)	0.0384 (5)
C3C	0.52062 (7)	0.41680 (7)	0.13534 (19)	0.0568 (6)
H3C	0.5209	0.3982	0.0852	0.068*
C4	0.55767 (7)	0.43756 (8)	0.1585 (2)	0.0696 (8)
H4	0.5832	0.4329	0.1244	0.083*
C5C	0.55746 (8)	0.46472 (8)	0.2303 (2)	0.0672 (8)
H5C	0.5829	0.4787	0.2462	0.081*
C6C	0.52063 (9)	0.47162 (8)	0.27891 (19)	0.0705 (8)
H6C	0.5203	0.4908	0.3278	0.085*
C7C	0.48369 (8)	0.45065 (7)	0.25692 (17)	0.0578 (6)
H7C	0.4583	0.4553	0.2917	0.069*
N1C	0.42638 (5)	0.37157 (4)	0.20806 (10)	0.0290 (3)
C8C	0.42788 (6)	0.44607 (6)	0.02949 (14)	0.0401 (5)
H8C	0.4501	0.4623	0.0623	0.048*
C9C	0.38766 (6)	0.47131 (6)	0.02092 (15)	0.0417 (5)
H9C1	0.3943	0.4962	−0.0121	0.063*
H9C2	0.3768	0.4776	0.0832	0.063*
H9C3	0.3659	0.4564	−0.0139	0.063*
C10C	0.44466 (8)	0.43558 (7)	−0.06678 (16)	0.0648 (7)
H10G	0.4708	0.4196	−0.0607	0.097*
H10H	0.4510	0.4602	−0.1011	0.097*
H10I	0.4230	0.4202	−0.1006	0.097*
N2C	0.41959 (5)	0.40996 (4)	0.08501 (11)	0.0325 (4)
C11C	0.44864 (6)	0.35231 (6)	0.28607 (13)	0.0353 (5)
H11C	0.4740	0.3692	0.3026	0.042*
C12C	0.42030 (7)	0.34970 (8)	0.37019 (15)	0.0637 (7)
H12G	0.4136	0.3767	0.3923	0.096*
H12H	0.4350	0.3348	0.4195	0.096*
H12I	0.3938	0.3358	0.3536	0.096*
C13C	0.46464 (9)	0.31132 (7)	0.25844 (18)	0.0791 (9)
H13G	0.4406	0.2951	0.2362	0.119*
H13H	0.4778	0.2983	0.3125	0.119*
H13I	0.4859	0.3140	0.2087	0.119*
Al2	0.37998 (2)	0.64639 (2)	0.36001 (4)	0.02457 (12)
C1D	0.31649 (5)	0.60332 (5)	0.34917 (12)	0.0274 (4)
C2D	0.27771 (5)	0.57700 (5)	0.34328 (12)	0.0282 (4)
C3D	0.24150 (6)	0.58567 (5)	0.39528 (13)	0.0345 (4)
H3D	0.2412	0.6086	0.4345	0.041*
C4D	0.20570 (6)	0.56131 (6)	0.39077 (14)	0.0384 (5)
H4D	0.1812	0.5676	0.4269	0.046*
C5D	0.20555 (6)	0.52816 (6)	0.33425 (14)	0.0376 (5)

H5D	0.1810	0.5115	0.3312	0.045*
C6D	0.24119 (6)	0.51914 (6)	0.28200 (15)	0.0424 (5)
H6D	0.2411	0.4962	0.2427	0.051*
C7D	0.27713 (6)	0.54332 (6)	0.28648 (14)	0.0386 (5)
H7D	0.3016	0.5368	0.2504	0.046*
N1D	0.32807 (5)	0.62932 (4)	0.28395 (10)	0.0307 (4)
C8D	0.29988 (6)	0.63924 (6)	0.20547 (13)	0.0381 (5)
H8D	0.2717	0.6260	0.2165	0.046*
C9D	0.29233 (6)	0.68411 (6)	0.20005 (14)	0.0447 (5)
H9D1	0.2790	0.6933	0.2580	0.067*
H9D2	0.2734	0.6901	0.1474	0.067*
H9D3	0.3197	0.6979	0.1913	0.067*
C10D	0.31777 (7)	0.62359 (7)	0.11355 (14)	0.0542 (6)
H10J	0.3465	0.6345	0.1037	0.081*
H10K	0.2991	0.6319	0.0623	0.081*
H10L	0.3193	0.5943	0.1156	0.081*
N2D	0.34371 (4)	0.60324 (4)	0.42005 (10)	0.0274 (3)
C11D	0.34084 (6)	0.57323 (5)	0.49438 (13)	0.0328 (4)
H11D	0.3217	0.5512	0.4723	0.039*
C12D	0.38475 (6)	0.55526 (6)	0.51400 (15)	0.0424 (5)
H12J	0.3949	0.5411	0.4585	0.064*
H12K	0.3827	0.5365	0.5662	0.064*
H12L	0.4048	0.5767	0.5299	0.064*
C13D	0.32180 (7)	0.59037 (6)	0.58335 (14)	0.0457 (5)
H13J	0.3404	0.6116	0.6073	0.069*
H13K	0.3193	0.5691	0.6301	0.069*
H13L	0.2934	0.6015	0.5700	0.069*
C1E	0.37174 (5)	0.71908 (5)	0.35371 (12)	0.0256 (4)
C2E	0.36747 (6)	0.76381 (5)	0.34912 (12)	0.0296 (4)
C3E	0.40107 (7)	0.78807 (6)	0.37688 (14)	0.0395 (5)
H3E	0.4266	0.7763	0.4000	0.047*
C4E	0.39782 (8)	0.82927 (6)	0.37125 (16)	0.0523 (6)
H4E	0.4210	0.8456	0.3911	0.063*
C5E	0.36123 (8)	0.84666 (6)	0.33711 (17)	0.0559 (6)
H5E	0.3593	0.8750	0.3321	0.067*
C6E	0.32771 (7)	0.82312 (7)	0.31042 (17)	0.0555 (6)
H6E	0.3022	0.8351	0.2878	0.067*
C7E	0.33065 (6)	0.78179 (6)	0.31620 (15)	0.0430 (5)
H7E	0.3072	0.7657	0.2974	0.052*
N1E	0.39597 (4)	0.69803 (4)	0.29583 (10)	0.0258 (3)
C8E	0.42244 (6)	0.71676 (5)	0.22381 (12)	0.0305 (4)
H8E	0.4153	0.7459	0.2215	0.037*
C9E	0.41301 (7)	0.69879 (6)	0.12889 (13)	0.0441 (5)
H9E1	0.4186	0.6699	0.1305	0.066*
H9E2	0.4314	0.7114	0.0819	0.066*
H9E3	0.3830	0.7035	0.1129	0.066*
C10E	0.46953 (6)	0.71261 (6)	0.24634 (14)	0.0437 (5)
H10M	0.4758	0.7268	0.3045	0.066*
H10N	0.4865	0.7241	0.1956	0.066*

H10O	0.4767	0.6842	0.2535	0.066*	
N2E	0.35260 (4)	0.69555 (4)	0.41534 (10)	0.0277 (3)	
C11E	0.32134 (12)	0.71432 (9)	0.4803 (2)	0.0287 (8)	0.669 (3)
H11E	0.3197	0.7437	0.4674	0.034*	0.669 (3)
C12E	0.2776 (3)	0.6956 (5)	0.4651 (9)	0.0474 (19)	0.669 (3)
H12M	0.2684	0.7003	0.4007	0.071*	0.669 (3)
H12N	0.2569	0.7077	0.5080	0.071*	0.669 (3)
H12O	0.2792	0.6667	0.4766	0.071*	0.669 (3)
C13E	0.33384 (10)	0.70779 (11)	0.5821 (2)	0.0458 (8)	0.669 (3)
H13M	0.3368	0.6791	0.5942	0.069*	0.669 (3)
H13N	0.3117	0.7190	0.6227	0.069*	0.669 (3)
H13O	0.3611	0.7212	0.5946	0.069*	0.669 (3)
C17E	0.3205 (3)	0.6996 (2)	0.4887 (6)	0.0287 (8)	0.331 (3)
H17E	0.3233	0.6759	0.5309	0.034*	0.331 (3)
C18E	0.2755 (5)	0.6997 (10)	0.450 (2)	0.0474 (19)	0.331 (3)
H18M	0.2718	0.7227	0.4087	0.071*	0.331 (3)
H18N	0.2550	0.7015	0.5019	0.071*	0.331 (3)
H18O	0.2705	0.6749	0.4155	0.071*	0.331 (3)
C19E	0.3304 (2)	0.7364 (2)	0.5451 (4)	0.0458 (8)	0.331 (3)
H19M	0.3114	0.7376	0.5993	0.069*	0.331 (3)
H19N	0.3261	0.7603	0.5065	0.069*	0.331 (3)
H19O	0.3602	0.7354	0.5661	0.069*	0.331 (3)
C1F	0.45074 (5)	0.61603 (5)	0.38032 (13)	0.0277 (4)	
C2F	0.49321 (6)	0.59610 (5)	0.39381 (14)	0.0323 (4)	
C3F	0.52564 (6)	0.60114 (5)	0.32799 (15)	0.0381 (5)	
H3F	0.5209	0.6178	0.2754	0.046*	
C4F	0.56468 (6)	0.58206 (6)	0.33873 (17)	0.0465 (6)	
H4F	0.5867	0.5860	0.2940	0.056*	
C5F	0.57158 (6)	0.55745 (6)	0.41426 (17)	0.0492 (6)	
H5F	0.5983	0.5443	0.4215	0.059*	
C6F	0.53976 (7)	0.55191 (6)	0.47929 (17)	0.0483 (6)	
H6F	0.5445	0.5348	0.5311	0.058*	
C7F	0.50078 (6)	0.57133 (6)	0.46940 (15)	0.0406 (5)	
H7F	0.4791	0.5676	0.5149	0.049*	
N1F	0.42561 (4)	0.60969 (4)	0.30707 (10)	0.0288 (3)	
C8F	0.43367 (6)	0.57660 (6)	0.24177 (14)	0.0384 (5)	
H8F	0.4595	0.5618	0.2638	0.046*	
C9F	0.39648 (8)	0.54767 (7)	0.24042 (17)	0.0628 (7)	
H9F1	0.3924	0.5365	0.3029	0.094*	
H9F2	0.4025	0.5260	0.1963	0.094*	
H9F3	0.3705	0.5618	0.2212	0.094*	
C10F	0.44222 (7)	0.59103 (7)	0.14327 (15)	0.0507 (6)	
H10P	0.4165	0.6040	0.1186	0.076*	
H10Q	0.4497	0.5682	0.1038	0.076*	
H10R	0.4659	0.6102	0.1438	0.076*	
N2F	0.43312 (4)	0.64145 (4)	0.44012 (10)	0.0262 (3)	
C11F	0.45671 (18)	0.65933 (17)	0.5185 (3)	0.0301 (5)	0.764 (14)
H11F	0.4865	0.6485	0.5173	0.036*	0.764 (14)
C12F	0.4593 (2)	0.70472 (13)	0.5101 (4)	0.0388 (11)	0.764 (14)

H12P	0.4761	0.7118	0.4550	0.058*	0.764 (14)
H12Q	0.4729	0.7158	0.5659	0.058*	0.764 (14)
H12R	0.4304	0.7158	0.5040	0.058*	0.764 (14)
C13F	0.43651 (18)	0.64762 (17)	0.6113 (3)	0.0400 (10)	0.764 (14)
H13P	0.4059	0.6539	0.6100	0.060*	0.764 (14)
H13Q	0.4503	0.6625	0.6618	0.060*	0.764 (14)
H13R	0.4403	0.6188	0.6216	0.060*	0.764 (14)
C17F	0.4560 (6)	0.6575 (5)	0.5216 (8)	0.0301 (5)	0.236 (14)
H17F	0.4805	0.6396	0.5377	0.036*	0.236 (14)
C18F	0.4727 (6)	0.6986 (5)	0.4939 (12)	0.0388 (11)	0.236 (14)
H18D	0.4957	0.6955	0.4482	0.058*	0.236 (14)
H18E	0.4837	0.7124	0.5492	0.058*	0.236 (14)
H18F	0.4494	0.7143	0.4665	0.058*	0.236 (14)
C19F	0.4254 (5)	0.6602 (5)	0.6042 (11)	0.0400 (10)	0.236 (14)
H19D	0.3999	0.6753	0.5859	0.060*	0.236 (14)
H19E	0.4396	0.6738	0.6561	0.060*	0.236 (14)
H19F	0.4171	0.6332	0.6235	0.060*	0.236 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0253 (3)	0.0241 (3)	0.0238 (3)	0.0048 (2)	−0.0012 (2)	0.0003 (2)
C1A	0.0315 (10)	0.0271 (9)	0.0265 (9)	0.0074 (8)	−0.0059 (8)	−0.0010 (8)
C2A	0.0423 (11)	0.0277 (10)	0.0313 (10)	0.0055 (9)	0.0032 (9)	−0.0021 (8)
C3A	0.0627 (15)	0.0315 (11)	0.0526 (14)	0.0119 (10)	−0.0115 (12)	−0.0035 (10)
C4A	0.0845 (19)	0.0311 (12)	0.0637 (16)	0.0194 (12)	−0.0080 (14)	0.0018 (11)
C5A	0.0870 (19)	0.0254 (11)	0.0579 (15)	−0.0006 (12)	0.0159 (14)	−0.0039 (11)
C6A	0.0624 (15)	0.0372 (12)	0.0585 (15)	−0.0069 (11)	0.0056 (12)	−0.0111 (11)
C7A	0.0481 (13)	0.0350 (11)	0.0421 (12)	0.0043 (10)	0.0024 (10)	−0.0048 (10)
N1A	0.0324 (8)	0.0259 (8)	0.0272 (8)	0.0050 (7)	0.0015 (7)	0.0006 (7)
C8A	0.0411 (13)	0.0387 (11)	0.0365 (14)	0.0117 (11)	0.0082 (11)	−0.0038 (11)
C9A	0.0438 (15)	0.082 (3)	0.0333 (13)	0.0136 (16)	0.0090 (11)	−0.0041 (16)
C10A	0.0319 (15)	0.147 (4)	0.047 (2)	0.0269 (19)	0.0039 (13)	−0.013 (2)
C14A	0.0411 (13)	0.0387 (11)	0.0365 (14)	0.0117 (11)	0.0082 (11)	−0.0038 (11)
C15A	0.0438 (15)	0.082 (3)	0.0333 (13)	0.0136 (16)	0.0090 (11)	−0.0041 (16)
C16A	0.0319 (15)	0.147 (4)	0.047 (2)	0.0269 (19)	0.0039 (13)	−0.013 (2)
N2A	0.0316 (8)	0.0285 (8)	0.0284 (8)	0.0065 (7)	0.0028 (7)	−0.0017 (7)
C11A	0.0471 (13)	0.0342 (17)	0.0279 (15)	0.0006 (11)	0.0094 (12)	−0.0019 (11)
C12A	0.0421 (14)	0.035 (2)	0.0508 (15)	−0.0102 (16)	0.0107 (11)	−0.0005 (17)
C13A	0.0726 (18)	0.0359 (16)	0.0384 (15)	−0.0073 (14)	0.0044 (13)	0.0073 (12)
C17A	0.0471 (13)	0.0342 (17)	0.0279 (15)	0.0006 (11)	0.0094 (12)	−0.0019 (11)
C18A	0.0421 (14)	0.035 (2)	0.0508 (15)	−0.0102 (16)	0.0107 (11)	−0.0005 (17)
C19A	0.0726 (18)	0.0359 (16)	0.0384 (15)	−0.0073 (14)	0.0044 (13)	0.0073 (12)
C1B	0.0258 (9)	0.0204 (9)	0.0302 (10)	0.0010 (7)	0.0025 (8)	0.0046 (8)
C2B	0.0271 (9)	0.0247 (9)	0.0304 (10)	0.0044 (8)	0.0000 (8)	−0.0005 (8)
C3B	0.0285 (10)	0.0349 (11)	0.0521 (13)	0.0068 (9)	0.0091 (9)	0.0129 (10)
C4B	0.0349 (11)	0.0346 (11)	0.0606 (14)	0.0109 (9)	0.0064 (10)	0.0192 (10)
C5B	0.0259 (10)	0.0340 (11)	0.0498 (13)	0.0094 (8)	−0.0016 (9)	0.0015 (9)
C6B	0.0244 (10)	0.0337 (11)	0.0495 (12)	0.0009 (8)	0.0030 (9)	0.0029 (9)

C7B	0.0311 (10)	0.0264 (10)	0.0424 (12)	0.0035 (8)	0.0006 (9)	0.0063 (9)
N1B	0.0296 (8)	0.0233 (8)	0.0237 (8)	0.0048 (6)	−0.0002 (6)	−0.0007 (6)
C8B	0.0382 (11)	0.0282 (10)	0.0316 (10)	0.0075 (8)	0.0016 (9)	−0.0063 (8)
C9B	0.0607 (14)	0.0376 (12)	0.0397 (12)	−0.0143 (10)	0.0088 (11)	−0.0122 (10)
C10B	0.0486 (13)	0.0547 (13)	0.0349 (12)	−0.0136 (11)	0.0137 (10)	−0.0155 (10)
C11B	0.0363 (11)	0.0408 (11)	0.0291 (10)	0.0110 (9)	−0.0076 (9)	−0.0013 (9)
C12B	0.0770 (17)	0.0590 (15)	0.0290 (12)	−0.0033 (13)	−0.0071 (11)	0.0049 (10)
N2B	0.0283 (8)	0.0288 (8)	0.0228 (8)	0.0067 (6)	−0.0025 (6)	0.0008 (6)
C13B	0.0442 (12)	0.0474 (13)	0.0342 (11)	0.0005 (10)	−0.0101 (9)	−0.0065 (10)
C1C	0.0288 (10)	0.0308 (10)	0.0362 (11)	0.0023 (8)	−0.0014 (9)	−0.0010 (9)
C2C	0.0326 (11)	0.0379 (11)	0.0448 (12)	−0.0037 (9)	−0.0094 (9)	0.0097 (10)
C3C	0.0345 (12)	0.0500 (14)	0.0860 (19)	−0.0015 (10)	−0.0036 (12)	−0.0006 (13)
C4	0.0317 (13)	0.0650 (17)	0.112 (2)	−0.0060 (12)	−0.0047 (14)	0.0138 (17)
C5C	0.0510 (16)	0.0610 (17)	0.090 (2)	−0.0246 (13)	−0.0288 (15)	0.0212 (15)
C6C	0.0722 (19)	0.0729 (18)	0.0663 (18)	−0.0340 (15)	−0.0143 (15)	−0.0027 (14)
C7C	0.0523 (15)	0.0671 (16)	0.0542 (15)	−0.0218 (12)	−0.0043 (12)	−0.0078 (13)
N1C	0.0290 (8)	0.0291 (8)	0.0288 (8)	0.0020 (7)	−0.0051 (7)	0.0018 (7)
C8C	0.0323 (11)	0.0416 (12)	0.0464 (13)	−0.0050 (9)	−0.0032 (9)	0.0160 (10)
C9C	0.0459 (12)	0.0335 (11)	0.0458 (13)	0.0002 (9)	0.0017 (10)	0.0111 (9)
C10C	0.0559 (15)	0.0760 (18)	0.0624 (16)	0.0209 (13)	0.0293 (13)	0.0333 (14)
N2C	0.0290 (8)	0.0351 (9)	0.0334 (9)	0.0008 (7)	−0.0029 (7)	0.0081 (7)
C11C	0.0373 (11)	0.0341 (11)	0.0345 (11)	−0.0012 (9)	−0.0135 (9)	0.0047 (9)
C12C	0.0582 (15)	0.0860 (18)	0.0470 (14)	0.0063 (14)	−0.0031 (12)	0.0311 (13)
C13C	0.114 (2)	0.0538 (15)	0.0697 (18)	0.0389 (16)	−0.0516 (17)	−0.0077 (14)
Al2	0.0230 (3)	0.0267 (3)	0.0240 (3)	−0.0040 (2)	−0.0014 (2)	0.0007 (2)
C1D	0.0246 (9)	0.0285 (9)	0.0292 (10)	−0.0024 (8)	0.0016 (8)	−0.0062 (8)
C2D	0.0240 (9)	0.0300 (10)	0.0304 (10)	−0.0038 (8)	−0.0023 (8)	−0.0024 (8)
C3D	0.0317 (11)	0.0319 (10)	0.0400 (12)	−0.0043 (8)	0.0020 (9)	−0.0059 (9)
C4D	0.0255 (10)	0.0406 (12)	0.0490 (13)	−0.0027 (9)	0.0029 (9)	−0.0003 (10)
C5D	0.0270 (10)	0.0346 (11)	0.0511 (13)	−0.0084 (8)	−0.0100 (9)	0.0029 (10)
C6D	0.0348 (12)	0.0359 (11)	0.0564 (14)	−0.0053 (9)	−0.0065 (10)	−0.0145 (10)
C7D	0.0271 (10)	0.0416 (12)	0.0472 (12)	−0.0030 (9)	−0.0001 (9)	−0.0130 (10)
N1D	0.0284 (8)	0.0395 (9)	0.0241 (8)	−0.0069 (7)	−0.0031 (7)	0.0010 (7)
C8D	0.0305 (10)	0.0565 (13)	0.0274 (10)	−0.0112 (10)	−0.0063 (8)	0.0028 (9)
C9D	0.0370 (12)	0.0638 (15)	0.0334 (11)	−0.0003 (10)	−0.0092 (9)	0.0116 (10)
C10D	0.0597 (15)	0.0732 (16)	0.0298 (11)	−0.0090 (12)	−0.0100 (11)	−0.0066 (11)
N2D	0.0264 (8)	0.0264 (8)	0.0293 (8)	−0.0056 (6)	−0.0032 (7)	0.0020 (7)
C11D	0.0311 (10)	0.0275 (10)	0.0398 (11)	−0.0093 (8)	−0.0041 (9)	0.0074 (9)
C12D	0.0402 (12)	0.0318 (10)	0.0552 (13)	−0.0055 (9)	−0.0093 (10)	0.0106 (10)
C13D	0.0490 (13)	0.0501 (13)	0.0380 (12)	−0.0064 (10)	0.0033 (10)	0.0151 (10)
C1E	0.0229 (9)	0.0311 (10)	0.0227 (9)	0.0007 (7)	−0.0040 (8)	0.0011 (8)
C2E	0.0330 (10)	0.0302 (10)	0.0255 (10)	0.0068 (8)	0.0067 (8)	0.0031 (8)
C3E	0.0449 (12)	0.0318 (11)	0.0419 (12)	0.0039 (9)	−0.0067 (10)	−0.0029 (9)
C4E	0.0622 (15)	0.0304 (11)	0.0643 (15)	0.0008 (11)	−0.0064 (13)	−0.0042 (11)
C5E	0.0653 (16)	0.0306 (12)	0.0718 (17)	0.0098 (11)	0.0083 (13)	0.0072 (11)
C6E	0.0461 (14)	0.0461 (14)	0.0742 (17)	0.0143 (11)	0.0049 (12)	0.0209 (12)
C7E	0.0339 (11)	0.0411 (12)	0.0541 (13)	0.0018 (9)	0.0023 (10)	0.0132 (10)
N1E	0.0252 (8)	0.0277 (8)	0.0246 (8)	−0.0006 (6)	0.0039 (6)	0.0015 (6)
C8E	0.0341 (10)	0.0262 (9)	0.0312 (10)	−0.0020 (8)	0.0081 (8)	0.0019 (8)

C9E	0.0456 (12)	0.0573 (13)	0.0293 (11)	−0.0098 (10)	0.0085 (9)	0.0023 (10)
C10E	0.0364 (12)	0.0534 (13)	0.0413 (12)	−0.0103 (10)	0.0090 (10)	0.0023 (10)
N2E	0.0249 (8)	0.0357 (9)	0.0225 (8)	−0.0022 (7)	0.0019 (6)	0.0018 (7)
C11E	0.0370 (12)	0.020 (2)	0.0289 (13)	−0.0057 (18)	0.0117 (10)	0.0067 (17)
C12E	0.0303 (14)	0.073 (3)	0.039 (5)	0.0018 (16)	0.0073 (14)	−0.004 (3)
C13E	0.0498 (17)	0.058 (2)	0.0295 (16)	−0.0005 (17)	0.0079 (14)	−0.0090 (14)
C17E	0.0370 (12)	0.020 (2)	0.0289 (13)	−0.0057 (18)	0.0117 (10)	0.0067 (17)
C18E	0.0303 (14)	0.073 (3)	0.039 (5)	0.0018 (16)	0.0073 (14)	−0.004 (3)
C19E	0.0498 (17)	0.058 (2)	0.0295 (16)	−0.0005 (17)	0.0079 (14)	−0.0090 (14)
C1F	0.0241 (9)	0.0207 (9)	0.0383 (11)	−0.0049 (7)	0.0006 (8)	0.0029 (8)
C2F	0.0283 (10)	0.0213 (9)	0.0472 (12)	−0.0022 (8)	−0.0019 (9)	−0.0039 (9)
C3F	0.0307 (11)	0.0287 (10)	0.0549 (13)	−0.0046 (8)	0.0008 (10)	−0.0013 (9)
C4F	0.0283 (11)	0.0370 (11)	0.0742 (16)	−0.0025 (9)	0.0069 (11)	−0.0048 (11)
C5F	0.0280 (11)	0.0376 (12)	0.0819 (18)	0.0047 (9)	−0.0029 (11)	−0.0031 (12)
C6F	0.0388 (12)	0.0401 (12)	0.0659 (16)	0.0062 (10)	−0.0067 (11)	0.0064 (11)
C7F	0.0308 (11)	0.0366 (11)	0.0544 (14)	0.0006 (9)	0.0001 (10)	0.0011 (10)
N1F	0.0277 (8)	0.0247 (8)	0.0339 (9)	−0.0039 (6)	−0.0006 (7)	−0.0057 (7)
C8F	0.0385 (11)	0.0297 (10)	0.0471 (12)	−0.0021 (9)	0.0013 (10)	−0.0121 (9)
C9F	0.0778 (18)	0.0485 (14)	0.0622 (16)	−0.0260 (13)	0.0190 (14)	−0.0264 (12)
C10F	0.0494 (13)	0.0539 (14)	0.0490 (14)	−0.0049 (11)	0.0136 (11)	−0.0199 (11)
N2F	0.0242 (8)	0.0246 (8)	0.0297 (8)	−0.0021 (6)	−0.0032 (6)	−0.0012 (6)
C11F	0.0284 (10)	0.0277 (11)	0.0342 (11)	0.0001 (8)	−0.0085 (8)	−0.0006 (9)
C12F	0.047 (3)	0.0295 (17)	0.040 (2)	−0.0042 (17)	−0.014 (2)	−0.0041 (15)
C13F	0.044 (2)	0.041 (2)	0.0354 (14)	−0.0033 (18)	−0.0091 (15)	−0.0017 (17)
C17F	0.0284 (10)	0.0277 (11)	0.0342 (11)	0.0001 (8)	−0.0085 (8)	−0.0006 (9)
C18F	0.047 (3)	0.0295 (17)	0.040 (2)	−0.0042 (17)	−0.014 (2)	−0.0041 (15)
C19F	0.044 (2)	0.041 (2)	0.0354 (14)	−0.0033 (18)	−0.0091 (15)	−0.0017 (17)

Geometric parameters (Å, º)

Al1—N1A	1.9826 (15)	Al2—N2E	2.0156 (15)
Al1—N1C	2.0168 (15)	Al2—N1E	2.0185 (15)
Al1—N2B	2.0220 (14)	Al2—N2D	2.0267 (15)
Al1—N1B	2.0299 (14)	Al2—N2F	2.0279 (14)
Al1—N2C	2.0310 (16)	Al2—N1F	2.0295 (15)
Al1—N2A	2.0344 (15)	Al2—N1D	2.0382 (15)
C1A—N2A	1.327 (2)	C1D—N2D	1.326 (2)
C1A—N1A	1.329 (2)	C1D—N1D	1.327 (2)
C1A—C2A	1.496 (2)	C1D—C2D	1.501 (2)
C2A—C7A	1.383 (3)	C2D—C3D	1.387 (2)
C2A—C3A	1.384 (3)	C2D—C7D	1.389 (2)
C3A—C4A	1.384 (3)	C3D—C4D	1.386 (2)
C3A—H3A	0.9500	C3D—H3D	0.9500
C4A—C5A	1.375 (3)	C4D—C5D	1.373 (3)
C4A—H4A	0.9500	C4D—H4D	0.9500
C5A—C6A	1.369 (3)	C5D—C6D	1.377 (3)
C5A—H5A	0.9500	C5D—H5D	0.9500
C6A—C7A	1.388 (3)	C6D—C7D	1.386 (3)
C6A—H6A	0.9500	C6D—H6D	0.9500
C7A—H7A	0.9500	C7D—H7D	0.9500

N1A—C11A	1.461 (3)	N1D—C8D	1.468 (2)
N1A—C17A	1.490 (7)	C8D—C9D	1.519 (3)
C8A—N2A	1.469 (3)	C8D—C10D	1.525 (3)
C8A—C9A	1.508 (4)	C8D—H8D	1.0000
C8A—C10A	1.522 (4)	C9D—H9D1	0.9800
C8A—H8A	1.0000	C9D—H9D2	0.9800
C9A—H9A1	0.9800	C9D—H9D3	0.9800
C9A—H9A2	0.9800	C10D—H10J	0.9800
C9A—H9A3	0.9800	C10D—H10K	0.9800
C10A—H10A	0.9800	C10D—H10L	0.9800
C10A—H10B	0.9800	N2D—C11D	1.467 (2)
C10A—H10C	0.9800	C11D—C13D	1.521 (3)
C14A—N2A	1.475 (8)	C11D—C12D	1.525 (3)
C14A—C15A	1.509 (10)	C11D—H11D	1.0000
C14A—C16A	1.522 (10)	C12D—H12J	0.9800
C14A—H14A	1.0000	C12D—H12K	0.9800
C15A—H15A	0.9800	C12D—H12L	0.9800
C15A—H15B	0.9800	C13D—H13J	0.9800
C15A—H15C	0.9800	C13D—H13K	0.9800
C16A—H16A	0.9800	C13D—H13L	0.9800
C16A—H16B	0.9800	C1E—N2E	1.326 (2)
C16A—H16C	0.9800	C1E—N1E	1.326 (2)
C11A—C13A	1.522 (3)	C1E—C2E	1.502 (2)
C11A—C12A	1.523 (3)	C2E—C7E	1.382 (3)
C11A—H11A	1.0000	C2E—C3E	1.386 (3)
C12A—H12A	0.9800	C3E—C4E	1.383 (3)
C12A—H12B	0.9800	C3E—H3E	0.9500
C12A—H12C	0.9800	C4E—C5E	1.374 (3)
C13A—H13A	0.9800	C4E—H4E	0.9500
C13A—H13B	0.9800	C5E—C6E	1.366 (3)
C13A—H13C	0.9800	C5E—H5E	0.9500
C17A—C18A	1.527 (10)	C6E—C7E	1.387 (3)
C17A—C19A	1.532 (9)	C6E—H6E	0.9500
C17A—H17A	1.0000	C7E—H7E	0.9500
C18A—H18A	0.9800	N1E—C8E	1.465 (2)
C18A—H18B	0.9800	C8E—C10E	1.515 (3)
C18A—H18C	0.9800	C8E—C9E	1.517 (3)
C19A—H19A	0.9800	C8E—H8E	1.0000
C19A—H19B	0.9800	C9E—H9E1	0.9800
C19A—H19C	0.9800	C9E—H9E2	0.9800
C1B—N1B	1.320 (2)	C9E—H9E3	0.9800
C1B—N2B	1.329 (2)	C10E—H10M	0.9800
C1B—C2B	1.500 (2)	C10E—H10N	0.9800
C2B—C3B	1.384 (2)	C10E—H10O	0.9800
C2B—C7B	1.385 (2)	N2E—C17E	1.461 (6)
C3B—C4B	1.384 (2)	N2E—C11E	1.490 (3)
C3B—H3B	0.9500	C11E—C12E	1.521 (7)
C4B—C5B	1.377 (3)	C11E—C13E	1.527 (4)
C4B—H4B	0.9500	C11E—H11E	1.0000

C5B—C6B	1.376 (3)	C12E—H12M	0.9800
C5B—H5B	0.9500	C12E—H12N	0.9800
C6B—C7B	1.384 (2)	C12E—H12O	0.9800
C6B—H6B	0.9500	C13E—H13M	0.9800
C7B—H7B	0.9500	C13E—H13N	0.9800
N1B—C8B	1.468 (2)	C13E—H13O	0.9800
C8B—C9B	1.516 (3)	C17E—C19E	1.505 (7)
C8B—C10B	1.520 (3)	C17E—C18E	1.512 (9)
C8B—H8B	1.0000	C17E—H17E	1.0000
C9B—H9B1	0.9800	C18E—H18M	0.9800
C9B—H9B2	0.9800	C18E—H18N	0.9800
C9B—H9B3	0.9800	C18E—H18O	0.9800
C10B—H10D	0.9800	C19E—H19M	0.9800
C10B—H10E	0.9800	C19E—H19N	0.9800
C10B—H10F	0.9800	C19E—H19O	0.9800
C11B—N2B	1.469 (2)	C1F—N2F	1.327 (2)
C11B—C12B	1.516 (3)	C1F—N1F	1.329 (2)
C11B—C13B	1.519 (3)	C1F—C2F	1.499 (2)
C11B—H11B	1.0000	C2F—C7F	1.385 (3)
C12B—H12D	0.9800	C2F—C3F	1.396 (3)
C12B—H12E	0.9800	C3F—C4F	1.386 (3)
C12B—H12F	0.9800	C3F—H3F	0.9500
C13B—H13D	0.9800	C4F—C5F	1.377 (3)
C13B—H13E	0.9800	C4F—H4F	0.9500
C13B—H13F	0.9800	C5F—C6F	1.377 (3)
C1C—N1C	1.322 (2)	C5F—H5F	0.9500
C1C—N2C	1.330 (2)	C6F—C7F	1.389 (3)
C1C—C2C	1.499 (3)	C6F—H6F	0.9500
C2C—C7C	1.380 (3)	C7F—H7F	0.9500
C2C—C3C	1.386 (3)	N1F—C8F	1.471 (2)
C3C—C4	1.391 (3)	C8F—C9F	1.513 (3)
C3C—H3C	0.9500	C8F—C10F	1.517 (3)
C4—C5C	1.373 (4)	C8F—H8F	1.0000
C4—H4	0.9500	C9F—H9F1	0.9800
C5C—C6C	1.367 (4)	C9F—H9F2	0.9800
C5C—H5C	0.9500	C9F—H9F3	0.9800
C6C—C7C	1.388 (3)	C10F—H10P	0.9800
C6C—H6C	0.9500	C10F—H10Q	0.9800
C7C—H7C	0.9500	C10F—H10R	0.9800
N1C—C11C	1.467 (2)	N2F—C11F	1.472 (3)
C8C—N2C	1.469 (2)	N2F—C17F	1.473 (7)
C8C—C10C	1.519 (3)	C11F—C12F	1.523 (4)
C8C—C9C	1.520 (3)	C11F—C13F	1.525 (4)
C8C—H8C	1.0000	C11F—H11F	1.0000
C9C—H9C1	0.9800	C12F—H12P	0.9800
C9C—H9C2	0.9800	C12F—H12Q	0.9800
C9C—H9C3	0.9800	C12F—H12R	0.9800
C10C—H10G	0.9800	C13F—H13P	0.9800
C10C—H10H	0.9800	C13F—H13Q	0.9800

C10C—H10I	0.9800	C13F—H13R	0.9800
C11C—C12C	1.500 (3)	C17F—C18F	1.520 (8)
C11C—C13C	1.511 (3)	C17F—C19F	1.526 (9)
C11C—H11C	1.0000	C17F—H17F	1.0000
C12C—H12G	0.9800	C18F—H18D	0.9800
C12C—H12H	0.9800	C18F—H18E	0.9800
C12C—H12I	0.9800	C18F—H18F	0.9800
C13C—H13G	0.9800	C19F—H19D	0.9800
C13C—H13H	0.9800	C19F—H19E	0.9800
C13C—H13I	0.9800	C19F—H19F	0.9800

N1A—Al1—N1C	100.06 (6)	N2E—Al2—N1E	65.70 (6)
N1A—Al1—N2B	96.82 (6)	N2E—Al2—N2D	100.03 (6)
N1C—Al1—N2B	159.54 (6)	N1E—Al2—N2D	160.14 (6)
N1A—Al1—N1B	97.10 (6)	N2E—Al2—N2F	101.04 (6)
N1C—Al1—N1B	100.60 (6)	N1E—Al2—N2F	97.19 (6)
N2B—Al1—N1B	65.71 (6)	N2D—Al2—N2F	99.21 (6)
N1A—Al1—N2C	161.62 (6)	N2E—Al2—N1F	159.86 (6)
N1C—Al1—N2C	65.60 (6)	N1E—Al2—N1F	99.87 (6)
N2B—Al1—N2C	99.77 (6)	N2D—Al2—N1F	97.08 (6)
N1B—Al1—N2C	96.88 (6)	N2F—Al2—N1F	65.56 (6)
N1A—Al1—N2A	65.85 (6)	N2E—Al2—N1D	95.75 (6)
N1C—Al1—N2A	97.58 (6)	N1E—Al2—N1D	101.08 (6)
N2B—Al1—N2A	99.83 (6)	N2D—Al2—N1D	65.32 (6)
N1B—Al1—N2A	157.07 (6)	N2F—Al2—N1D	159.07 (6)
N2C—Al1—N2A	103.32 (6)	N1F—Al2—N1D	101.02 (6)
N2A—C1A—N1A	110.66 (15)	N2D—C1D—N1D	111.51 (15)
N2A—C1A—C2A	124.81 (16)	N2D—C1D—C2D	124.13 (16)
N1A—C1A—C2A	124.53 (16)	N1D—C1D—C2D	124.36 (16)
C7A—C2A—C3A	118.75 (18)	C3D—C2D—C7D	118.31 (16)
C7A—C2A—C1A	120.65 (17)	C3D—C2D—C1D	120.49 (16)
C3A—C2A—C1A	120.57 (18)	C7D—C2D—C1D	121.20 (16)
C2A—C3A—C4A	120.3 (2)	C4D—C3D—C2D	120.81 (17)
C2A—C3A—H3A	119.9	C4D—C3D—H3D	119.6
C4A—C3A—H3A	119.9	C2D—C3D—H3D	119.6
C5A—C4A—C3A	120.4 (2)	C5D—C4D—C3D	120.28 (18)
C5A—C4A—H4A	119.8	C5D—C4D—H4D	119.9
C3A—C4A—H4A	119.8	C3D—C4D—H4D	119.9
C6A—C5A—C4A	120.0 (2)	C4D—C5D—C6D	119.69 (17)
C6A—C5A—H5A	120.0	C4D—C5D—H5D	120.2
C4A—C5A—H5A	120.0	C6D—C5D—H5D	120.2
C5A—C6A—C7A	119.9 (2)	C5D—C6D—C7D	120.27 (18)
C5A—C6A—H6A	120.1	C5D—C6D—H6D	119.9
C7A—C6A—H6A	120.1	C7D—C6D—H6D	119.9
C2A—C7A—C6A	120.7 (2)	C6D—C7D—C2D	120.65 (18)
C2A—C7A—H7A	119.6	C6D—C7D—H7D	119.7
C6A—C7A—H7A	119.6	C2D—C7D—H7D	119.7
C1A—N1A—C11A	130.33 (17)	C1D—N1D—C8D	121.64 (15)
C1A—N1A—C17A	115.0 (8)	C1D—N1D—Al2	91.32 (11)

C1A—N1A—Al1	92.86 (11)	C8D—N1D—Al2	145.71 (12)
C11A—N1A—Al1	136.74 (14)	N1D—C8D—C9D	110.81 (15)
C17A—N1A—Al1	149.2 (8)	N1D—C8D—C10D	111.43 (16)
N2A—C8A—C9A	112.1 (2)	C9D—C8D—C10D	110.55 (17)
N2A—C8A—C10A	109.3 (2)	N1D—C8D—H8D	108.0
C9A—C8A—C10A	110.7 (3)	C9D—C8D—H8D	108.0
N2A—C8A—H8A	108.2	C10D—C8D—H8D	108.0
C9A—C8A—H8A	108.2	C8D—C9D—H9D1	109.5
C10A—C8A—H8A	108.2	C8D—C9D—H9D2	109.5
C8A—C9A—H9A1	109.5	H9D1—C9D—H9D2	109.5
C8A—C9A—H9A2	109.5	C8D—C9D—H9D3	109.5
H9A1—C9A—H9A2	109.5	H9D1—C9D—H9D3	109.5
C8A—C9A—H9A3	109.5	H9D2—C9D—H9D3	109.5
H9A1—C9A—H9A3	109.5	C8D—C10D—H10J	109.5
H9A2—C9A—H9A3	109.5	C8D—C10D—H10K	109.5
C8A—C10A—H10A	109.5	H10J—C10D—H10K	109.5
C8A—C10A—H10B	109.5	C8D—C10D—H10L	109.5
H10A—C10A—H10B	109.5	H10J—C10D—H10L	109.5
C8A—C10A—H10C	109.5	H10K—C10D—H10L	109.5
H10A—C10A—H10C	109.5	C1D—N2D—C11D	121.30 (14)
H10B—C10A—H10C	109.5	C1D—N2D—Al2	91.84 (11)
N2A—C14A—C15A	109.1 (13)	C11D—N2D—Al2	146.06 (11)
N2A—C14A—C16A	111.6 (16)	N2D—C11D—C13D	112.15 (15)
C15A—C14A—C16A	109.3 (13)	N2D—C11D—C12D	110.37 (15)
N2A—C14A—H14A	108.9	C13D—C11D—C12D	110.24 (16)
C15A—C14A—H14A	108.9	N2D—C11D—H11D	108.0
C16A—C14A—H14A	108.9	C13D—C11D—H11D	108.0
C14A—C15A—H15A	109.5	C12D—C11D—H11D	108.0
C14A—C15A—H15B	109.5	C11D—C12D—H12J	109.5
H15A—C15A—H15B	109.5	C11D—C12D—H12K	109.5
C14A—C15A—H15C	109.5	H12J—C12D—H12K	109.5
H15A—C15A—H15C	109.5	C11D—C12D—H12L	109.5
H15B—C15A—H15C	109.5	H12J—C12D—H12L	109.5
C14A—C16A—H16A	109.5	H12K—C12D—H12L	109.5
C14A—C16A—H16B	109.5	C11D—C13D—H13J	109.5
H16A—C16A—H16B	109.5	C11D—C13D—H13K	109.5
C14A—C16A—H16C	109.5	H13J—C13D—H13K	109.5
H16A—C16A—H16C	109.5	C11D—C13D—H13L	109.5
H16B—C16A—H16C	109.5	H13J—C13D—H13L	109.5
C1A—N2A—C8A	122.2 (2)	H13K—C13D—H13L	109.5
C1A—N2A—C14A	122.5 (11)	N2E—C1E—N1E	111.20 (15)
C1A—N2A—Al1	90.62 (10)	N2E—C1E—C2E	125.37 (15)
C8A—N2A—Al1	146.9 (2)	N1E—C1E—C2E	123.43 (15)
C14A—N2A—Al1	144.0 (10)	C7E—C2E—C3E	118.45 (17)
N1A—C11A—C13A	115.9 (2)	C7E—C2E—C1E	121.43 (17)
N1A—C11A—C12A	111.3 (3)	C3E—C2E—C1E	120.11 (16)
C13A—C11A—C12A	111.3 (2)	C4E—C3E—C2E	120.63 (19)
N1A—C11A—H11A	105.9	C4E—C3E—H3E	119.7
C13A—C11A—H11A	105.9	C2E—C3E—H3E	119.7

C12A—C11A—H11A	105.9	C5E—C4E—C3E	120.2 (2)
C11A—C12A—H12A	109.5	C5E—C4E—H4E	119.9
C11A—C12A—H12B	109.5	C3E—C4E—H4E	119.9
H12A—C12A—H12B	109.5	C6E—C5E—C4E	119.8 (2)
C11A—C12A—H12C	109.5	C6E—C5E—H5E	120.1
H12A—C12A—H12C	109.5	C4E—C5E—H5E	120.1
H12B—C12A—H12C	109.5	C5E—C6E—C7E	120.4 (2)
C11A—C13A—H13A	109.5	C5E—C6E—H6E	119.8
C11A—C13A—H13B	109.5	C7E—C6E—H6E	119.8
H13A—C13A—H13B	109.5	C2E—C7E—C6E	120.6 (2)
C11A—C13A—H13C	109.5	C2E—C7E—H7E	119.7
H13A—C13A—H13C	109.5	C6E—C7E—H7E	119.7
H13B—C13A—H13C	109.5	C1E—N1E—C8E	122.58 (14)
N1A—C17A—C18A	112.4 (18)	C1E—N1E—Al2	91.48 (10)
N1A—C17A—C19A	112.5 (10)	C8E—N1E—Al2	145.80 (12)
C18A—C17A—C19A	109.6 (12)	N1E—C8E—C10E	111.12 (15)
N1A—C17A—H17A	107.4	N1E—C8E—C9E	110.76 (14)
C18A—C17A—H17A	107.4	C10E—C8E—C9E	110.15 (16)
C19A—C17A—H17A	107.4	N1E—C8E—H8E	108.2
C17A—C18A—H18A	109.5	C10E—C8E—H8E	108.2
C17A—C18A—H18B	109.5	C9E—C8E—H8E	108.2
H18A—C18A—H18B	109.5	C8E—C9E—H9E1	109.5
C17A—C18A—H18C	109.5	C8E—C9E—H9E2	109.5
H18A—C18A—H18C	109.5	H9E1—C9E—H9E2	109.5
H18B—C18A—H18C	109.5	C8E—C9E—H9E3	109.5
C17A—C19A—H19A	109.5	H9E1—C9E—H9E3	109.5
C17A—C19A—H19B	109.5	H9E2—C9E—H9E3	109.5
H19A—C19A—H19B	109.5	C8E—C10E—H10M	109.5
C17A—C19A—H19C	109.5	C8E—C10E—H10N	109.5
H19A—C19A—H19C	109.5	H10M—C10E—H10N	109.5
H19B—C19A—H19C	109.5	C8E—C10E—H10O	109.5
N1B—C1B—N2B	112.13 (15)	H10M—C10E—H10O	109.5
N1B—C1B—C2B	124.56 (15)	H10N—C10E—H10O	109.5
N2B—C1B—C2B	123.29 (15)	C1E—N2E—C17E	137.4 (3)
C3B—C2B—C7B	118.69 (16)	C1E—N2E—C11E	117.69 (17)
C3B—C2B—C1B	120.04 (16)	C1E—N2E—Al2	91.62 (10)
C7B—C2B—C1B	121.27 (15)	C17E—N2E—Al2	130.6 (3)
C2B—C3B—C4B	120.71 (18)	C11E—N2E—Al2	150.30 (15)
C2B—C3B—H3B	119.6	N2E—C11E—C12E	109.1 (6)
C4B—C3B—H3B	119.6	N2E—C11E—C13E	111.7 (3)
C5B—C4B—C3B	120.00 (18)	C12E—C11E—C13E	108.0 (6)
C5B—C4B—H4B	120.0	N2E—C11E—H11E	109.3
C3B—C4B—H4B	120.0	C12E—C11E—H11E	109.3
C6B—C5B—C4B	119.94 (17)	C13E—C11E—H11E	109.3
C6B—C5B—H5B	120.0	C11E—C12E—H12M	109.5
C4B—C5B—H5B	120.0	C11E—C12E—H12N	109.5
C5B—C6B—C7B	120.01 (17)	H12M—C12E—H12N	109.5
C5B—C6B—H6B	120.0	C11E—C12E—H12O	109.5
C7B—C6B—H6B	120.0	H12M—C12E—H12O	109.5

C6B—C7B—C2B	120.65 (17)	H12N—C12E—H12O	109.5
C6B—C7B—H7B	119.7	C11E—C13E—H13M	109.5
C2B—C7B—H7B	119.7	C11E—C13E—H13N	109.5
C1B—N1B—C8B	121.75 (14)	H13M—C13E—H13N	109.5
C1B—N1B—Al1	91.05 (10)	C11E—C13E—H13O	109.5
C8B—N1B—Al1	146.75 (12)	H13M—C13E—H13O	109.5
N1B—C8B—C9B	110.45 (15)	H13N—C13E—H13O	109.5
N1B—C8B—C10B	111.82 (15)	N2E—C17E—C19E	108.7 (5)
C9B—C8B—C10B	109.92 (16)	N2E—C17E—C18E	112.2 (14)
N1B—C8B—H8B	108.2	C19E—C17E—C18E	112.8 (11)
C9B—C8B—H8B	108.2	N2E—C17E—H17E	107.6
C10B—C8B—H8B	108.2	C19E—C17E—H17E	107.6
C8B—C9B—H9B1	109.5	C18E—C17E—H17E	107.6
C8B—C9B—H9B2	109.5	C17E—C18E—H18M	109.5
H9B1—C9B—H9B2	109.5	C17E—C18E—H18N	109.5
C8B—C9B—H9B3	109.5	H18M—C18E—H18N	109.5
H9B1—C9B—H9B3	109.5	C17E—C18E—H18O	109.5
H9B2—C9B—H9B3	109.5	H18M—C18E—H18O	109.5
C8B—C10B—H10D	109.5	H18N—C18E—H18O	109.5
C8B—C10B—H10E	109.5	C17E—C19E—H19M	109.5
H10D—C10B—H10E	109.5	C17E—C19E—H19N	109.5
C8B—C10B—H10F	109.5	H19M—C19E—H19N	109.5
H10D—C10B—H10F	109.5	C17E—C19E—H19O	109.5
H10E—C10B—H10F	109.5	H19M—C19E—H19O	109.5
N2B—C11B—C12B	111.38 (16)	H19N—C19E—H19O	109.5
N2B—C11B—C13B	110.85 (15)	N2F—C1F—N1F	111.56 (15)
C12B—C11B—C13B	110.97 (17)	N2F—C1F—C2F	124.68 (16)
N2B—C11B—H11B	107.8	N1F—C1F—C2F	123.75 (16)
C12B—C11B—H11B	107.8	C7F—C2F—C3F	118.52 (18)
C13B—C11B—H11B	107.8	C7F—C2F—C1F	121.23 (17)
C11B—C12B—H12D	109.5	C3F—C2F—C1F	120.22 (17)
C11B—C12B—H12E	109.5	C4F—C3F—C2F	120.6 (2)
H12D—C12B—H12E	109.5	C4F—C3F—H3F	119.7
C11B—C12B—H12F	109.5	C2F—C3F—H3F	119.7
H12D—C12B—H12F	109.5	C5F—C4F—C3F	120.0 (2)
H12E—C12B—H12F	109.5	C5F—C4F—H4F	120.0
C1B—N2B—C11B	121.61 (14)	C3F—C4F—H4F	120.0
C1B—N2B—Al1	91.12 (10)	C6F—C5F—C4F	120.01 (19)
C11B—N2B—Al1	146.07 (12)	C6F—C5F—H5F	120.0
C11B—C13B—H13D	109.5	C4F—C5F—H5F	120.0
C11B—C13B—H13E	109.5	C5F—C6F—C7F	120.2 (2)
H13D—C13B—H13E	109.5	C5F—C6F—H6F	119.9
C11B—C13B—H13F	109.5	C7F—C6F—H6F	119.9
H13D—C13B—H13F	109.5	C2F—C7F—C6F	120.6 (2)
H13E—C13B—H13F	109.5	C2F—C7F—H7F	119.7
N1C—C1C—N2C	111.56 (16)	C6F—C7F—H7F	119.7
N1C—C1C—C2C	124.64 (17)	C1F—N1F—C8F	121.47 (15)
N2C—C1C—C2C	123.80 (17)	C1F—N1F—Al2	91.36 (11)
C7C—C2C—C3C	118.6 (2)	C8F—N1F—Al2	144.40 (12)

C7C—C2C—C1C	121.05 (19)	N1F—C8F—C9F	110.87 (16)
C3C—C2C—C1C	120.32 (19)	N1F—C8F—C10F	112.63 (16)
C2C—C3C—C4	120.2 (2)	C9F—C8F—C10F	109.06 (18)
C2C—C3C—H3C	119.9	N1F—C8F—H8F	108.0
C4—C3C—H3C	119.9	C9F—C8F—H8F	108.0
C5C—C4—C3C	120.3 (3)	C10F—C8F—H8F	108.0
C5C—C4—H4	119.8	C8F—C9F—H9F1	109.5
C3C—C4—H4	119.8	C8F—C9F—H9F2	109.5
C6C—C5C—C4	119.9 (2)	H9F1—C9F—H9F2	109.5
C6C—C5C—H5C	120.0	C8F—C9F—H9F3	109.5
C4—C5C—H5C	120.0	H9F1—C9F—H9F3	109.5
C5C—C6C—C7C	120.1 (3)	H9F2—C9F—H9F3	109.5
C5C—C6C—H6C	120.0	C8F—C10F—H10P	109.5
C7C—C6C—H6C	120.0	C8F—C10F—H10Q	109.5
C2C—C7C—C6C	120.9 (2)	H10P—C10F—H10Q	109.5
C2C—C7C—H7C	119.5	C8F—C10F—H10R	109.5
C6C—C7C—H7C	119.5	H10P—C10F—H10R	109.5
C1C—N1C—C11C	122.93 (15)	H10Q—C10F—H10R	109.5
C1C—N1C—Al1	91.86 (11)	C1F—N2F—C11F	123.1 (3)
C11C—N1C—Al1	144.32 (12)	C1F—N2F—C17F	123.0 (8)
N2C—C8C—C10C	111.39 (17)	C1F—N2F—Al2	91.50 (11)
N2C—C8C—C9C	110.70 (15)	C11F—N2F—Al2	144.2 (3)
C10C—C8C—C9C	109.91 (17)	C17F—N2F—Al2	145.0 (8)
N2C—C8C—H8C	108.2	N2F—C11F—C12F	111.7 (4)
C10C—C8C—H8C	108.2	N2F—C11F—C13F	110.8 (3)
C9C—C8C—H8C	108.2	C12F—C11F—C13F	110.3 (3)
C8C—C9C—H9C1	109.5	N2F—C11F—H11F	108.0
C8C—C9C—H9C2	109.5	C12F—C11F—H11F	108.0
H9C1—C9C—H9C2	109.5	C13F—C11F—H11F	108.0
C8C—C9C—H9C3	109.5	C11F—C12F—H12P	109.5
H9C1—C9C—H9C3	109.5	C11F—C12F—H12Q	109.5
H9C2—C9C—H9C3	109.5	H12P—C12F—H12Q	109.5
C8C—C10C—H10G	109.5	C11F—C12F—H12R	109.5
C8C—C10C—H10H	109.5	H12P—C12F—H12R	109.5
H10G—C10C—H10H	109.5	H12Q—C12F—H12R	109.5
C8C—C10C—H10I	109.5	C11F—C13F—H13P	109.5
H10G—C10C—H10I	109.5	C11F—C13F—H13Q	109.5
H10H—C10C—H10I	109.5	H13P—C13F—H13Q	109.5
C1C—N2C—C8C	121.12 (16)	C11F—C13F—H13R	109.5
C1C—N2C—Al1	90.98 (11)	H13P—C13F—H13R	109.5
C8C—N2C—Al1	146.38 (12)	H13Q—C13F—H13R	109.5
N1C—C11C—C12C	111.03 (16)	N2F—C17F—C18F	106.8 (12)
N1C—C11C—C13C	110.77 (16)	N2F—C17F—C19F	109.4 (12)
C12C—C11C—C13C	110.7 (2)	C18F—C17F—C19F	111.4 (11)
N1C—C11C—H11C	108.1	N2F—C17F—H17F	109.7
C12C—C11C—H11C	108.1	C18F—C17F—H17F	109.7
C13C—C11C—H11C	108.1	C19F—C17F—H17F	109.7
C11C—C12C—H12G	109.5	C17F—C18F—H18D	109.5
C11C—C12C—H12H	109.5	C17F—C18F—H18E	109.5

H12G—C12C—H12H	109.5	H18D—C18F—H18E	109.5
C11C—C12C—H12I	109.5	C17F—C18F—H18F	109.5
H12G—C12C—H12I	109.5	H18D—C18F—H18F	109.5
H12H—C12C—H12I	109.5	H18E—C18F—H18F	109.5
C11C—C13C—H13G	109.5	C17F—C19F—H19D	109.5
C11C—C13C—H13H	109.5	C17F—C19F—H19E	109.5
H13G—C13C—H13H	109.5	H19D—C19F—H19E	109.5
C11C—C13C—H13I	109.5	C17F—C19F—H19F	109.5
H13G—C13C—H13I	109.5	H19D—C19F—H19F	109.5
H13H—C13C—H13I	109.5	H19E—C19F—H19F	109.5

N2A—C1A—C2A—C7A	−103.1 (2)	N2D—C1D—C2D—C3D	76.0 (2)
N1A—C1A—C2A—C7A	77.6 (2)	N1D—C1D—C2D—C3D	−104.6 (2)
N2A—C1A—C2A—C3A	78.9 (2)	N2D—C1D—C2D—C7D	−103.5 (2)
N1A—C1A—C2A—C3A	−100.5 (2)	N1D—C1D—C2D—C7D	75.9 (2)
C7A—C2A—C3A—C4A	−1.4 (3)	C7D—C2D—C3D—C4D	0.1 (3)
C1A—C2A—C3A—C4A	176.6 (2)	C1D—C2D—C3D—C4D	−179.46 (17)
C2A—C3A—C4A—C5A	0.1 (4)	C2D—C3D—C4D—C5D	−0.2 (3)
C3A—C4A—C5A—C6A	1.1 (4)	C3D—C4D—C5D—C6D	0.1 (3)
C4A—C5A—C6A—C7A	−1.1 (4)	C4D—C5D—C6D—C7D	0.1 (3)
C3A—C2A—C7A—C6A	1.4 (3)	C5D—C6D—C7D—C2D	−0.2 (3)
C1A—C2A—C7A—C6A	−176.62 (19)	C3D—C2D—C7D—C6D	0.1 (3)
C5A—C6A—C7A—C2A	−0.2 (3)	C1D—C2D—C7D—C6D	179.68 (18)
N2A—C1A—N1A—C11A	178.1 (2)	N2D—C1D—N1D—C8D	−170.76 (16)
C2A—C1A—N1A—C11A	−2.4 (3)	C2D—C1D—N1D—C8D	9.8 (3)
N2A—C1A—N1A—C17A	167.2 (7)	N2D—C1D—N1D—Al2	−0.72 (15)
C2A—C1A—N1A—C17A	−13.3 (7)	C2D—C1D—N1D—Al2	179.81 (15)
N2A—C1A—N1A—Al1	0.87 (15)	C1D—N1D—C8D—C9D	124.70 (18)
C2A—C1A—N1A—Al1	−179.68 (15)	Al2—N1D—C8D—C9D	−37.4 (3)
N1A—C1A—N2A—C8A	175.16 (19)	C1D—N1D—C8D—C10D	−111.8 (2)
C2A—C1A—N2A—C8A	−4.3 (3)	Al2—N1D—C8D—C10D	86.1 (3)
N1A—C1A—N2A—C14A	164.0 (9)	N1D—C1D—N2D—C11D	−171.62 (15)
C2A—C1A—N2A—C14A	−15.4 (9)	C2D—C1D—N2D—C11D	7.9 (3)
N1A—C1A—N2A—Al1	−0.85 (14)	N1D—C1D—N2D—Al2	0.72 (15)
C2A—C1A—N2A—Al1	179.70 (16)	C2D—C1D—N2D—Al2	−179.80 (15)
C9A—C8A—N2A—C1A	120.5 (3)	C1D—N2D—C11D—C13D	−104.30 (19)
C10A—C8A—N2A—C1A	−116.3 (3)	Al2—N2D—C11D—C13D	89.5 (2)
C9A—C8A—N2A—C14A	−145 (8)	C1D—N2D—C11D—C12D	132.35 (17)
C10A—C8A—N2A—C14A	−22 (7)	Al2—N2D—C11D—C12D	−33.8 (3)
C9A—C8A—N2A—Al1	−66.9 (4)	N2E—C1E—C2E—C7E	−73.9 (2)
C10A—C8A—N2A—Al1	56.3 (5)	N1E—C1E—C2E—C7E	106.8 (2)
C15A—C14A—N2A—C1A	87.2 (18)	N2E—C1E—C2E—C3E	107.1 (2)
C16A—C14A—N2A—C1A	−152.0 (12)	N1E—C1E—C2E—C3E	−72.3 (2)
C15A—C14A—N2A—C8A	−4 (6)	C7E—C2E—C3E—C4E	−0.3 (3)
C16A—C14A—N2A—C8A	116 (8)	C1E—C2E—C3E—C4E	178.73 (18)
C15A—C14A—N2A—Al1	−119.1 (15)	C2E—C3E—C4E—C5E	−0.6 (3)
C16A—C14A—N2A—Al1	2 (2)	C3E—C4E—C5E—C6E	1.3 (4)
C1A—N1A—C11A—C13A	40.9 (4)	C4E—C5E—C6E—C7E	−1.0 (4)
C17A—N1A—C11A—C13A	75 (3)	C3E—C2E—C7E—C6E	0.6 (3)

Al1—N1A—C11A—C13A	−143.0 (2)	C1E—C2E—C7E—C6E	−178.46 (19)
C1A—N1A—C11A—C12A	−87.5 (3)	C5E—C6E—C7E—C2E	0.1 (3)
C17A—N1A—C11A—C12A	−53 (3)	N2E—C1E—N1E—C8E	−176.80 (15)
Al1—N1A—C11A—C12A	88.5 (3)	C2E—C1E—N1E—C8E	2.6 (3)
C1A—N1A—C17A—C18A	−120.7 (14)	N2E—C1E—N1E—Al2	−0.01 (14)
C11A—N1A—C17A—C18A	87 (3)	C2E—C1E—N1E—Al2	179.40 (15)
Al1—N1A—C17A—C18A	32 (2)	C1E—N1E—C8E—C10E	110.61 (19)
C1A—N1A—C17A—C19A	115.1 (13)	Al2—N1E—C8E—C10E	−63.7 (3)
C11A—N1A—C17A—C19A	−36.8 (18)	C1E—N1E—C8E—C9E	−126.61 (18)
Al1—N1A—C17A—C19A	−92.3 (17)	Al2—N1E—C8E—C9E	59.1 (3)
N1B—C1B—C2B—C3B	103.6 (2)	N1E—C1E—N2E—C17E	−173.4 (6)
N2B—C1B—C2B—C3B	−74.5 (2)	C2E—C1E—N2E—C17E	7.2 (6)
N1B—C1B—C2B—C7B	−76.8 (2)	N1E—C1E—N2E—C11E	−175.0 (2)
N2B—C1B—C2B—C7B	105.1 (2)	C2E—C1E—N2E—C11E	5.6 (3)
C7B—C2B—C3B—C4B	0.0 (3)	N1E—C1E—N2E—Al2	0.01 (14)
C1B—C2B—C3B—C4B	179.67 (18)	C2E—C1E—N2E—Al2	−179.39 (15)
C2B—C3B—C4B—C5B	0.2 (3)	C1E—N2E—C11E—C12E	118.7 (6)
C3B—C4B—C5B—C6B	−0.4 (3)	C17E—N2E—C11E—C12E	−58.1 (16)
C4B—C5B—C6B—C7B	0.4 (3)	Al2—N2E—C11E—C12E	−51.1 (8)
C5B—C6B—C7B—C2B	−0.1 (3)	C1E—N2E—C11E—C13E	−121.9 (3)
C3B—C2B—C7B—C6B	−0.1 (3)	C17E—N2E—C11E—C13E	61.3 (14)
C1B—C2B—C7B—C6B	−179.73 (17)	Al2—N2E—C11E—C13E	68.3 (5)
N2B—C1B—N1B—C8B	173.84 (15)	C1E—N2E—C17E—C19E	−44.8 (10)
C2B—C1B—N1B—C8B	−4.5 (3)	C11E—N2E—C17E—C19E	−40.6 (10)
N2B—C1B—N1B—Al1	−0.36 (14)	Al2—N2E—C17E—C19E	143.9 (4)
C2B—C1B—N1B—Al1	−178.70 (15)	C1E—N2E—C17E—C18E	80.7 (15)
C1B—N1B—C8B—C9B	−131.79 (18)	C11E—N2E—C17E—C18E	85 (2)
Al1—N1B—C8B—C9B	37.6 (3)	Al2—N2E—C17E—C18E	−90.6 (14)
C1B—N1B—C8B—C10B	105.45 (19)	N2F—C1F—C2F—C7F	60.3 (2)
Al1—N1B—C8B—C10B	−85.2 (2)	N1F—C1F—C2F—C7F	−118.3 (2)
N1B—C1B—N2B—C11B	170.92 (15)	N2F—C1F—C2F—C3F	−121.9 (2)
C2B—C1B—N2B—C11B	−10.7 (2)	N1F—C1F—C2F—C3F	59.4 (2)
N1B—C1B—N2B—Al1	0.36 (14)	C7F—C2F—C3F—C4F	−0.6 (3)
C2B—C1B—N2B—Al1	178.73 (14)	C1F—C2F—C3F—C4F	−178.45 (17)
C12B—C11B—N2B—C1B	118.59 (19)	C2F—C3F—C4F—C5F	0.8 (3)
C13B—C11B—N2B—C1B	−117.33 (18)	C3F—C4F—C5F—C6F	−0.2 (3)
C12B—C11B—N2B—Al1	−78.5 (3)	C4F—C5F—C6F—C7F	−0.5 (3)
C13B—C11B—N2B—Al1	45.6 (3)	C3F—C2F—C7F—C6F	−0.1 (3)
N1C—C1C—C2C—C7C	−75.1 (3)	C1F—C2F—C7F—C6F	177.67 (18)
N2C—C1C—C2C—C7C	104.0 (2)	C5F—C6F—C7F—C2F	0.7 (3)
N1C—C1C—C2C—C3C	106.8 (2)	N2F—C1F—N1F—C8F	−166.75 (15)
N2C—C1C—C2C—C3C	−74.2 (3)	C2F—C1F—N1F—C8F	12.1 (3)
C7C—C2C—C3C—C4	0.8 (3)	N2F—C1F—N1F—Al2	−1.25 (14)
C1C—C2C—C3C—C4	179.0 (2)	C2F—C1F—N1F—Al2	177.56 (15)
C2C—C3C—C4—C5C	−0.6 (4)	C1F—N1F—C8F—C9F	118.5 (2)
C3C—C4—C5C—C6C	−0.5 (4)	Al2—N1F—C8F—C9F	−36.0 (3)
C4—C5C—C6C—C7C	1.2 (4)	C1F—N1F—C8F—C10F	−118.93 (19)
C3C—C2C—C7C—C6C	0.0 (3)	Al2—N1F—C8F—C10F	86.5 (2)
C1C—C2C—C7C—C6C	−178.2 (2)	N1F—C1F—N2F—C11F	−168.8 (3)

C5C—C6C—C7C—C2C	−1.0 (4)	C2F—C1F—N2F—C11F	12.4 (3)
N2C—C1C—N1C—C11C	171.40 (15)	N1F—C1F—N2F—C17F	−172.5 (8)
C2C—C1C—N1C—C11C	−9.4 (3)	C2F—C1F—N2F—C17F	8.7 (8)
N2C—C1C—N1C—Al1	−0.18 (16)	N1F—C1F—N2F—Al2	1.26 (14)
C2C—C1C—N1C—Al1	178.99 (17)	C2F—C1F—N2F—Al2	−177.55 (15)
N1C—C1C—N2C—C8C	169.67 (16)	C1F—N2F—C11F—C12F	117.7 (4)
C2C—C1C—N2C—C8C	−9.5 (3)	C17F—N2F—C11F—C12F	−152 (21)
N1C—C1C—N2C—Al1	0.17 (15)	Al2—N2F—C11F—C12F	−45.2 (6)
C2C—C1C—N2C—Al1	−179.00 (17)	C1F—N2F—C11F—C13F	−118.9 (5)
C10C—C8C—N2C—C1C	112.2 (2)	C17F—N2F—C11F—C13F	−29 (20)
C9C—C8C—N2C—C1C	−125.21 (19)	Al2—N2F—C11F—C13F	78.2 (6)
C10C—C8C—N2C—Al1	−87.1 (3)	C1F—N2F—C17F—C18F	97.8 (13)
C9C—C8C—N2C—Al1	35.6 (3)	C11F—N2F—C17F—C18F	6 (19)
C1C—N1C—C11C—C12C	130.3 (2)	Al2—N2F—C17F—C18F	−71.2 (16)
Al1—N1C—C11C—C12C	−64.2 (3)	C1F—N2F—C17F—C19F	−141.5 (10)
C1C—N1C—C11C—C13C	−106.2 (2)	C11F—N2F—C17F—C19F	127 (21)
Al1—N1C—C11C—C13C	59.3 (3)	Al2—N2F—C17F—C19F	49.5 (18)

(AlPhCNiPr22Cl) Chloridobis(*N*,*N*′-diisopropylbenzimidamido)aluminium(III)

Crystal data

$[Al(C_{13}H_{19}N_2)_2Cl]$
M_r = 469.03
Monoclinic, $P2_1/c$
a = 19.205 (1) Å
b = 16.4832 (9) Å
c = 17.8498 (10) Å
β = 106.287 (1)°
V = 5423.8 (5) Å^3
Z = 8
$F(000)$ = 2016
D_x = 1.149 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8832 reflections
θ = 2.2–25.1°
μ = 0.19 mm^{-1}
T = 100 K
Prism, yellow
0.21 × 0.20 × 0.14 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (TWINABS; Sheldrick, 2008)
T_{min} = 0.858, T_{max} = 0.973
100296 measured reflections
10641 independent reflections
7375 reflections with $I > 2\sigma(I)$
R_{int} = 0.080
θ_{max} = 26.0°, θ_{min} = 1.7°
h = 0→23
k = −20→0
l = −22→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.090
S = 1.00
10641 reflections
593 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 4.680P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Special details

Experimental. Integrated as non-merohedrally split crystal. Single reflection set is generated based on the reflections of the first component and overlapped reflections of the first and second components.

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. H atoms were positioned from geometric considerations and refined as riding on the attached atoms with orientation of CH3 groups optimized. U_{iso} of H atoms were contrained to be 20% larger than Ueqv of the attached atom (50% larger for CH3 groups).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.40996 (3)	0.30415 (4)	0.46657 (4)	0.02013 (15)
Cl1	0.48446 (3)	0.33724 (3)	0.39740 (3)	0.02442 (13)
C1A	0.45647 (11)	0.34633 (12)	0.59834 (13)	0.0226 (5)
C2A	0.48630 (12)	0.37850 (13)	0.67933 (12)	0.0229 (5)
C3A	0.51624 (12)	0.45585 (13)	0.69101 (13)	0.0269 (5)
H3A	0.5171	0.4886	0.6475	0.032*
C4A	0.54482 (12)	0.48525 (14)	0.76596 (14)	0.0311 (6)
H4A	0.5661	0.5377	0.7738	0.037*
C5A	0.54242 (13)	0.43847 (15)	0.82921 (14)	0.0362 (6)
H5A	0.5614	0.4591	0.8806	0.043*
C6A	0.51261 (14)	0.36187 (15)	0.81813 (14)	0.0382 (6)
H6A	0.5114	0.3298	0.8619	0.046*
C7A	0.48443 (13)	0.33143 (14)	0.74348 (13)	0.0312 (6)
H7A	0.4639	0.2786	0.7360	0.037*
N1A	0.39906 (9)	0.37715 (10)	0.54562 (10)	0.0239 (4)
C11A	0.34861 (12)	0.43629 (14)	0.56244 (13)	0.0281 (5)
H11A	0.3687	0.4558	0.6173	0.034*
C12A	0.27567 (13)	0.39630 (16)	0.55493 (16)	0.0400 (6)
H12A	0.2558	0.3759	0.5016	0.060*
H12B	0.2422	0.4361	0.5665	0.060*
H12C	0.2820	0.3511	0.5919	0.060*
C13A	0.34198 (13)	0.50824 (14)	0.50763 (15)	0.0356 (6)
H13A	0.3898	0.5329	0.5148	0.053*
H13B	0.3088	0.5484	0.5192	0.053*
H13C	0.3230	0.4898	0.4535	0.053*
N2A	0.48408 (9)	0.28481 (10)	0.56825 (10)	0.0223 (4)
C21A	0.55718 (12)	0.25225 (13)	0.60462 (14)	0.0276 (5)
H21A	0.5635	0.2450	0.6618	0.033*
C22A	0.56353 (13)	0.16986 (14)	0.56882 (14)	0.0338 (6)
H22A	0.5286	0.1322	0.5808	0.051*
H22B	0.6128	0.1488	0.5905	0.051*
H22C	0.5533	0.1755	0.5121	0.051*
C23A	0.61602 (13)	0.30916 (15)	0.59374 (16)	0.0415 (7)
H23A	0.6106	0.3164	0.5379	0.062*
H23B	0.6638	0.2859	0.6189	0.062*
H23C	0.6116	0.3618	0.6174	0.062*

C1B	0.30417 (11)	0.24168 (13)	0.38434 (12)	0.0212 (5)
C2B	0.24110 (11)	0.19646 (13)	0.33379 (12)	0.0227 (5)
C3B	0.25077 (12)	0.14563 (14)	0.27549 (13)	0.0283 (5)
H3B	0.2971	0.1412	0.2666	0.034*
C4B	0.19276 (13)	0.10123 (15)	0.23016 (14)	0.0344 (6)
H4B	0.1992	0.0675	0.1894	0.041*
C5B	0.12579 (14)	0.10598 (16)	0.24418 (15)	0.0393 (6)
H5B	0.0863	0.0749	0.2136	0.047*
C6B	0.11620 (13)	0.15570 (16)	0.30243 (15)	0.0388 (6)
H6B	0.0701	0.1587	0.3121	0.047*
C7B	0.17323 (12)	0.20128 (14)	0.34691 (13)	0.0295 (5)
H7B	0.1661	0.2360	0.3866	0.035*
N1B	0.35512 (9)	0.20577 (10)	0.44238 (10)	0.0213 (4)
C11B	0.34447 (12)	0.12476 (13)	0.47142 (13)	0.0256 (5)
H11B	0.2934	0.1079	0.4452	0.031*
C12B	0.35318 (13)	0.12823 (15)	0.55884 (13)	0.0348 (6)
H12D	0.4028	0.1447	0.5862	0.052*
H12E	0.3435	0.0745	0.5773	0.052*
H12F	0.3189	0.1676	0.5693	0.052*
C13B	0.39439 (13)	0.06279 (13)	0.45069 (14)	0.0329 (6)
H13D	0.3859	0.0616	0.3939	0.049*
H13E	0.3845	0.0091	0.4689	0.049*
H13F	0.4450	0.0777	0.4758	0.049*
N2B	0.31993 (9)	0.31941 (10)	0.38067 (10)	0.0220 (4)
C21B	0.28949 (12)	0.37497 (13)	0.31475 (13)	0.0272 (5)
H21B	0.3180	0.4264	0.3275	0.033*
C22B	0.21167 (13)	0.39796 (15)	0.30638 (15)	0.0383 (6)
H22D	0.1804	0.3506	0.2892	0.058*
H22E	0.1971	0.4414	0.2677	0.058*
H22F	0.2069	0.4168	0.3568	0.058*
C23B	0.30095 (13)	0.34464 (14)	0.23853 (13)	0.0319 (6)
H23D	0.3521	0.3306	0.2468	0.048*
H23E	0.2872	0.3873	0.1988	0.048*
H23F	0.2709	0.2965	0.2209	0.048*
Al2	0.09906 (3)	0.69869 (4)	0.04045 (4)	0.01958 (14)
Cl2	0.03433 (3)	0.64402 (3)	0.11154 (3)	0.02421 (13)
C1C	0.19838 (11)	0.77567 (12)	0.11760 (12)	0.0207 (5)
C2C	0.25703 (11)	0.82799 (13)	0.16634 (12)	0.0212 (5)
C3C	0.32648 (12)	0.82681 (13)	0.15708 (13)	0.0265 (5)
H3C	0.3376	0.7907	0.1206	0.032*
C4C	0.37958 (13)	0.87813 (14)	0.20084 (13)	0.0308 (6)
H4C	0.4268	0.8776	0.1938	0.037*
C5C	0.36378 (13)	0.93017 (14)	0.25483 (13)	0.0308 (6)
H5C	0.4001	0.9658	0.2844	0.037*
C6C	0.29541 (13)	0.93037 (14)	0.26565 (13)	0.0309 (6)
H6C	0.2851	0.9650	0.3037	0.037*
C7C	0.24181 (12)	0.88011 (13)	0.22103 (13)	0.0267 (5)
H7C	0.1945	0.8812	0.2278	0.032*
N1C	0.19321 (9)	0.69659 (10)	0.12535 (10)	0.0217 (4)

C11C	0.23760 (12)	0.65363 (13)	0.19509 (13)	0.0272 (5)
H11C	0.2856	0.6817	0.2133	0.033*
C12C	0.25070 (15)	0.56752 (14)	0.17359 (15)	0.0420 (7)
H12G	0.2041	0.5394	0.1543	0.063*
H12H	0.2806	0.5393	0.2197	0.063*
H12I	0.2758	0.5680	0.1328	0.063*
C13C	0.20164 (13)	0.65577 (15)	0.26103 (13)	0.0359 (6)
H13G	0.1967	0.7122	0.2761	0.054*
H13H	0.2315	0.6258	0.3060	0.054*
H13I	0.1535	0.6307	0.2434	0.054*
N2C	0.14207 (9)	0.80444 (10)	0.06068 (10)	0.0201 (4)
C21C	0.14526 (12)	0.88486 (13)	0.02560 (13)	0.0247 (5)
H21C	0.1954	0.9067	0.0478	0.030*
C22C	0.13202 (14)	0.87677 (14)	−0.06213 (13)	0.0347 (6)
H22G	0.1676	0.8392	−0.0729	0.052*
H22H	0.1370	0.9300	−0.0845	0.052*
H22I	0.0830	0.8558	−0.0856	0.052*
C23C	0.09284 (13)	0.94365 (13)	0.04646 (14)	0.0303 (6)
H23G	0.0432	0.9233	0.0260	0.045*
H23H	0.0969	0.9969	0.0236	0.045*
H23I	0.1046	0.9487	0.1033	0.045*
C1D	0.04966 (11)	0.66175 (12)	−0.09242 (12)	0.0209 (5)
C2D	0.02093 (11)	0.63235 (13)	−0.17414 (12)	0.0214 (5)
C3D	0.02412 (12)	0.68126 (14)	−0.23634 (13)	0.0283 (5)
H3D	0.0435	0.7345	−0.2269	0.034*
C4D	−0.00084 (13)	0.65272 (14)	−0.31228 (14)	0.0329 (6)
H4D	0.0019	0.6862	−0.3547	0.039*
C5D	−0.02962 (12)	0.57563 (14)	−0.32616 (13)	0.0309 (6)
H5D	−0.0469	0.5562	−0.3782	0.037*
C6D	−0.03325 (12)	0.52686 (14)	−0.26466 (13)	0.0286 (5)
H6D	−0.0534	0.4740	−0.2745	0.034*
C7D	−0.00768 (12)	0.55463 (13)	−0.18853 (13)	0.0263 (5)
H7D	−0.0097	0.5206	−0.1463	0.032*
N1D	0.01586 (9)	0.71126 (10)	−0.05597 (10)	0.0227 (4)
C11D	−0.06152 (12)	0.73053 (14)	−0.08691 (13)	0.0282 (5)
H11D	−0.0729	0.7380	−0.1447	0.034*
C12D	−0.07695 (13)	0.80964 (16)	−0.05082 (14)	0.0407 (7)
H12J	−0.0628	0.8044	0.0061	0.061*
H12K	−0.1289	0.8220	−0.0696	0.061*
H12L	−0.0491	0.8536	−0.0657	0.061*
C13D	−0.10924 (13)	0.66258 (16)	−0.07050 (15)	0.0421 (7)
H13J	−0.0988	0.6121	−0.0943	0.063*
H13K	−0.1604	0.6769	−0.0927	0.063*
H13L	−0.0991	0.6551	−0.0140	0.063*
N2D	0.11453 (9)	0.63989 (11)	−0.04533 (10)	0.0227 (4)
C21D	0.16736 (13)	0.59264 (15)	−0.07247 (14)	0.0355 (6)
H21D	0.1514	0.5919	−0.1308	0.043*
C22D	0.24112 (13)	0.63313 (18)	−0.04624 (16)	0.0460 (7)
H22J	0.2386	0.6866	−0.0708	0.069*

H22K	0.2769	0.5995	−0.0616	0.069*
H22L	0.2555	0.6394	0.0106	0.069*
C23D	0.16898 (15)	0.50588 (16)	−0.04362 (18)	0.0570 (9)
H23J	0.1840	0.5054	0.0136	0.086*
H23K	0.2035	0.4742	−0.0630	0.086*
H23L	0.1205	0.4820	−0.0628	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0243 (3)	0.0176 (3)	0.0185 (3)	0.0012 (3)	0.0061 (3)	−0.0007 (3)
Cl1	0.0279 (3)	0.0244 (3)	0.0238 (3)	−0.0044 (2)	0.0118 (2)	0.0012 (2)
C1A	0.0272 (12)	0.0177 (11)	0.0240 (12)	−0.0022 (9)	0.0088 (10)	0.0009 (9)
C2A	0.0270 (12)	0.0220 (12)	0.0192 (12)	0.0010 (9)	0.0056 (9)	−0.0022 (9)
C3A	0.0319 (13)	0.0223 (12)	0.0260 (13)	0.0006 (10)	0.0071 (10)	−0.0006 (10)
C4A	0.0342 (14)	0.0247 (13)	0.0323 (14)	−0.0038 (11)	0.0058 (11)	−0.0062 (11)
C5A	0.0458 (16)	0.0365 (15)	0.0225 (13)	−0.0030 (12)	0.0034 (11)	−0.0093 (11)
C6A	0.0579 (17)	0.0338 (14)	0.0222 (13)	−0.0019 (13)	0.0102 (12)	0.0031 (11)
C7A	0.0418 (15)	0.0236 (12)	0.0276 (13)	−0.0065 (11)	0.0086 (11)	−0.0004 (10)
N1A	0.0276 (10)	0.0213 (10)	0.0221 (10)	0.0072 (8)	0.0057 (8)	−0.0026 (8)
C11A	0.0302 (13)	0.0292 (13)	0.0247 (13)	0.0075 (10)	0.0074 (10)	−0.0060 (10)
C12A	0.0387 (15)	0.0424 (16)	0.0443 (16)	0.0083 (12)	0.0201 (13)	0.0004 (13)
C13A	0.0384 (15)	0.0240 (13)	0.0438 (16)	0.0084 (11)	0.0106 (12)	−0.0027 (11)
N2A	0.0257 (10)	0.0187 (9)	0.0209 (10)	0.0031 (8)	0.0037 (8)	−0.0015 (8)
C21A	0.0253 (12)	0.0270 (12)	0.0264 (13)	0.0055 (10)	0.0004 (10)	−0.0015 (10)
C22A	0.0336 (14)	0.0313 (13)	0.0321 (14)	0.0105 (11)	0.0017 (11)	−0.0036 (11)
C23A	0.0277 (14)	0.0375 (15)	0.0548 (18)	0.0023 (12)	0.0044 (12)	−0.0082 (13)
C1B	0.0213 (11)	0.0263 (12)	0.0175 (11)	0.0017 (9)	0.0079 (9)	−0.0010 (9)
C2B	0.0262 (12)	0.0210 (11)	0.0198 (12)	−0.0003 (10)	0.0045 (9)	0.0056 (9)
C3B	0.0258 (12)	0.0320 (13)	0.0259 (13)	−0.0011 (10)	0.0054 (10)	0.0022 (10)
C4B	0.0389 (15)	0.0341 (14)	0.0257 (13)	−0.0047 (12)	0.0020 (11)	−0.0011 (11)
C5B	0.0338 (15)	0.0415 (15)	0.0356 (15)	−0.0142 (12)	−0.0018 (12)	0.0086 (12)
C6B	0.0281 (13)	0.0473 (16)	0.0403 (16)	−0.0046 (12)	0.0082 (11)	0.0138 (13)
C7B	0.0277 (13)	0.0335 (13)	0.0278 (13)	0.0017 (11)	0.0085 (10)	0.0056 (11)
N1B	0.0241 (10)	0.0198 (9)	0.0193 (10)	0.0009 (8)	0.0051 (8)	0.0042 (8)
C11B	0.0276 (12)	0.0212 (12)	0.0265 (13)	−0.0042 (10)	0.0052 (10)	0.0065 (10)
C12B	0.0443 (15)	0.0322 (14)	0.0305 (14)	0.0056 (12)	0.0146 (12)	0.0117 (11)
C13B	0.0461 (15)	0.0202 (12)	0.0300 (14)	−0.0035 (11)	0.0070 (12)	0.0007 (10)
N2B	0.0295 (10)	0.0172 (9)	0.0191 (10)	0.0033 (8)	0.0066 (8)	0.0021 (7)
C21B	0.0347 (13)	0.0219 (12)	0.0244 (13)	0.0042 (10)	0.0073 (10)	0.0052 (10)
C22B	0.0385 (15)	0.0381 (15)	0.0379 (15)	0.0080 (12)	0.0099 (12)	0.0133 (12)
C23B	0.0419 (14)	0.0289 (13)	0.0237 (13)	0.0024 (11)	0.0071 (11)	0.0045 (10)
Al2	0.0237 (3)	0.0166 (3)	0.0190 (3)	0.0011 (3)	0.0068 (3)	0.0000 (3)
Cl2	0.0264 (3)	0.0266 (3)	0.0213 (3)	−0.0061 (2)	0.0096 (2)	0.0024 (2)
C1C	0.0255 (12)	0.0221 (12)	0.0179 (11)	0.0014 (9)	0.0116 (9)	0.0005 (9)
C2C	0.0246 (11)	0.0190 (11)	0.0191 (11)	−0.0012 (9)	0.0044 (9)	0.0040 (9)
C3C	0.0320 (13)	0.0261 (12)	0.0232 (12)	0.0007 (10)	0.0109 (10)	−0.0008 (10)
C4C	0.0294 (13)	0.0336 (14)	0.0306 (14)	−0.0058 (11)	0.0107 (11)	0.0024 (11)
C5C	0.0360 (14)	0.0287 (13)	0.0247 (13)	−0.0096 (11)	0.0034 (11)	−0.0005 (10)
C6C	0.0371 (14)	0.0298 (13)	0.0250 (13)	−0.0024 (11)	0.0073 (11)	−0.0046 (10)

C7C	0.0265 (12)	0.0305 (13)	0.0235 (12)	0.0003 (10)	0.0075 (10)	−0.0014 (10)
N1C	0.0249 (10)	0.0178 (9)	0.0214 (10)	0.0018 (8)	0.0048 (8)	0.0032 (8)
C11C	0.0293 (12)	0.0236 (12)	0.0255 (13)	0.0014 (10)	0.0024 (10)	0.0075 (10)
C12C	0.0542 (17)	0.0272 (14)	0.0401 (16)	0.0095 (12)	0.0060 (13)	0.0113 (12)
C13C	0.0395 (14)	0.0409 (15)	0.0245 (13)	0.0002 (12)	0.0043 (11)	0.0081 (11)
N2C	0.0234 (9)	0.0172 (9)	0.0192 (10)	0.0012 (8)	0.0051 (8)	0.0032 (8)
C21C	0.0285 (12)	0.0190 (11)	0.0272 (13)	0.0010 (10)	0.0089 (10)	0.0047 (9)
C22C	0.0518 (16)	0.0281 (13)	0.0272 (14)	0.0052 (12)	0.0159 (12)	0.0077 (11)
C23C	0.0362 (14)	0.0203 (12)	0.0329 (14)	0.0025 (10)	0.0071 (11)	0.0010 (10)
C1D	0.0268 (12)	0.0156 (11)	0.0213 (12)	−0.0010 (9)	0.0082 (9)	0.0005 (9)
C2D	0.0221 (11)	0.0207 (11)	0.0219 (12)	0.0024 (9)	0.0070 (9)	−0.0021 (9)
C3D	0.0356 (14)	0.0245 (12)	0.0251 (13)	−0.0038 (10)	0.0090 (10)	−0.0020 (10)
C4D	0.0427 (15)	0.0339 (14)	0.0233 (13)	−0.0026 (12)	0.0111 (11)	0.0021 (11)
C5D	0.0348 (14)	0.0380 (14)	0.0206 (13)	−0.0026 (11)	0.0088 (10)	−0.0085 (11)
C6D	0.0302 (13)	0.0237 (12)	0.0312 (14)	−0.0036 (10)	0.0073 (11)	−0.0077 (10)
C7D	0.0308 (13)	0.0229 (12)	0.0253 (13)	0.0000 (10)	0.0078 (10)	0.0017 (10)
N1D	0.0226 (10)	0.0217 (10)	0.0233 (10)	0.0037 (8)	0.0056 (8)	−0.0020 (8)
C11D	0.0252 (12)	0.0345 (13)	0.0225 (12)	0.0078 (10)	0.0027 (10)	−0.0044 (10)
C12D	0.0341 (14)	0.0491 (16)	0.0333 (15)	0.0189 (13)	0.0001 (11)	−0.0098 (12)
C13D	0.0254 (13)	0.0557 (18)	0.0434 (16)	−0.0025 (13)	0.0065 (11)	−0.0035 (14)
N2D	0.0236 (10)	0.0227 (10)	0.0218 (10)	0.0038 (8)	0.0066 (8)	−0.0020 (8)
C21D	0.0312 (14)	0.0446 (16)	0.0294 (14)	0.0120 (12)	0.0063 (11)	−0.0124 (12)
C22D	0.0268 (14)	0.072 (2)	0.0414 (16)	0.0052 (14)	0.0137 (12)	−0.0041 (15)
C23D	0.0465 (18)	0.0330 (16)	0.077 (2)	0.0167 (13)	−0.0068 (15)	−0.0219 (15)

Geometric parameters (Å, º)

Al1—N1A	1.9102 (18)	Al2—N2D	1.9046 (18)
Al1—N1B	1.9157 (18)	Al2—N2C	1.9194 (18)
Al1—N2B	1.9791 (18)	Al2—N1D	2.0039 (18)
Al1—N2A	1.9932 (18)	Al2—N1C	2.0076 (18)
Al1—Cl1	2.2046 (8)	Al2—Cl2	2.2027 (8)
C1A—N2A	1.326 (3)	C1C—N1C	1.317 (3)
C1A—N1A	1.333 (3)	C1C—N2C	1.345 (3)
C1A—C2A	1.495 (3)	C1C—C2C	1.490 (3)
C2A—C3A	1.390 (3)	C2C—C3C	1.389 (3)
C2A—C7A	1.392 (3)	C2C—C7C	1.392 (3)
C3A—C4A	1.383 (3)	C3C—C4C	1.385 (3)
C3A—H3A	0.9500	C3C—H3C	0.9500
C4A—C5A	1.379 (3)	C4C—C5C	1.386 (3)
C4A—H4A	0.9500	C4C—H4C	0.9500
C5A—C6A	1.378 (3)	C5C—C6C	1.380 (3)
C5A—H5A	0.9500	C5C—H5C	0.9500
C6A—C7A	1.384 (3)	C6C—C7C	1.386 (3)
C6A—H6A	0.9500	C6C—H6C	0.9500
C7A—H7A	0.9500	C7C—H7C	0.9500
N1A—C11A	1.464 (3)	N1C—C11C	1.477 (3)
C11A—C12A	1.520 (3)	C11C—C12C	1.510 (3)
C11A—C13A	1.520 (3)	C11C—C13C	1.523 (3)
C11A—H11A	1.0000	C11C—H11C	1.0000

C12A—H12A	0.9800	C12C—H12G	0.9800
C12A—H12B	0.9800	C12C—H12H	0.9800
C12A—H12C	0.9800	C12C—H12I	0.9800
C13A—H13A	0.9800	C13C—H13G	0.9800
C13A—H13B	0.9800	C13C—H13H	0.9800
C13A—H13C	0.9800	C13C—H13I	0.9800
N2A—C21A	1.473 (3)	N2C—C21C	1.475 (3)
C21A—C22A	1.520 (3)	C21C—C23C	1.517 (3)
C21A—C23A	1.522 (3)	C21C—C22C	1.520 (3)
C21A—H21A	1.0000	C21C—H21C	1.0000
C22A—H22A	0.9800	C22C—H22G	0.9800
C22A—H22B	0.9800	C22C—H22H	0.9800
C22A—H22C	0.9800	C22C—H22I	0.9800
C23A—H23A	0.9800	C23C—H23G	0.9800
C23A—H23B	0.9800	C23C—H23H	0.9800
C23A—H23C	0.9800	C23C—H23I	0.9800
C1B—N2B	1.322 (3)	C1D—N1D	1.322 (3)
C1B—N1B	1.346 (3)	C1D—N2D	1.342 (3)
C1B—C2B	1.491 (3)	C1D—C2D	1.489 (3)
C2B—C3B	1.388 (3)	C2D—C3D	1.387 (3)
C2B—C7B	1.390 (3)	C2D—C7D	1.389 (3)
C3B—C4B	1.388 (3)	C3D—C4D	1.387 (3)
C3B—H3B	0.9500	C3D—H3D	0.9500
C4B—C5B	1.380 (3)	C4D—C5D	1.380 (3)
C4B—H4B	0.9500	C4D—H4D	0.9500
C5B—C6B	1.376 (4)	C5D—C6D	1.378 (3)
C5B—H5B	0.9500	C5D—H5D	0.9500
C6B—C7B	1.381 (3)	C6D—C7D	1.387 (3)
C6B—H6B	0.9500	C6D—H6D	0.9500
C7B—H7B	0.9500	C7D—H7D	0.9500
N1B—C11B	1.467 (3)	N1D—C11D	1.468 (3)
C11B—C13B	1.516 (3)	C11D—C12D	1.520 (3)
C11B—C12B	1.523 (3)	C11D—C13D	1.527 (3)
C11B—H11B	1.0000	C11D—H11D	1.0000
C12B—H12D	0.9800	C12D—H12J	0.9800
C12B—H12E	0.9800	C12D—H12K	0.9800
C12B—H12F	0.9800	C12D—H12L	0.9800
C13B—H13D	0.9800	C13D—H13J	0.9800
C13B—H13E	0.9800	C13D—H13K	0.9800
C13B—H13F	0.9800	C13D—H13L	0.9800
N2B—C21B	1.476 (3)	N2D—C21D	1.465 (3)
C21B—C22B	1.508 (3)	C21D—C22D	1.516 (3)
C21B—C23B	1.522 (3)	C21D—C23D	1.517 (4)
C21B—H21B	1.0000	C21D—H21D	1.0000
C22B—H22D	0.9800	C22D—H22J	0.9800
C22B—H22E	0.9800	C22D—H22K	0.9800
C22B—H22F	0.9800	C22D—H22L	0.9800
C23B—H23D	0.9800	C23D—H23J	0.9800
C23B—H23E	0.9800	C23D—H23K	0.9800

C23B—H23F	0.9800	C23D—H23L	0.9800
N1A—Al1—N1B	122.18 (8)	N2D—Al2—N2C	117.22 (8)
N1A—Al1—N2B	103.84 (8)	N2D—Al2—N1D	68.20 (7)
N1B—Al1—N2B	68.12 (7)	N2C—Al2—N1D	105.37 (8)
N1A—Al1—N2A	68.06 (7)	N2D—Al2—N1C	106.71 (8)
N1B—Al1—N2A	106.08 (8)	N2C—Al2—N1C	67.95 (7)
N2B—Al1—N2A	166.28 (8)	N1D—Al2—N1C	169.27 (8)
N1A—Al1—Cl1	118.73 (6)	N2D—Al2—Cl2	119.70 (6)
N1B—Al1—Cl1	119.03 (6)	N2C—Al2—Cl2	123.08 (6)
N2B—Al1—Cl1	95.62 (6)	N1D—Al2—Cl2	95.41 (6)
N2A—Al1—Cl1	98.02 (6)	N1C—Al2—Cl2	95.31 (6)
N2A—C1A—N1A	110.55 (19)	N1C—C1C—N2C	111.09 (19)
N2A—C1A—C2A	125.08 (19)	N1C—C1C—C2C	125.32 (19)
N1A—C1A—C2A	124.35 (19)	N2C—C1C—C2C	123.57 (18)
C3A—C2A—C7A	119.5 (2)	C3C—C2C—C7C	119.3 (2)
C3A—C2A—C1A	120.04 (19)	C3C—C2C—C1C	121.08 (19)
C7A—C2A—C1A	120.43 (19)	C7C—C2C—C1C	119.59 (19)
C4A—C3A—C2A	120.1 (2)	C4C—C3C—C2C	120.3 (2)
C4A—C3A—H3A	119.9	C4C—C3C—H3C	119.9
C2A—C3A—H3A	119.9	C2C—C3C—H3C	119.9
C5A—C4A—C3A	120.0 (2)	C3C—C4C—C5C	120.0 (2)
C5A—C4A—H4A	120.0	C3C—C4C—H4C	120.0
C3A—C4A—H4A	120.0	C5C—C4C—H4C	120.0
C6A—C5A—C4A	120.2 (2)	C6C—C5C—C4C	120.1 (2)
C6A—C5A—H5A	119.9	C6C—C5C—H5C	120.0
C4A—C5A—H5A	119.9	C4C—C5C—H5C	120.0
C5A—C6A—C7A	120.3 (2)	C5C—C6C—C7C	120.1 (2)
C5A—C6A—H6A	119.8	C5C—C6C—H6C	120.0
C7A—C6A—H6A	119.8	C7C—C6C—H6C	120.0
C6A—C7A—C2A	119.8 (2)	C6C—C7C—C2C	120.3 (2)
C6A—C7A—H7A	120.1	C6C—C7C—H7C	119.9
C2A—C7A—H7A	120.1	C2C—C7C—H7C	119.9
C1A—N1A—C11A	124.96 (18)	C1C—N1C—C11C	121.34 (18)
C1A—N1A—Al1	92.36 (13)	C1C—N1C—Al2	88.97 (13)
C11A—N1A—Al1	141.91 (15)	C11C—N1C—Al2	146.00 (14)
N1A—C11A—C12A	109.87 (19)	N1C—C11C—C12C	109.53 (19)
N1A—C11A—C13A	109.18 (18)	N1C—C11C—C13C	111.13 (18)
C12A—C11A—C13A	111.9 (2)	C12C—C11C—C13C	111.2 (2)
N1A—C11A—H11A	108.6	N1C—C11C—H11C	108.3
C12A—C11A—H11A	108.6	C12C—C11C—H11C	108.3
C13A—C11A—H11A	108.6	C13C—C11C—H11C	108.3
C11A—C12A—H12A	109.5	C11C—C12C—H12G	109.5
C11A—C12A—H12B	109.5	C11C—C12C—H12H	109.5
H12A—C12A—H12B	109.5	H12G—C12C—H12H	109.5
C11A—C12A—H12C	109.5	C11C—C12C—H12I	109.5
H12A—C12A—H12C	109.5	H12G—C12C—H12I	109.5
H12B—C12A—H12C	109.5	H12H—C12C—H12I	109.5
C11A—C13A—H13A	109.5	C11C—C13C—H13G	109.5

C11A—C13A—H13B	109.5	C11C—C13C—H13H	109.5
H13A—C13A—H13B	109.5	H13G—C13C—H13H	109.5
C11A—C13A—H13C	109.5	C11C—C13C—H13I	109.5
H13A—C13A—H13C	109.5	H13G—C13C—H13I	109.5
H13B—C13A—H13C	109.5	H13H—C13C—H13I	109.5
C1A—N2A—C21A	122.71 (18)	C1C—N2C—C21C	121.15 (17)
C1A—N2A—Al1	88.97 (13)	C1C—N2C—Al2	91.97 (13)
C21A—N2A—Al1	143.97 (15)	C21C—N2C—Al2	143.46 (14)
N2A—C21A—C22A	108.62 (18)	N2C—C21C—C23C	111.14 (18)
N2A—C21A—C23A	111.66 (19)	N2C—C21C—C22C	110.10 (18)
C22A—C21A—C23A	110.3 (2)	C23C—C21C—C22C	112.21 (19)
N2A—C21A—H21A	108.7	N2C—C21C—H21C	107.7
C22A—C21A—H21A	108.7	C23C—C21C—H21C	107.7
C23A—C21A—H21A	108.7	C22C—C21C—H21C	107.7
C21A—C22A—H22A	109.5	C21C—C22C—H22G	109.5
C21A—C22A—H22B	109.5	C21C—C22C—H22H	109.5
H22A—C22A—H22B	109.5	H22G—C22C—H22H	109.5
C21A—C22A—H22C	109.5	C21C—C22C—H22I	109.5
H22A—C22A—H22C	109.5	H22G—C22C—H22I	109.5
H22B—C22A—H22C	109.5	H22H—C22C—H22I	109.5
C21A—C23A—H23A	109.5	C21C—C23C—H23G	109.5
C21A—C23A—H23B	109.5	C21C—C23C—H23H	109.5
H23A—C23A—H23B	109.5	H23G—C23C—H23H	109.5
C21A—C23A—H23C	109.5	C21C—C23C—H23I	109.5
H23A—C23A—H23C	109.5	H23G—C23C—H23I	109.5
H23B—C23A—H23C	109.5	H23H—C23C—H23I	109.5
N2B—C1B—N1B	109.70 (18)	N1D—C1D—N2D	110.81 (18)
N2B—C1B—C2B	127.78 (19)	N1D—C1D—C2D	125.81 (19)
N1B—C1B—C2B	122.53 (19)	N2D—C1D—C2D	123.38 (18)
C3B—C2B—C7B	119.3 (2)	C3D—C2D—C7D	119.5 (2)
C3B—C2B—C1B	119.90 (19)	C3D—C2D—C1D	120.51 (19)
C7B—C2B—C1B	120.7 (2)	C7D—C2D—C1D	120.01 (19)
C4B—C3B—C2B	120.1 (2)	C4D—C3D—C2D	120.3 (2)
C4B—C3B—H3B	120.0	C4D—C3D—H3D	119.9
C2B—C3B—H3B	120.0	C2D—C3D—H3D	119.9
C5B—C4B—C3B	120.1 (2)	C5D—C4D—C3D	119.9 (2)
C5B—C4B—H4B	120.0	C5D—C4D—H4D	120.0
C3B—C4B—H4B	120.0	C3D—C4D—H4D	120.0
C6B—C5B—C4B	120.0 (2)	C6D—C5D—C4D	120.1 (2)
C6B—C5B—H5B	120.0	C6D—C5D—H5D	120.0
C4B—C5B—H5B	120.0	C4D—C5D—H5D	120.0
C5B—C6B—C7B	120.4 (2)	C5D—C6D—C7D	120.3 (2)
C5B—C6B—H6B	119.8	C5D—C6D—H6D	119.8
C7B—C6B—H6B	119.8	C7D—C6D—H6D	119.8
C6B—C7B—C2B	120.1 (2)	C6D—C7D—C2D	119.9 (2)
C6B—C7B—H7B	119.9	C6D—C7D—H7D	120.0
C2B—C7B—H7B	119.9	C2D—C7D—H7D	120.0
C1B—N1B—C11B	121.91 (18)	C1D—N1D—C11D	122.25 (18)
C1B—N1B—Al1	92.08 (13)	C1D—N1D—Al2	88.60 (13)

C11B—N1B—Al1	144.38 (14)	C11D—N1D—Al2	145.58 (15)
N1B—C11B—C13B	111.50 (18)	N1D—C11D—C12D	108.87 (18)
N1B—C11B—C12B	109.98 (18)	N1D—C11D—C13D	111.59 (19)
C13B—C11B—C12B	112.34 (19)	C12D—C11D—C13D	110.4 (2)
N1B—C11B—H11B	107.6	N1D—C11D—H11D	108.6
C13B—C11B—H11B	107.6	C12D—C11D—H11D	108.6
C12B—C11B—H11B	107.6	C13D—C11D—H11D	108.6
C11B—C12B—H12D	109.5	C11D—C12D—H12J	109.5
C11B—C12B—H12E	109.5	C11D—C12D—H12K	109.5
H12D—C12B—H12E	109.5	H12J—C12D—H12K	109.5
C11B—C12B—H12F	109.5	C11D—C12D—H12L	109.5
H12D—C12B—H12F	109.5	H12J—C12D—H12L	109.5
H12E—C12B—H12F	109.5	H12K—C12D—H12L	109.5
C11B—C13B—H13D	109.5	C11D—C13D—H13J	109.5
C11B—C13B—H13E	109.5	C11D—C13D—H13K	109.5
H13D—C13B—H13E	109.5	H13J—C13D—H13K	109.5
C11B—C13B—H13F	109.5	C11D—C13D—H13L	109.5
H13D—C13B—H13F	109.5	H13J—C13D—H13L	109.5
H13E—C13B—H13F	109.5	H13K—C13D—H13L	109.5
C1B—N2B—C21B	126.56 (18)	C1D—N2D—C21D	122.89 (18)
C1B—N2B—Al1	90.04 (13)	C1D—N2D—Al2	92.30 (13)
C21B—N2B—Al1	139.55 (15)	C21D—N2D—Al2	144.59 (15)
N2B—C21B—C22B	113.25 (18)	N2D—C21D—C22D	109.7 (2)
N2B—C21B—C23B	112.61 (18)	N2D—C21D—C23D	109.8 (2)
C22B—C21B—C23B	112.4 (2)	C22D—C21D—C23D	112.4 (2)
N2B—C21B—H21B	105.9	N2D—C21D—H21D	108.2
C22B—C21B—H21B	105.9	C22D—C21D—H21D	108.2
C23B—C21B—H21B	105.9	C23D—C21D—H21D	108.2
C21B—C22B—H22D	109.5	C21D—C22D—H22J	109.5
C21B—C22B—H22E	109.5	C21D—C22D—H22K	109.5
H22D—C22B—H22E	109.5	H22J—C22D—H22K	109.5
C21B—C22B—H22F	109.5	C21D—C22D—H22L	109.5
H22D—C22B—H22F	109.5	H22J—C22D—H22L	109.5
H22E—C22B—H22F	109.5	H22K—C22D—H22L	109.5
C21B—C23B—H23D	109.5	C21D—C23D—H23J	109.5
C21B—C23B—H23E	109.5	C21D—C23D—H23K	109.5
H23D—C23B—H23E	109.5	H23J—C23D—H23K	109.5
C21B—C23B—H23F	109.5	C21D—C23D—H23L	109.5
H23D—C23B—H23F	109.5	H23J—C23D—H23L	109.5
H23E—C23B—H23F	109.5	H23K—C23D—H23L	109.5

N2A—C1A—C2A—C3A	113.2 (2)	N1C—C1C—C2C—C3C	73.6 (3)
N1A—C1A—C2A—C3A	−65.1 (3)	N2C—C1C—C2C—C3C	−108.4 (2)
N2A—C1A—C2A—C7A	−66.8 (3)	N1C—C1C—C2C—C7C	−107.6 (3)
N1A—C1A—C2A—C7A	115.0 (3)	N2C—C1C—C2C—C7C	70.4 (3)
C7A—C2A—C3A—C4A	0.9 (3)	C7C—C2C—C3C—C4C	−1.2 (3)
C1A—C2A—C3A—C4A	−179.1 (2)	C1C—C2C—C3C—C4C	177.5 (2)
C2A—C3A—C4A—C5A	−1.2 (3)	C2C—C3C—C4C—C5C	0.8 (3)
C3A—C4A—C5A—C6A	1.0 (4)	C3C—C4C—C5C—C6C	0.7 (4)

C4A—C5A—C6A—C7A	−0.4 (4)	C4C—C5C—C6C—C7C	−1.8 (4)
C5A—C6A—C7A—C2A	0.0 (4)	C5C—C6C—C7C—C2C	1.4 (3)
C3A—C2A—C7A—C6A	−0.3 (3)	C3C—C2C—C7C—C6C	0.1 (3)
C1A—C2A—C7A—C6A	179.7 (2)	C1C—C2C—C7C—C6C	−178.7 (2)
N2A—C1A—N1A—C11A	169.42 (19)	N2C—C1C—N1C—C11C	−165.00 (18)
C2A—C1A—N1A—C11A	−12.1 (3)	C2C—C1C—N1C—C11C	13.2 (3)
N2A—C1A—N1A—Al1	−2.45 (18)	N2C—C1C—N1C—Al2	−1.29 (17)
C2A—C1A—N1A—Al1	176.06 (18)	C2C—C1C—N1C—Al2	176.93 (19)
C1A—N1A—C11A—C12A	−109.8 (2)	C1C—N1C—C11C—C12C	−151.4 (2)
Al1—N1A—C11A—C12A	56.9 (3)	Al2—N1C—C11C—C12C	58.7 (3)
C1A—N1A—C11A—C13A	127.1 (2)	C1C—N1C—C11C—C13C	85.3 (2)
Al1—N1A—C11A—C13A	−66.1 (3)	Al2—N1C—C11C—C13C	−64.6 (3)
N1A—C1A—N2A—C21A	164.08 (19)	N1C—C1C—N2C—C21C	−162.41 (18)
C2A—C1A—N2A—C21A	−14.4 (3)	C2C—C1C—N2C—C21C	19.3 (3)
N1A—C1A—N2A—Al1	2.35 (17)	N1C—C1C—N2C—Al2	1.35 (18)
C2A—C1A—N2A—Al1	−176.15 (19)	C2C—C1C—N2C—Al2	−176.91 (17)
C1A—N2A—C21A—C22A	164.8 (2)	C1C—N2C—C21C—C23C	−112.2 (2)
Al1—N2A—C21A—C22A	−47.4 (3)	Al2—N2C—C21C—C23C	95.8 (3)
C1A—N2A—C21A—C23A	−73.4 (3)	C1C—N2C—C21C—C22C	122.8 (2)
Al1—N2A—C21A—C23A	74.4 (3)	Al2—N2C—C21C—C22C	−29.1 (3)
N2B—C1B—C2B—C3B	103.6 (3)	N1D—C1D—C2D—C3D	79.8 (3)
N1B—C1B—C2B—C3B	−75.9 (3)	N2D—C1D—C2D—C3D	−100.9 (3)
N2B—C1B—C2B—C7B	−79.7 (3)	N1D—C1D—C2D—C7D	−101.8 (3)
N1B—C1B—C2B—C7B	100.7 (3)	N2D—C1D—C2D—C7D	77.4 (3)
C7B—C2B—C3B—C4B	1.0 (3)	C7D—C2D—C3D—C4D	−0.2 (3)
C1B—C2B—C3B—C4B	177.7 (2)	C1D—C2D—C3D—C4D	178.2 (2)
C2B—C3B—C4B—C5B	−1.6 (4)	C2D—C3D—C4D—C5D	0.6 (4)
C3B—C4B—C5B—C6B	1.0 (4)	C3D—C4D—C5D—C6D	−0.3 (4)
C4B—C5B—C6B—C7B	0.2 (4)	C4D—C5D—C6D—C7D	−0.4 (3)
C5B—C6B—C7B—C2B	−0.8 (4)	C5D—C6D—C7D—C2D	0.8 (3)
C3B—C2B—C7B—C6B	0.2 (3)	C3D—C2D—C7D—C6D	−0.5 (3)
C1B—C2B—C7B—C6B	−176.5 (2)	C1D—C2D—C7D—C6D	−178.9 (2)
N2B—C1B—N1B—C11B	166.65 (18)	N2D—C1D—N1D—C11D	−166.39 (19)
C2B—C1B—N1B—C11B	−13.7 (3)	C2D—C1D—N1D—C11D	13.0 (3)
N2B—C1B—N1B—Al1	−2.16 (17)	N2D—C1D—N1D—Al2	−2.60 (17)
C2B—C1B—N1B—Al1	177.48 (17)	C2D—C1D—N1D—Al2	176.75 (19)
C1B—N1B—C11B—C13B	111.4 (2)	C1D—N1D—C11D—C12D	−158.9 (2)
Al1—N1B—C11B—C13B	−88.1 (3)	Al2—N1D—C11D—C12D	50.7 (3)
C1B—N1B—C11B—C12B	−123.3 (2)	C1D—N1D—C11D—C13D	79.0 (3)
Al1—N1B—C11B—C12B	37.2 (3)	Al2—N1D—C11D—C13D	−71.5 (3)
N1B—C1B—N2B—C21B	163.53 (19)	N1D—C1D—N2D—C21D	−173.06 (19)
C2B—C1B—N2B—C21B	−16.1 (3)	C2D—C1D—N2D—C21D	7.6 (3)
N1B—C1B—N2B—Al1	2.08 (17)	N1D—C1D—N2D—Al2	2.74 (18)
C2B—C1B—N2B—Al1	−177.5 (2)	C2D—C1D—N2D—Al2	−176.63 (18)
C1B—N2B—C21B—C22B	72.6 (3)	C1D—N2D—C21D—C22D	130.6 (2)
Al1—N2B—C21B—C22B	−136.8 (2)	Al2—N2D—C21D—C22D	−42.1 (4)
C1B—N2B—C21B—C23B	−56.4 (3)	C1D—N2D—C21D—C23D	−105.3 (2)
Al1—N2B—C21B—C23B	94.2 (2)	Al2—N2D—C21D—C23D	81.9 (3)

(AlPhCNCy22Cl) Chloridobis(*N*,*N*′-dicyclohexylbenzimidamido)aluminium(III) tetrahydrofuran 0.675-solvate

Crystal data

$[Al(C_{19}H_{27}N_2)_2Cl]\cdot 0.675C_4H_8O$
$M_r = 677.95$
Monoclinic, *C*2/*c*
$a = 22.042$ (4) Å
$b = 16.007$ (3) Å
$c = 12.852$ (2) Å
$\beta = 115.396$ (2)°
$V = 4096.6$ (12) Å^3
$Z = 4$
$F(000) = 1468$
$D_x = 1.099$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10954 reflections
$\theta = 2.5$–30.4°
$\mu = 0.15$ mm^{-1}
$T = 150$ K
Plate, colourless
0.40 × 0.34 × 0.12 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 11.198 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min} = 0.872$, $T_{max} = 0.982$
20863 measured reflections
4038 independent reflections
3577 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -27\rightarrow27$
$k = -19\rightarrow19$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.082$
$S = 1.00$
4038 reflections
200 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 6.580P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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. C4H8O solvent showed strong disorder along 0, 1/2,*z* channels and was was treated using SQUEEZE procedure from *PLATON* software (Spek, 2009). See details in platon_squeeze_void_*).
Total removed eletron density corresponds to 108 electrons which in turn corresponds to 2.7 THF molecues of solvent.
H atoms were positioned from geometric consideration and refined as riding on the attached atom. U_{iso} of H atoms were constrained to be 20% larger than Ueqv of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.5000	0.48000 (3)	0.2500	0.03380 (14)
Al1	0.5000	0.61653 (4)	0.2500	0.02219 (14)
N1	0.41384 (6)	0.62964 (7)	0.10908 (10)	0.0240 (3)
N2	0.51084 (6)	0.68318 (7)	0.13434 (10)	0.0242 (3)

C1	0.44562 (7)	0.67531 (9)	0.06238 (12)	0.0235 (3)
C2	0.41364 (7)	0.71313 (9)	−0.05510 (12)	0.0253 (3)
C3	0.42589 (8)	0.67932 (11)	−0.14389 (13)	0.0351 (4)
H3	0.4554	0.6330	−0.1295	0.042*
C4	0.39503 (9)	0.71323 (12)	−0.25332 (14)	0.0419 (4)
H4	0.4030	0.6897	−0.3142	0.050*
C5	0.35279 (9)	0.78104 (12)	−0.27447 (14)	0.0407 (4)
H5	0.3317	0.8041	−0.3498	0.049*
C6	0.34115 (9)	0.81544 (11)	−0.18641 (15)	0.0411 (4)
H6	0.3125	0.8626	−0.2009	0.049*
C7	0.37119 (8)	0.78128 (10)	−0.07669 (13)	0.0332 (4)
H7	0.3627	0.8046	−0.0163	0.040*
C11	0.34714 (7)	0.59362 (9)	0.04118 (12)	0.0255 (3)
H11	0.3193	0.6359	−0.0170	0.031*
C12	0.35123 (7)	0.51470 (10)	−0.02295 (13)	0.0300 (3)
H12A	0.3716	0.5287	−0.0761	0.036*
H12B	0.3805	0.4731	0.0332	0.036*
C13	0.28158 (8)	0.47686 (10)	−0.09147 (14)	0.0345 (4)
H13A	0.2535	0.5165	−0.1521	0.041*
H13B	0.2858	0.4249	−0.1296	0.041*
C14	0.24766 (9)	0.45747 (11)	−0.01311 (17)	0.0430 (4)
H14A	0.2731	0.4131	0.0421	0.052*
H14B	0.2017	0.4364	−0.0600	0.052*
C15	0.24402 (9)	0.53480 (12)	0.05303 (16)	0.0416 (4)
H15A	0.2251	0.5192	0.1077	0.050*
H15B	0.2135	0.5762	−0.0016	0.050*
C16	0.31316 (8)	0.57422 (11)	0.11943 (14)	0.0341 (4)
H16A	0.3083	0.6265	0.1564	0.041*
H16B	0.3418	0.5355	0.1810	0.041*
C21	0.55462 (7)	0.74495 (9)	0.11687 (12)	0.0254 (3)
H21	0.5263	0.7811	0.0502	0.030*
C22	0.60763 (8)	0.70273 (10)	0.08836 (14)	0.0325 (3)
H22A	0.5852	0.6718	0.0149	0.039*
H22B	0.6329	0.6619	0.1495	0.039*
C23	0.65675 (9)	0.76595 (12)	0.07778 (15)	0.0412 (4)
H23A	0.6924	0.7357	0.0658	0.049*
H23B	0.6326	0.8019	0.0097	0.049*
C24	0.68864 (9)	0.82035 (12)	0.18457 (16)	0.0443 (4)
H24A	0.7167	0.7853	0.2514	0.053*
H24B	0.7180	0.8625	0.1730	0.053*
C25	0.63515 (9)	0.86403 (11)	0.20905 (16)	0.0398 (4)
H25A	0.6094	0.9025	0.1449	0.048*
H25B	0.6568	0.8975	0.2804	0.048*
C26	0.58753 (8)	0.80053 (10)	0.22304 (13)	0.0316 (3)
H26A	0.5522	0.8304	0.2365	0.038*
H26B	0.6128	0.7652	0.2913	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0398 (3)	0.0233 (3)	0.0315 (3)	0.000	0.0088 (2)	0.000
Al1	0.0253 (3)	0.0220 (3)	0.0178 (3)	0.000	0.0078 (2)	0.000
N1	0.0254 (6)	0.0251 (6)	0.0188 (6)	−0.0020 (5)	0.0069 (5)	−0.0015 (5)
N2	0.0260 (6)	0.0251 (6)	0.0198 (6)	−0.0009 (5)	0.0082 (5)	0.0020 (5)
C1	0.0282 (7)	0.0212 (7)	0.0203 (7)	0.0021 (6)	0.0096 (6)	−0.0031 (5)
C2	0.0258 (7)	0.0263 (7)	0.0218 (7)	−0.0010 (6)	0.0082 (6)	0.0009 (6)
C3	0.0413 (9)	0.0360 (9)	0.0278 (8)	0.0093 (7)	0.0146 (7)	0.0015 (7)
C4	0.0516 (10)	0.0513 (11)	0.0239 (8)	0.0052 (9)	0.0173 (8)	0.0010 (7)
C5	0.0434 (10)	0.0484 (11)	0.0256 (8)	0.0041 (8)	0.0102 (7)	0.0121 (7)
C6	0.0414 (10)	0.0410 (10)	0.0366 (9)	0.0148 (8)	0.0128 (8)	0.0122 (8)
C7	0.0374 (9)	0.0350 (9)	0.0276 (8)	0.0077 (7)	0.0141 (7)	0.0026 (7)
C11	0.0251 (7)	0.0258 (7)	0.0220 (7)	−0.0009 (6)	0.0069 (6)	−0.0025 (6)
C12	0.0284 (8)	0.0315 (8)	0.0278 (8)	−0.0007 (6)	0.0100 (6)	−0.0075 (6)
C13	0.0294 (8)	0.0326 (9)	0.0346 (8)	−0.0008 (7)	0.0072 (7)	−0.0128 (7)
C14	0.0360 (9)	0.0384 (10)	0.0539 (11)	−0.0121 (8)	0.0187 (8)	−0.0145 (8)
C15	0.0369 (9)	0.0465 (11)	0.0478 (10)	−0.0113 (8)	0.0242 (8)	−0.0144 (8)
C16	0.0360 (9)	0.0373 (9)	0.0319 (8)	−0.0083 (7)	0.0174 (7)	−0.0098 (7)
C21	0.0265 (7)	0.0261 (7)	0.0227 (7)	0.0002 (6)	0.0097 (6)	0.0036 (6)
C22	0.0385 (9)	0.0341 (9)	0.0306 (8)	0.0032 (7)	0.0202 (7)	0.0022 (7)
C23	0.0419 (10)	0.0496 (11)	0.0430 (10)	0.0018 (8)	0.0285 (8)	0.0074 (8)
C24	0.0344 (9)	0.0551 (12)	0.0463 (10)	−0.0106 (8)	0.0200 (8)	0.0049 (9)
C25	0.0397 (9)	0.0378 (9)	0.0412 (9)	−0.0117 (8)	0.0167 (8)	−0.0040 (8)
C26	0.0321 (8)	0.0330 (8)	0.0330 (8)	−0.0045 (7)	0.0170 (7)	−0.0048 (7)

Geometric parameters (Å, º)

Cl1—Al1	2.1855 (9)	C13—C14	1.522 (2)
Al1—N2	1.9260 (12)	C13—H13A	0.9900
Al1—N2^{i}	1.9261 (12)	C13—H13B	0.9900
Al1—N1	1.9952 (12)	C14—C15	1.523 (2)
Al1—N1^{i}	1.9953 (12)	C14—H14A	0.9900
Al1—C1^{i}	2.3785 (14)	C14—H14B	0.9900
N1—C1	1.3213 (18)	C15—C16	1.528 (2)
N1—C11	1.4680 (18)	C15—H15A	0.9900
N2—C1	1.3407 (18)	C15—H15B	0.9900
N2—C21	1.4647 (18)	C16—H16A	0.9900
C1—C2	1.4935 (19)	C16—H16B	0.9900
C2—C7	1.386 (2)	C21—C22	1.524 (2)
C2—C3	1.390 (2)	C21—C26	1.527 (2)
C3—C4	1.384 (2)	C21—H21	1.0000
C3—H3	0.9500	C22—C23	1.530 (2)
C4—C5	1.379 (3)	C22—H22A	0.9900
C4—H4	0.9500	C22—H22B	0.9900
C5—C6	1.378 (2)	C23—C24	1.519 (3)
C5—H5	0.9500	C23—H23A	0.9900
C6—C7	1.388 (2)	C23—H23B	0.9900
C6—H6	0.9500	C24—C25	1.515 (2)

C7—H7	0.9500	C24—H24A	0.9900
C11—C16	1.521 (2)	C24—H24B	0.9900
C11—C12	1.532 (2)	C25—C26	1.526 (2)
C11—H11	1.0000	C25—H25A	0.9900
C12—C13	1.530 (2)	C25—H25B	0.9900
C12—H12A	0.9900	C26—H26A	0.9900
C12—H12B	0.9900	C26—H26B	0.9900

N2—Al1—N2^{i}	112.73 (8)	C14—C13—H13B	109.5
N2—Al1—N1	68.04 (5)	C12—C13—H13B	109.5
N2^{i}—Al1—N1	104.92 (5)	H13A—C13—H13B	108.1
N2—Al1—N1^{i}	104.92 (5)	C13—C14—C15	111.23 (14)
N2^{i}—Al1—N1^{i}	68.04 (5)	C13—C14—H14A	109.4
N1—Al1—N1^{i}	167.92 (8)	C15—C14—H14A	109.4
N2—Al1—Cl1	123.64 (4)	C13—C14—H14B	109.4
N2^{i}—Al1—Cl1	123.64 (4)	C15—C14—H14B	109.4
N1—Al1—Cl1	96.04 (4)	H14A—C14—H14B	108.0
N1^{i}—Al1—Cl1	96.04 (4)	C14—C15—C16	111.64 (14)
N2—Al1—C1^{i}	112.83 (5)	C14—C15—H15A	109.3
N2^{i}—Al1—C1^{i}	34.30 (5)	C16—C15—H15A	109.3
N1—Al1—C1^{i}	138.45 (5)	C14—C15—H15B	109.3
N1^{i}—Al1—C1^{i}	33.74 (5)	C16—C15—H15B	109.3
Cl1—Al1—C1^{i}	113.30 (4)	H15A—C15—H15B	108.0
C1—N1—C11	122.56 (12)	C11—C16—C15	111.78 (13)
C1—N1—Al1	89.24 (9)	C11—C16—H16A	109.3
C11—N1—Al1	144.99 (10)	C15—C16—H16A	109.3
C1—N2—C21	122.66 (12)	C11—C16—H16B	109.3
C1—N2—Al1	91.67 (9)	C15—C16—H16B	109.3
C21—N2—Al1	143.16 (9)	H16A—C16—H16B	107.9
N1—C1—N2	111.05 (12)	N2—C21—C22	111.15 (12)
N1—C1—C2	124.84 (13)	N2—C21—C26	110.37 (11)
N2—C1—C2	124.11 (13)	C22—C21—C26	110.72 (12)
C7—C2—C3	119.63 (14)	N2—C21—H21	108.2
C7—C2—C1	120.46 (13)	C22—C21—H21	108.2
C3—C2—C1	119.91 (13)	C26—C21—H21	108.2
C4—C3—C2	119.85 (15)	C21—C22—C23	111.88 (13)
C4—C3—H3	120.1	C21—C22—H22A	109.2
C2—C3—H3	120.1	C23—C22—H22A	109.2
C5—C4—C3	120.34 (16)	C21—C22—H22B	109.2
C5—C4—H4	119.8	C23—C22—H22B	109.2
C3—C4—H4	119.8	H22A—C22—H22B	107.9
C6—C5—C4	120.03 (15)	C24—C23—C22	111.69 (13)
C6—C5—H5	120.0	C24—C23—H23A	109.3
C4—C5—H5	120.0	C22—C23—H23A	109.3
C5—C6—C7	120.09 (16)	C24—C23—H23B	109.3
C5—C6—H6	120.0	C22—C23—H23B	109.3
C7—C6—H6	120.0	H23A—C23—H23B	107.9
C2—C7—C6	120.05 (15)	C25—C24—C23	110.63 (14)
C2—C7—H7	120.0	C25—C24—H24A	109.5

C6—C7—H7	120.0	C23—C24—H24A	109.5
N1—C11—C16	109.79 (12)	C25—C24—H24B	109.5
N1—C11—C12	111.63 (12)	C23—C24—H24B	109.5
C16—C11—C12	110.28 (13)	H24A—C24—H24B	108.1
N1—C11—H11	108.4	C24—C25—C26	110.66 (14)
C16—C11—H11	108.4	C24—C25—H25A	109.5
C12—C11—H11	108.4	C26—C25—H25A	109.5
C13—C12—C11	111.11 (12)	C24—C25—H25B	109.5
C13—C12—H12A	109.4	C26—C25—H25B	109.5
C11—C12—H12A	109.4	H25A—C25—H25B	108.1
C13—C12—H12B	109.4	C25—C26—C21	111.72 (13)
C11—C12—H12B	109.4	C25—C26—H26A	109.3
H12A—C12—H12B	108.0	C21—C26—H26A	109.3
C14—C13—C12	110.88 (13)	C25—C26—H26B	109.3
C14—C13—H13A	109.5	C21—C26—H26B	109.3
C12—C13—H13A	109.5	H26A—C26—H26B	107.9

C11—N1—C1—N2	−164.48 (12)	C1—N1—C11—C12	78.85 (17)
Al1—N1—C1—N2	−0.02 (11)	Al1—N1—C11—C12	−73.3 (2)
C11—N1—C1—C2	15.3 (2)	N1—C11—C12—C13	178.91 (13)
Al1—N1—C1—C2	179.75 (13)	C16—C11—C12—C13	56.57 (17)
C21—N2—C1—N1	−165.84 (12)	C11—C12—C13—C14	−56.96 (18)
Al1—N2—C1—N1	0.02 (12)	C12—C13—C14—C15	55.59 (19)
C21—N2—C1—C2	14.4 (2)	C13—C14—C15—C16	−54.5 (2)
Al1—N2—C1—C2	−179.75 (12)	N1—C11—C16—C15	−178.78 (13)
N1—C1—C2—C7	73.0 (2)	C12—C11—C16—C15	−55.38 (18)
N2—C1—C2—C7	−107.29 (17)	C14—C15—C16—C11	54.7 (2)
N1—C1—C2—C3	−106.33 (18)	C1—N2—C21—C22	−112.74 (15)
N2—C1—C2—C3	73.4 (2)	Al1—N2—C21—C22	91.30 (18)
C7—C2—C3—C4	−0.8 (2)	C1—N2—C21—C26	124.01 (14)
C1—C2—C3—C4	178.53 (15)	Al1—N2—C21—C26	−31.9 (2)
C2—C3—C4—C5	0.8 (3)	N2—C21—C22—C23	−176.17 (12)
C3—C4—C5—C6	0.0 (3)	C26—C21—C22—C23	−53.12 (17)
C4—C5—C6—C7	−0.8 (3)	C21—C22—C23—C24	54.26 (19)
C3—C2—C7—C6	0.0 (2)	C22—C23—C24—C25	−56.0 (2)
C1—C2—C7—C6	−179.31 (15)	C23—C24—C25—C26	57.18 (19)
C5—C6—C7—C2	0.8 (3)	C24—C25—C26—C21	−57.18 (19)
C1—N1—C11—C16	−158.54 (13)	N2—C21—C26—C25	178.32 (13)
Al1—N1—C11—C16	49.3 (2)	C22—C21—C26—C25	54.82 (17)

Symmetry code: (i) $-x+1, y, -z+1/2$.