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Synthesis, characterization and crystal structure of a 2-(diethylaminomethyl)indole ligated dimethylaluminium complex

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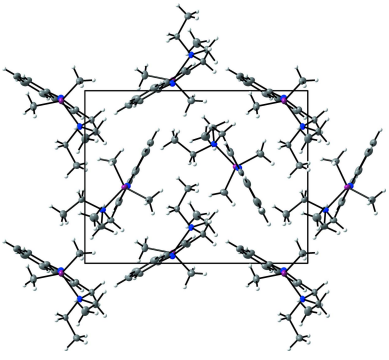
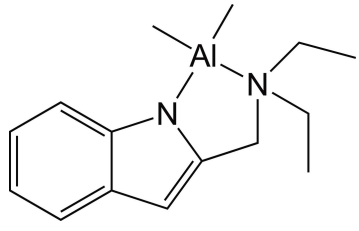
The title compound, $[Al(CH_3)_2(C_{13}H_{17}N_2)]$ (systematic name; {2-[(diethylamino)methyl]indol-1-yl-κ^2N,N'}dimethylaluminium), was prepared by methane elimination from the reaction of 2-(diethylaminomethyl)indole and trimethylaluminium. The complex crystallizes readily from a concentrated toluene solution in high yield. The asymmetric unit contains two crystallographically independent molecules. Each molecule has a four-coordinate aluminium atom that has pseudo-tetrahedral geometry. C—H$\cdots\pi$ interactions link the independent molecules into chains extending along the *b*-axis direction.

1. Chemical context

Organoaluminium chemistry has a long history of active research that has led to numerous applications in industry (Mason, 2005). Organoaluminium compounds have garnered much attention in recent years for their use in the formation of polyactides, (Liu *et al.*, 2010; Chisholm *et al.*, 2003, 2005; Zhang *et al.*, 2014; Chen *et al.*, 2012; Schwarz *et al.*, 2010) and hydroamination (Koller & Bergman, 2010*a*,*b*; Khandelwal & Wehmschulte, 2012). While many varieties of ancillary ligands on aluminium have been employed in such reactions, a majority of these systems have nitrogen-donor arms as a component. Our group is interested in particular in the use of 2-(dialkylaminomethyl)indoles (Nagarathnam, 1992) as ligands for organoaluminium complexes. Herein we report the synthesis, characterization and crystal structure of the first 2-(dialkylaminomethyl)indolyl–aluminium complex, $[Al(CH_3)_2(C_{13}H_{17}N_2)]$.





2. Structural commentary

The asymmetric unit of the title complex contains two independent molecules (Fig. 1). They are structurally different with regard to the chelate rings that are formed around the aluminium atoms by the indolyl moiety. The most obvious difference between the two crystallographically independent molecules is the displacement of the Al atom from the plane of the chelate ring. Al1 deviates by 0.6831 (5) Å from the plane

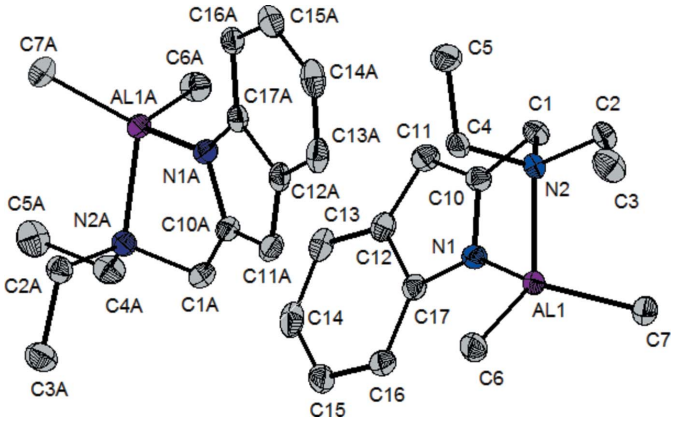


Figure 1
A view of the asymmetric unit of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

defined by atoms N1/C10/C1/N2 while Al1*A* deviates by 0.6150 (5) Å from the plane N1*A*/C10*A*/C1*A*/N2*A*. Each molecule contains a four-coordinate, pseudo-tetrahedral, aluminium atom. There are two distinct bond lengths for the Al—N bonds in the molecule. The Al—$N_{indolyl}$ bond lengths are 1.8879 (14) Å for Al1—N1 and 1.8779 (15) Å for Al1*A*—N1*A*. These lengths are in the range expected for anionically bound indolyl or pyrrolyl moieties (Huang *et al.*, 2001). As expected, these lengths are significantly shorter than those found for the dative Al—N_{imine} bonds, 2.0355 (15) Å for Al1—N2 and 2.0397 (16) Å for Al1*A*—N2*A* [see Huang *et al.* (2001) for typical values].

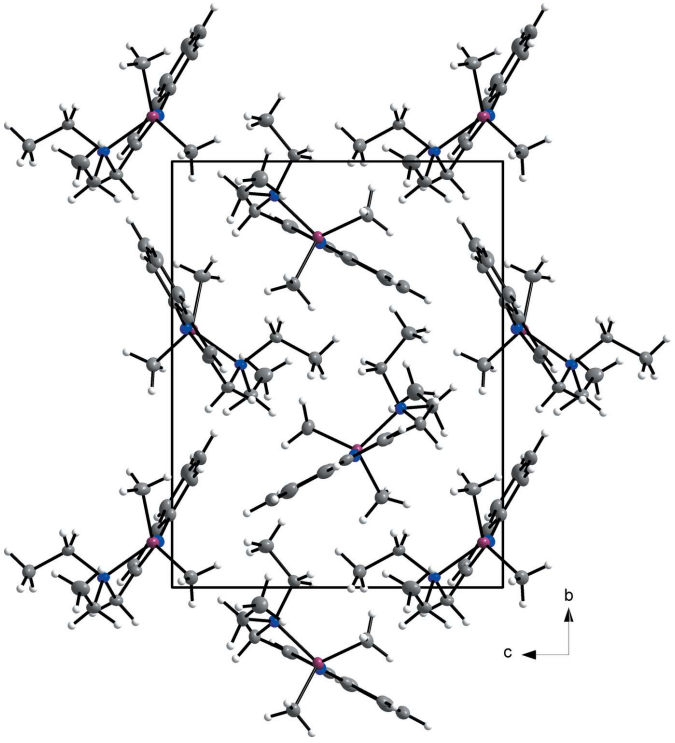


Figure 2
Crystal packing diagram of the title compound viewed along the *a* axis.

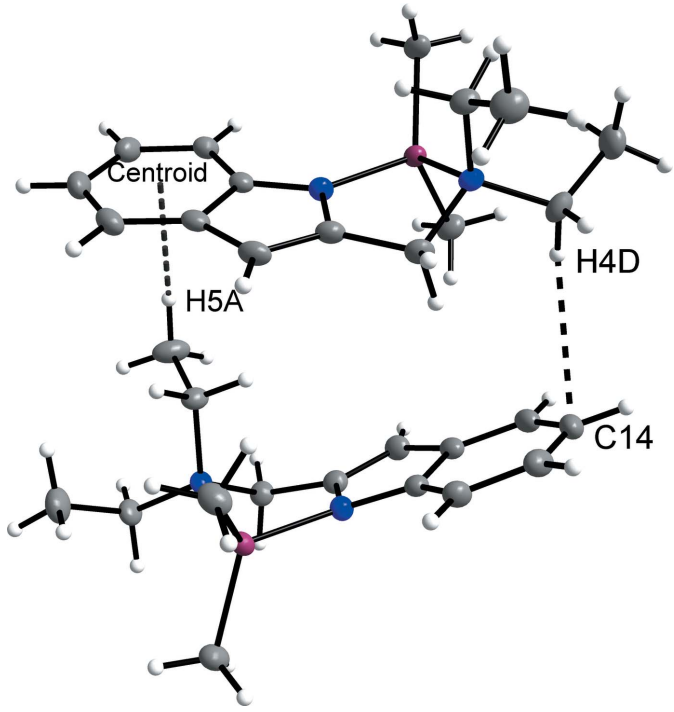


Figure 3
C—H···π interactions between molecules in the asymmetric unit.

3. Supramolecular features

The crystal packing is illustrated in Fig. 2. In the crystal, molecules associate *via* three different types of C—H···π interactions, as shown in Figs. 3 and 4. There is one interaction between the methyl proton H5*A* and the centroid of the (C12*A*–C17*A*) aromatic ring of 2.57 Å (Table 1) and another between the methylene proton H4*D* and the aromatic C14 of 2.88 Å. The third interaction is between H2*B* and the centroid of C12A^{i}–C17A^{i} [Table 1; symmetry code: (i) $1-x, -\frac{1}{2}+y, 1-z$]. This interaction links the two independent molecules in the asymmetric unit into chains that extend along the *b*-axis direction.

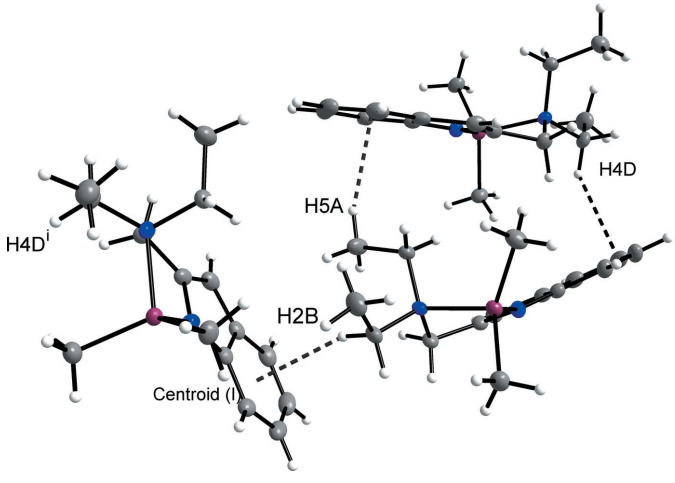


Figure 4
All C—H···π interactions between molecules of the title compound. [Symmetry code: (i) $1-x, -\frac{1}{2}+y, 1-z$.]

Table 1
C—H···π interactions (Å, °).

*Cg*1 is the centroid of the C12*A*–C17*A* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···*Cg*1	0.98	2.57	3.470 (2)	153
C2—H2*B*···*Cg*1^{i}	0.99	2.55	3.434 (2)	149

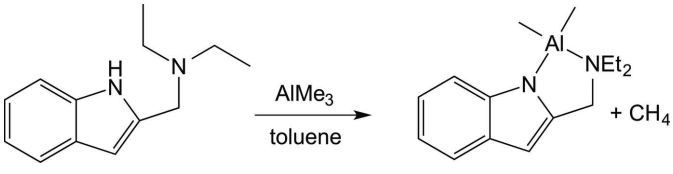
Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+1$.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.36; Groom & Allen, 2014) for indolyl gave 500 hits. A search for indolide generated 18 hits. Neither of these sets of hits included structures involving indolyl moieties bound to aluminium. A substructure search for N-bound indolyl-coordinating aluminium complexes resulted in only five hits (Kingsley *et al.*, 2010), all of which contained bridging μ^2:η^1:η^1 coordination modes. The title compound is the first structurally characterized complex with a monomeric μ^1:η^1-coordinating indole moiety to aluminium.

5. Synthesis and crystallization

To a 100 mL side-arm flask was added 2-(diethylaminomethyl)indole (0.402 g, 2.0 mmol) and 25 mL of toluene. A toluene solution of trimethylaluminium (1.0 mL, 2.0 *M*, 2.0 mmol) was added *via* syringe. The reaction solution turned bright yellow, which darkened as the solution was stirred for 12 h. The solvent was then removed *in vacuo* resulting in a yellow solid, which was dissolved in a mixture of 10 mL of hot toluene, followed by cooling to 243 K for 48 h. The resulting yellow crystalline material was isolated by filtration. Yield: 0.462 g, 1.78 mmol, 90%. ^{1}H NMR ($CDCl_3$, 600 MHz): δ 7.55 (*d*, $^3J_{HH}$ = 7.8 Hz, 1H, H16), 7.36 (*d*, $^3J_{HH}$ = 7.8 Hz, 1H, H13), 7.07 (*t*, $^3J_{HH}$ = 7.8 Hz, 1H, H15), 7.00 (*t*, $^3J_{HH}$ = 7.8 Hz, 1H, H14), 6.31 (*s*, 1H, H11), 4.00 (*s*, 2H, indole CH_2), 2.88 (*q*, $^3J_{HH}$ = 7.2 Hz, 4H, amino CH_2CH_3), 1.13 (*t*, $^3J_{HH}$ = 7.2 Hz, 6H, amino CH_2CH_3), −0.59 (*s*, 6H, $AlCH_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 150.8 MHz): δ 141.7 (C17), 139.4 (C10), 131.8 (C12), 120.2 (C15), 119.6 (C16), 118.5 (C15), 113.7 (C14), 98.1 (C11), 53.2 (indole CH_2), 44.7 (amino CH_2CH_3), 8.3 (amino CH_2CH_3), −11.10 (*br*, $AlCH_3$) (Kingsley *et al.*, 2010). Analysis calculated for $C_{15}H_{23}N_2Al$: C, 69.74; H, 8.97; N, 10.84. Found: C, 69.67; H, 8.70; N, 10.63.



X-ray quality crystals were grown from a concentrated solution in hot toluene followed by slow cooling to room temperature followed by storage at 243 K for 72 h.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Al(CH_3)_2(C_{13}H_{17}N_2)]$
M_r	258.33
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, *b*, *c* (Å)	9.7467 (5), 14.1245 (7), 10.9866 (5)
β (°)	94.206 (1)
V (Å^3)	1508.42 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.12
Crystal size (mm)	0.20 × 0.20 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)
T_{min}, T_{max}	0.697, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13157, 5440, 5366
R_{int}	0.025
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.024, 0.068, 1.05
No. of reflections	5440
No. of parameters	333
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.19
Absolute structure	Flack *x* determined using 2203 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.05 (3)

Computer programs: *APEX2* (Bruker, 2005), *SAINT* (Bruker, 2003), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010)..

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined using a riding model with C—H = 0.05–0.99 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

Acknowledgements

The authors would like to thank the University of Michigan-Flint Office of Research and Sponsored Programs for their support of this project. Special acknowledgement is given to Dr Chris Gianopoulos for assistance in data collection and structure refinement and to the University of Toledo Instrumentation Center for the use of their Bruker APEXII diffractometer.

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supporting information

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Synthesis, characterization and crystal structure of a 2-(diethylaminomethyl)-indole ligated dimethylaluminium complex

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Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *publCIF* (Westrip, 2010)..

{2-[(Diethylamino)methyl]indol-1-yl-κ^2N,N'}dimethylaluminium

Crystal data

$[Al(CH_3)_2(C_{13}H_{17}N_2)]$
M_r = 258.33
Monoclinic, $P2_1$
a = 9.7467 (5) Å
b = 14.1245 (7) Å
c = 10.9866 (5) Å
β = 94.206 (1)°
V = 1508.42 (13) Å^3
Z = 4
$F(000)$ = 560
D_x = 1.138 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5904 reflections
θ = 2.4–26.4°
μ = 0.12 mm^{-1}
T = 150 K
Irregular, yellow
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.697, T_{max} = 0.745
13157 measured reflections
5440 independent reflections
5366 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.3°, θ_{min} = 1.9°
h = −12→10
k = −16→17
l = −13→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.068
S = 1.05
5440 reflections
333 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.2513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack x determined using 2203 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.05 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.49235 (5)	0.10530 (4)	0.05845 (4)	0.01712 (12)
Al1A	0.00034 (5)	0.32156 (4)	0.44114 (4)	0.01652 (12)
N1	0.29822 (14)	0.10862 (11)	0.04241 (13)	0.0187 (3)
N1A	0.19261 (14)	0.30931 (11)	0.44801 (12)	0.0185 (3)
N2	0.46863 (14)	0.02289 (10)	0.20745 (13)	0.0166 (3)
N2A	0.02362 (15)	0.42016 (11)	0.30859 (12)	0.0185 (3)
C1	0.33910 (17)	−0.03044 (13)	0.16893 (16)	0.0194 (3)
H1A	0.3588	−0.0811	0.1105	0.023*
H1B	0.3005	−0.0598	0.2408	0.023*
C2	0.58090 (17)	−0.04771 (13)	0.23735 (16)	0.0210 (4)
H2A	0.5922	−0.0876	0.1647	0.025*
H2B	0.5532	−0.0896	0.3035	0.025*
C3	0.7178 (2)	−0.00237 (15)	0.2769 (2)	0.0311 (4)
H3A	0.7883	−0.0516	0.2893	0.047*
H3B	0.7099	0.0322	0.3534	0.047*
H3C	0.7439	0.0417	0.2136	0.047*
C4	0.44570 (18)	0.08681 (13)	0.31419 (15)	0.0201 (3)
H4A	0.3664	0.1285	0.2912	0.024*
H4B	0.5276	0.1278	0.3291	0.024*
C5	0.4190 (2)	0.03699 (15)	0.43275 (17)	0.0319 (4)
H5A	0.4053	0.0843	0.4960	0.048*
H5B	0.4981	−0.0030	0.4585	0.048*
H5C	0.3365	−0.0025	0.4202	0.048*
C6	0.57142 (19)	0.23092 (14)	0.09103 (18)	0.0263 (4)
H6A	0.6534	0.2252	0.1478	0.039*
H6B	0.5035	0.2713	0.1272	0.039*
H6C	0.5969	0.2592	0.0144	0.039*
C7	0.58197 (19)	0.02303 (15)	−0.05668 (16)	0.0254 (4)
H7A	0.6789	0.0143	−0.0284	0.038*
H7B	0.5760	0.0524	−0.1377	0.038*
H7C	0.5357	−0.0386	−0.0613	0.038*
C10	0.23890 (17)	0.03923 (13)	0.11001 (15)	0.0190 (3)
C11	0.10054 (18)	0.05168 (13)	0.11525 (16)	0.0215 (4)
H11	0.0391	0.0126	0.1559	0.026*
C12	0.06711 (17)	0.13596 (14)	0.04673 (16)	0.0204 (4)
C13	−0.05440 (18)	0.18738 (15)	0.01868 (16)	0.0256 (4)
H13	−0.1397	0.1651	0.0442	0.031*
C14	−0.0484 (2)	0.27035 (16)	−0.04612 (17)	0.0283 (4)
H14	−0.1304	0.3053	−0.0655	0.034*

C15	0.0767 (2)	0.30439 (15)	−0.08420 (16)	0.0281 (4)
H15	0.0783	0.3624	−0.1277	0.034*
C16	0.19806 (19)	0.25458 (14)	−0.05925 (16)	0.0238 (4)
H16	0.2827	0.2777	−0.0852	0.029*
C17	0.19268 (17)	0.16992 (13)	0.00483 (15)	0.0188 (3)
C1A	0.14884 (18)	0.38445 (14)	0.24981 (15)	0.0219 (4)
H1D	0.1228	0.3324	0.1924	0.026*
H1E	0.1900	0.4361	0.2037	0.026*
C2A	0.05447 (18)	0.51442 (13)	0.36912 (15)	0.0216 (4)
H2D	0.1376	0.5072	0.4258	0.026*
H2E	−0.0229	0.5309	0.4187	0.026*
C3A	0.0777 (2)	0.59665 (15)	0.28370 (18)	0.0299 (4)
H3D	0.0966	0.6543	0.3317	0.045*
H3E	−0.0047	0.6061	0.2284	0.045*
H3F	0.1563	0.5826	0.2359	0.045*
C4A	−0.09529 (19)	0.42606 (15)	0.21401 (16)	0.0252 (4)
H4D	−0.1106	0.3629	0.1764	0.030*
H4E	−0.0714	0.4704	0.1490	0.030*
C5A	−0.2272 (2)	0.45879 (17)	0.26472 (19)	0.0327 (5)
H5D	−0.3030	0.4539	0.2013	0.049*
H5E	−0.2173	0.5248	0.2914	0.049*
H5F	−0.2470	0.4190	0.3343	0.049*
C6A	−0.0962 (2)	0.21207 (14)	0.36621 (17)	0.0259 (4)
H6D	−0.1936	0.2277	0.3485	0.039*
H6E	−0.0880	0.1582	0.4225	0.039*
H6F	−0.0553	0.1955	0.2902	0.039*
C7A	−0.06954 (18)	0.37556 (15)	0.58896 (16)	0.0234 (4)
H7D	−0.1698	0.3820	0.5775	0.035*
H7E	−0.0281	0.4380	0.6048	0.035*
H7F	−0.0456	0.3337	0.6585	0.035*
C10A	0.25049 (18)	0.34955 (13)	0.34895 (15)	0.0198 (3)
C11A	0.39089 (18)	0.34640 (14)	0.36008 (16)	0.0223 (4)
H11A	0.4520	0.3707	0.3042	0.027*
C12A	0.42739 (18)	0.29896 (12)	0.47316 (16)	0.0202 (4)
C13A	0.55142 (18)	0.27146 (14)	0.53626 (18)	0.0261 (4)
H13A	0.6369	0.2843	0.5032	0.031*
C14A	0.54780 (19)	0.22547 (15)	0.64699 (18)	0.0284 (4)
H14A	0.6316	0.2067	0.6899	0.034*
C15A	0.4220 (2)	0.20598 (14)	0.69735 (17)	0.0256 (4)
H15A	0.4225	0.1744	0.7737	0.031*
C16A	0.29816 (18)	0.23198 (13)	0.63774 (16)	0.0205 (3)
H16A	0.2135	0.2192	0.6723	0.025*
C17A	0.30091 (17)	0.27766 (13)	0.52507 (15)	0.0179 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0165 (2)	0.0158 (3)	0.0194 (2)	0.00128 (19)	0.00356 (18)	0.00057 (19)

Al1A	0.0162 (2)	0.0184 (3)	0.0150 (2)	−0.00063 (19)	0.00145 (18)	−0.00094 (19)
N1	0.0183 (6)	0.0191 (8)	0.0189 (7)	0.0012 (6)	0.0020 (5)	0.0021 (6)
N1A	0.0193 (7)	0.0195 (8)	0.0168 (6)	0.0008 (6)	0.0031 (5)	0.0009 (6)
N2	0.0177 (6)	0.0129 (7)	0.0192 (6)	0.0013 (6)	0.0003 (5)	−0.0014 (6)
N2A	0.0219 (7)	0.0181 (7)	0.0152 (6)	0.0007 (6)	0.0000 (5)	−0.0016 (5)
C1	0.0208 (8)	0.0148 (8)	0.0225 (8)	−0.0028 (7)	0.0007 (6)	0.0005 (6)
C2	0.0212 (8)	0.0159 (9)	0.0258 (8)	0.0046 (7)	−0.0001 (7)	0.0011 (7)
C3	0.0231 (9)	0.0283 (11)	0.0409 (11)	0.0037 (8)	−0.0039 (8)	0.0035 (9)
C4	0.0265 (8)	0.0148 (9)	0.0191 (8)	0.0010 (7)	0.0022 (6)	−0.0021 (6)
C5	0.0516 (12)	0.0236 (10)	0.0216 (9)	−0.0026 (9)	0.0099 (8)	−0.0019 (8)
C6	0.0255 (9)	0.0194 (10)	0.0348 (10)	−0.0016 (7)	0.0083 (8)	0.0002 (8)
C7	0.0277 (9)	0.0250 (10)	0.0241 (9)	0.0055 (8)	0.0061 (7)	0.0005 (7)
C10	0.0209 (8)	0.0165 (8)	0.0194 (7)	−0.0024 (7)	0.0012 (6)	−0.0009 (6)
C11	0.0194 (8)	0.0227 (10)	0.0225 (8)	−0.0037 (7)	0.0024 (6)	−0.0004 (7)
C12	0.0194 (8)	0.0235 (9)	0.0182 (8)	0.0007 (7)	0.0011 (6)	−0.0046 (7)
C13	0.0211 (8)	0.0341 (11)	0.0216 (8)	0.0050 (8)	0.0013 (7)	−0.0061 (7)
C14	0.0283 (9)	0.0345 (11)	0.0216 (8)	0.0148 (8)	−0.0018 (7)	−0.0042 (8)
C15	0.0390 (10)	0.0253 (10)	0.0201 (8)	0.0117 (8)	0.0026 (7)	0.0031 (7)
C16	0.0275 (9)	0.0256 (10)	0.0189 (8)	0.0042 (7)	0.0048 (7)	0.0027 (7)
C17	0.0206 (8)	0.0206 (9)	0.0152 (7)	0.0024 (7)	0.0011 (6)	−0.0019 (6)
C1A	0.0253 (8)	0.0244 (9)	0.0166 (8)	0.0014 (7)	0.0053 (6)	0.0000 (7)
C2A	0.0268 (8)	0.0181 (9)	0.0197 (8)	−0.0009 (7)	0.0006 (7)	−0.0026 (7)
C3A	0.0372 (10)	0.0223 (10)	0.0301 (9)	−0.0035 (8)	0.0034 (8)	0.0017 (8)
C4A	0.0296 (9)	0.0271 (10)	0.0177 (8)	−0.0012 (8)	−0.0064 (7)	0.0010 (7)
C5A	0.0275 (9)	0.0354 (12)	0.0338 (10)	0.0040 (8)	−0.0064 (8)	0.0004 (9)
C6A	0.0291 (9)	0.0246 (10)	0.0237 (9)	−0.0051 (8)	−0.0004 (7)	−0.0022 (8)
C7A	0.0211 (8)	0.0295 (10)	0.0198 (8)	−0.0006 (7)	0.0034 (6)	−0.0037 (7)
C10A	0.0239 (8)	0.0183 (8)	0.0177 (8)	−0.0005 (7)	0.0063 (6)	−0.0015 (6)
C11A	0.0225 (8)	0.0211 (9)	0.0244 (8)	−0.0027 (7)	0.0097 (7)	−0.0041 (7)
C12A	0.0209 (8)	0.0158 (9)	0.0242 (8)	−0.0003 (6)	0.0050 (7)	−0.0067 (6)
C13A	0.0182 (8)	0.0244 (10)	0.0358 (10)	0.0015 (7)	0.0040 (7)	−0.0085 (8)
C14A	0.0227 (9)	0.0277 (10)	0.0335 (10)	0.0079 (7)	−0.0063 (7)	−0.0081 (8)
C15A	0.0307 (9)	0.0213 (10)	0.0239 (8)	0.0056 (8)	−0.0031 (7)	−0.0024 (7)
C16A	0.0226 (8)	0.0172 (9)	0.0218 (8)	0.0021 (7)	0.0028 (6)	−0.0024 (6)
C17A	0.0188 (8)	0.0148 (8)	0.0203 (8)	0.0008 (6)	0.0021 (6)	−0.0047 (7)

Geometric parameters (Å, º)

Al1—N1	1.8879 (14)	C12—C17	1.422 (2)
Al1—C6	1.957 (2)	C13—C14	1.375 (3)
Al1—C7	1.9686 (19)	C13—H13	0.9500
Al1—N2	2.0355 (15)	C14—C15	1.403 (3)
Al1A—N1A	1.8779 (15)	C14—H14	0.9500
Al1A—C6A	1.960 (2)	C15—C16	1.386 (3)
Al1A—C7A	1.9610 (18)	C15—H15	0.9500
Al1A—N2A	2.0397 (16)	C16—C17	1.391 (3)
N1—C10	1.382 (2)	C16—H16	0.9500
N1—C17	1.384 (2)	C1A—C10A	1.501 (2)

N1A—C17A	1.378 (2)	C1A—H1D	0.9900
N1A—C10A	1.384 (2)	C1A—H1E	0.9900
N2—C2	1.499 (2)	C2A—C3A	1.521 (3)
N2—C1	1.504 (2)	C2A—H2D	0.9900
N2—C4	1.510 (2)	C2A—H2E	0.9900
N2A—C4A	1.501 (2)	C3A—H3D	0.9800
N2A—C2A	1.509 (2)	C3A—H3E	0.9800
N2A—C1A	1.509 (2)	C3A—H3F	0.9800
C1—C10	1.500 (2)	C4A—C5A	1.511 (3)
C1—H1A	0.9900	C4A—H4D	0.9900
C1—H1B	0.9900	C4A—H4E	0.9900
C2—C3	1.515 (3)	C5A—H5D	0.9800
C2—H2A	0.9900	C5A—H5E	0.9800
C2—H2B	0.9900	C5A—H5F	0.9800
C3—H3A	0.9800	C6A—H6D	0.9800
C3—H3B	0.9800	C6A—H6E	0.9800
C3—H3C	0.9800	C6A—H6F	0.9800
C4—C5	1.520 (2)	C7A—H7D	0.9800
C4—H4A	0.9900	C7A—H7E	0.9800
C4—H4B	0.9900	C7A—H7F	0.9800
C5—H5A	0.9800	C10A—C11A	1.366 (2)
C5—H5B	0.9800	C11A—C12A	1.433 (3)
C5—H5C	0.9800	C11A—H11A	0.9500
C6—H6A	0.9800	C12A—C13A	1.404 (2)
C6—H6B	0.9800	C12A—C17A	1.428 (2)
C6—H6C	0.9800	C13A—C14A	1.382 (3)
C7—H7A	0.9800	C13A—H13A	0.9500
C7—H7B	0.9800	C14A—C15A	1.409 (3)
C7—H7C	0.9800	C14A—H14A	0.9500
C10—C11	1.365 (2)	C15A—C16A	1.380 (2)
C11—C12	1.433 (3)	C15A—H15A	0.9500
C11—H11	0.9500	C16A—C17A	1.398 (2)
C12—C13	1.404 (2)	C16A—H16A	0.9500

N1—Al1—C6	111.91 (8)	C14—C13—C12	119.17 (18)
N1—Al1—C7	116.33 (8)	C14—C13—H13	120.4
C6—Al1—C7	117.73 (8)	C12—C13—H13	120.4
N1—Al1—N2	85.25 (6)	C13—C14—C15	121.16 (17)
C6—Al1—N2	115.96 (7)	C13—C14—H14	119.4
C7—Al1—N2	105.14 (7)	C15—C14—H14	119.4
N1A—Al1A—C6A	113.03 (8)	C16—C15—C14	120.99 (19)
N1A—Al1A—C7A	114.12 (7)	C16—C15—H15	119.5
C6A—Al1A—C7A	118.00 (8)	C14—C15—H15	119.5
N1A—Al1A—N2A	85.91 (6)	C15—C16—C17	118.25 (17)
C6A—Al1A—N2A	108.30 (7)	C15—C16—H16	120.9
C7A—Al1A—N2A	112.91 (8)	C17—C16—H16	120.9
C10—N1—C17	105.83 (13)	N1—C17—C16	129.35 (16)
C10—N1—Al1	112.84 (11)	N1—C17—C12	109.32 (16)

C17—N1—Al1	139.57 (13)	C16—C17—C12	121.28 (16)
C17A—N1A—C10A	106.15 (14)	C10A—C1A—N2A	108.11 (13)
C17A—N1A—Al1A	140.50 (12)	C10A—C1A—H1D	110.1
C10A—N1A—Al1A	113.18 (11)	N2A—C1A—H1D	110.1
C2—N2—C1	108.22 (13)	C10A—C1A—H1E	110.1
C2—N2—C4	112.02 (12)	N2A—C1A—H1E	110.1
C1—N2—C4	110.43 (13)	H1D—C1A—H1E	108.4
C2—N2—Al1	115.63 (10)	N2A—C2A—C3A	115.85 (14)
C1—N2—Al1	101.69 (10)	N2A—C2A—H2D	108.3
C4—N2—Al1	108.35 (10)	C3A—C2A—H2D	108.3
C4A—N2A—C2A	112.02 (14)	N2A—C2A—H2E	108.3
C4A—N2A—C1A	109.27 (13)	C3A—C2A—H2E	108.3
C2A—N2A—C1A	110.02 (13)	H2D—C2A—H2E	107.4
C4A—N2A—Al1A	114.30 (11)	C2A—C3A—H3D	109.5
C2A—N2A—Al1A	108.47 (10)	C2A—C3A—H3E	109.5
C1A—N2A—Al1A	102.31 (11)	H3D—C3A—H3E	109.5
C10—C1—N2	107.43 (14)	C2A—C3A—H3F	109.5
C10—C1—H1A	110.2	H3D—C3A—H3F	109.5
N2—C1—H1A	110.2	H3E—C3A—H3F	109.5
C10—C1—H1B	110.2	N2A—C4A—C5A	113.37 (15)
N2—C1—H1B	110.2	N2A—C4A—H4D	108.9
H1A—C1—H1B	108.5	C5A—C4A—H4D	108.9
N2—C2—C3	113.28 (15)	N2A—C4A—H4E	108.9
N2—C2—H2A	108.9	C5A—C4A—H4E	108.9
C3—C2—H2A	108.9	H4D—C4A—H4E	107.7
N2—C2—H2B	108.9	C4A—C5A—H5D	109.5
C3—C2—H2B	108.9	C4A—C5A—H5E	109.5
H2A—C2—H2B	107.7	H5D—C5A—H5E	109.5
C2—C3—H3A	109.5	C4A—C5A—H5F	109.5
C2—C3—H3B	109.5	H5D—C5A—H5F	109.5
H3A—C3—H3B	109.5	H5E—C5A—H5F	109.5
C2—C3—H3C	109.5	Al1A—C6A—H6D	109.5
H3A—C3—H3C	109.5	Al1A—C6A—H6E	109.5
H3B—C3—H3C	109.5	H6D—C6A—H6E	109.5
N2—C4—C5	115.68 (15)	Al1A—C6A—H6F	109.5
N2—C4—H4A	108.4	H6D—C6A—H6F	109.5
C5—C4—H4A	108.4	H6E—C6A—H6F	109.5
N2—C4—H4B	108.4	Al1A—C7A—H7D	109.5
C5—C4—H4B	108.4	Al1A—C7A—H7E	109.5
H4A—C4—H4B	107.4	H7D—C7A—H7E	109.5
C4—C5—H5A	109.5	Al1A—C7A—H7F	109.5
C4—C5—H5B	109.5	H7D—C7A—H7F	109.5
H5A—C5—H5B	109.5	H7E—C7A—H7F	109.5
C4—C5—H5C	109.5	C11A—C10A—N1A	112.32 (15)
H5A—C5—H5C	109.5	C11A—C10A—C1A	132.80 (16)
H5B—C5—H5C	109.5	N1A—C10A—C1A	114.84 (14)
Al1—C6—H6A	109.5	C10A—C11A—C12A	106.03 (15)
Al1—C6—H6B	109.5	C10A—C11A—H11A	127.0

H6A—C6—H6B	109.5	C12A—C11A—H11A	127.0
Al1—C6—H6C	109.5	C13A—C12A—C17A	118.82 (17)
H6A—C6—H6C	109.5	C13A—C12A—C11A	135.04 (17)
H6B—C6—H6C	109.5	C17A—C12A—C11A	106.14 (15)
Al1—C7—H7A	109.5	C14A—C13A—C12A	119.22 (17)
Al1—C7—H7B	109.5	C14A—C13A—H13A	120.4
H7A—C7—H7B	109.5	C12A—C13A—H13A	120.4
Al1—C7—H7C	109.5	C13A—C14A—C15A	121.12 (17)
H7A—C7—H7C	109.5	C13A—C14A—H14A	119.4
H7B—C7—H7C	109.5	C15A—C14A—H14A	119.4
C11—C10—N1	112.64 (15)	C16A—C15A—C14A	121.18 (18)
C11—C10—C1	132.87 (16)	C16A—C15A—H15A	119.4
N1—C10—C1	114.36 (14)	C14A—C15A—H15A	119.4
C10—C11—C12	105.78 (15)	C15A—C16A—C17A	118.04 (17)
C10—C11—H11	127.1	C15A—C16A—H16A	121.0
C12—C11—H11	127.1	C17A—C16A—H16A	121.0
C13—C12—C17	119.11 (18)	N1A—C17A—C16A	129.05 (16)
C13—C12—C11	134.47 (17)	N1A—C17A—C12A	109.34 (15)
C17—C12—C11	106.40 (15)	C16A—C17A—C12A	121.61 (16)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C12*A*–C17*A* ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···*Cg*1	0.98	2.57	3.470 (2)	153
C2—H2*B*···*Cg*1^{i}	0.99	2.55	3.434 (2)	149

Symmetry code: (i) −*x*+1, *y*−1/2, −*z*+1.