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{*N*-[2-(2,6-Dimethylphenylamino)benzylidene]-2,6-dimethylaniline-κ^2N,N'}-dimethylaluminium(III)

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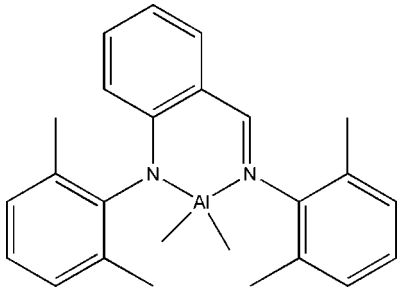
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.105; data-to-parameter ratio = 19.7.

In the title complex, $[Al(CH_3)_2(C_{23}H_{23}N_2)]$, a mononuclear Schiff base dimethylaluminium complex, the Al atom is four-coordinated by two N atoms from one Schiff base ligand and by the C atoms of the two methyl substituents. The Al atom exhibits a distorted tetrahedral coordination geometry.

Related literature

For related literature, see: Bochmann & Dawson (1996); Britovsek *et al.* (1999); Coles *et al.* (1997); Dias *et al.* (1995); Gameron *et al.* (1999, 2001); Huang *et al.* (2001); Jegier & Atwood (1997); Kuroki *et al.* (1991); Liu *et al.* (2005); Pappalardo *et al.* (2002); McKnight & Waymouth (1998).



Experimental

Crystal data

$[Al(CH_3)_2(C_{23}H_{23}N_2)]$
M_r = 384.48
Monoclinic, $P2_1/c$
a = 9.0483 (18) Å
b = 11.045 (2) Å
c = 24.192 (5) Å
β = 111.64 (3)°
V = 2247.3 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.19 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.981, T_{max} = 0.985
11340 measured reflections
5115 independent reflections
2682 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.106
S = 0.96
5115 reflections
259 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Al1—N1	1.8783 (15)	Al1—N2	1.9453 (15)
Al1—C25	1.943 (2)	Al1—C24	1.948 (2)
N1—Al1—C25	112.62 (8)	N1—Al1—C24	115.96 (8)
N1—Al1—N2	93.86 (6)	C25—Al1—C24	112.67 (10)
C25—Al1—N2	111.81 (8)	N2—Al1—C24	108.36 (8)

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2062).

References

Bochmann, M. & Dawson, D. (1996). *Angew. Chem. Int. Ed. Engl.* **35**, 2226–2228.
Britovsek, G. J. P., Gibson, V. C. & Wass, D. F. (1999). *Angew. Chem. Int. Ed.* **38**, 428–447.
Coles, M. P., Swenson, D. C., Jordan, R. F. & Young, V. G. Jr (1997). *Organometallics*, **16**, 5183–5194.
Dias, H. V., Jin, R. W. & Ratcliff, R. E. (1995). *Inorg. Chem.* **34**, 6100–6105.
Gameron, P. A., Gibson, V. C., Solan, G. A., White, A. J. P. & Williams, D. J. (1999). *Chem. Commun.* pp. 1883–1884.
Gameron, P. A., Gibson, V. C., Solan, G. A., White, A. J. P. & Williams, D. J. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1472–1476.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Huang, J. H., Chen, H. J., Zhou, C. C., Lee, G. H. & Peng, S. M. (2001). *Organometallics*, **20**, 2647–2650.
Jegier, J. A. & Atwood, D. A. (1997). *Inorg. Chem.* **36**, 2034–2039.
Kuroki, M., Watanabe, T., Aida, T. & Inoue, S. (1991). *J. Am. Chem. Soc.* **113**, 5903–5904.
Liu, X., Gao, W., Mu, Y., Li, G., Ye, L., Xia, H., Ren, Y. & Feng, S. (2005). *Organometallics*, **24**, 1614–1619.
McKnight, A. L. & Waymouth, R. M. (1998). *Chem. Rev.* **98**, 2587–2598.
Pappalardo, D., Tedesco, C. & Pellecchia, C. (2002). *Eur. J. Inorg. Chem.* pp. 621–628.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1993). *XP*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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{*N*-[2-(2,6-Dimethylphenylamino)benzylidene]-2,6-dimethylaniline-$\kappa^2 N,N'$}dimethylaluminium(III)

X.-M. Liu, W. Gao, B. Li, J.-G. Ni and Y. Mu

Comment

Organoaluminium complexes are currently generating considerable interest due to their increasing role in polymerization chemistry, such as cationic (Bochmann & Dawson, 1996), anionic (Kuroki *et al.*, 1991) and ring-opening polymerization, (Jegier & Atwood, 1997) and as cocatalysts in transition metal-catalysed olefin polymerization (McKnight & Waymouth, 1998; Britovsek *et al.*, 1999). Previously, a lot of alkylaluminium complexes with bidentate (Gameron *et al.*, 2001; Pappalardo *et al.*, 2002) or tridentate (Gameron *et al.*, 1999; Huang *et al.*, 2001) Schiff base ligands have been reported. Our current research efforts are focused on alkylaluminium complexes with new ligands. Herein we report the structure of the title complex, a mononuclear Schiff base dimethyl aluminium complex.

An *ORTEP* drawing of the molecular structure of the complex is shown in Fig. 1. The aluminium atom exhibits a distorted tetrahedral geometry. The N—Al—N angle (93.8°) in the complex is similar to that of *ortho*-$C_6H_4N(C_6H_4$-4-Me)(CH=NC_6H_4-4-Me)$AlMe_2$ (94.5°, Liu *et al.*, 2005), but larger than those in {tBuC$(NCy)_2$}$AlMe_2$ (Coles *et al.*, 1997) and {$(iPr)_2$ATI}$AlMe_2$ (Dias *et al.*, 1995) with four- and five- membered chelating rings, which exhibit angles of 69° and 84°, respectively. In the title compound the six membered chelating ring is nearly planar and the distance of the aluminium atom from the mean plane made up by the other five atoms of the six membered ring is only 0.1383 (7) Å. The imino C=N bond in the complex retains its double bond character with a bond length of 1.295 (2) Å.

Experimental

A solution of *ortho*-$C_6H_4NH(C_6H_3$-2,6-$Me_2)$(CH=NC_6H_3-2,6-Me_2) (0.20 g, 0.61 mmol) (Liu *et al.*, 2005) in 10 ml of n-hexane was slowly added to a solution of $AlMe_3$ (0.61 mmol) in 15 ml of n-hexane at 273 K with stirring. The mixture was stirred at 273 K for 30 min, and at room temperature for additional 2 h, was then concentrated to about 10 ml and kept at 253 K overnight to let the product crystallize. The product was obtained as orange-green crystals (0.21 g, 90%).

Refinement

The C-bound H atoms were positioned geometrically with C—H = 0.93–0.96 Å, and allowed to ride on their parent atoms with U_{iso}(H) = 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for all other hydrogen atoms.

Figures

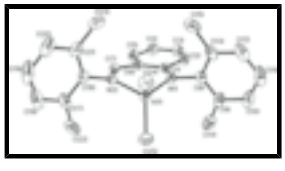


Fig. 1. View of the molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms were omitted for clarity.

{*N*-[2-(2,6-Dimethylphenylamino)benzylidene]-2,6-dimethylaniline- $\kappa^2 N,N'$}dimethylaluminium(III)

Crystal data

$[Al(CH_3)_2(C_{23}H_{23}N_2)]$	F_{000} = 824
M_r = 384.48	D_x = 1.136 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11340 reflections
a = 9.0483 (18) Å	θ = 5.8–54.9º
b = 11.045 (2) Å	μ = 0.10 mm^{-1}
c = 24.192 (5) Å	T = 293 (2) K
β = 111.64 (3)º	Block, yellow
V = 2247.3 (8) Å^3	0.19 × 0.18 × 0.15 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	5115 independent reflections
Radiation source: fine-focus sealed tube	2682 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −11→11
T_{min} = 0.981, T_{max} = 0.985	k = −14→14
11340 measured reflections	l = −28→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.106	$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.96	$(\Delta/\sigma)_{max}$ = 0.002
5115 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
259 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. (See detailed section in the paper)

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.26222 (6)	0.28378 (5)	0.10575 (2)	0.04098 (16)
N1	0.41224 (16)	0.39710 (13)	0.15157 (6)	0.0402 (4)
N2	0.39168 (17)	0.23307 (13)	0.06112 (6)	0.0405 (4)
C1	0.5702 (2)	0.40123 (15)	0.16054 (7)	0.0388 (4)
C2	0.6757 (2)	0.47997 (17)	0.20191 (8)	0.0499 (5)
H2	0.6370	0.5323	0.2235	0.060*
C3	0.8334 (2)	0.48160 (19)	0.21122 (9)	0.0563 (5)
H3	0.9001	0.5342	0.2395	0.068*
C4	0.8975 (2)	0.40686 (19)	0.17966 (9)	0.0600 (6)
H4	1.0057	0.4085	0.1867	0.072*
C5	0.7995 (2)	0.33225 (18)	0.13870 (9)	0.0539 (5)
H5	0.8413	0.2825	0.1171	0.065*
C6	0.6352 (2)	0.32662 (16)	0.12728 (8)	0.0410 (4)
C7	0.5424 (2)	0.25570 (16)	0.07846 (8)	0.0466 (5)
H7	0.5956	0.2210	0.0560	0.056*
C8	0.3519 (2)	0.48571 (17)	0.18158 (8)	0.0435 (5)
C9	0.3534 (2)	0.4627 (2)	0.23841 (9)	0.0545 (5)
C10	0.2850 (3)	0.5477 (3)	0.26395 (11)	0.0775 (8)
H10	0.2853	0.5347	0.3020	0.093*
C11	0.2172 (3)	0.6506 (3)	0.23360 (15)	0.0872 (9)
H11	0.1694	0.7057	0.2509	0.105*
C12	0.2188 (3)	0.6734 (2)	0.17843 (14)	0.0799 (8)
H12	0.1724	0.7439	0.1585	0.096*
C13	0.2891 (2)	0.59224 (18)	0.15176 (10)	0.0582 (6)
C14	0.4301 (3)	0.3531 (2)	0.27284 (9)	0.0817 (7)
H14A	0.4346	0.2906	0.2459	0.123*
H14B	0.3691	0.3252	0.2955	0.123*
H14C	0.5359	0.3728	0.2993	0.123*
C15	0.3006 (3)	0.6233 (2)	0.09329 (11)	0.0847 (8)
H15A	0.2323	0.6907	0.0759	0.127*
H15B	0.2685	0.5548	0.0671	0.127*
H15C	0.4084	0.6442	0.0993	0.127*
C16	0.3169 (2)	0.17614 (18)	0.00394 (9)	0.0485 (5)
C17	0.2837 (3)	0.0534 (2)	0.00084 (11)	0.0667 (6)
C18	0.1980 (3)	0.0062 (3)	−0.05477 (15)	0.0936 (9)

H18	0.1706	−0.0754	−0.0583	0.112*
C19	0.1535 (3)	0.0758 (4)	−0.10386 (15)	0.1062 (12)
H19	0.0949	0.0419	−0.1406	0.127*
C20	0.1932 (3)	0.1959 (3)	−0.10033 (11)	0.0879 (8)
H20	0.1643	0.2422	−0.1348	0.106*
C21	0.2751 (3)	0.2486 (2)	−0.04632 (9)	0.0607 (6)
C22	0.3397 (4)	−0.0260 (2)	0.05438 (13)	0.1026 (10)
H22A	0.3767	0.0232	0.0896	0.154*
H22B	0.4250	−0.0763	0.0531	0.154*
H22C	0.2535	−0.0761	0.0549	0.154*
C23	0.3145 (3)	0.3815 (2)	−0.04262 (11)	0.0872 (8)
H23A	0.2651	0.4178	−0.0811	0.131*
H23B	0.4277	0.3916	−0.0294	0.131*
H23C	0.2760	0.4199	−0.0150	0.131*
C24	0.0638 (2)	0.35035 (19)	0.05008 (9)	0.0601 (6)
H24A	0.0194	0.4049	0.0707	0.090*
H24B	−0.0098	0.2857	0.0330	0.090*
H24C	0.0841	0.3932	0.0191	0.090*
C25	0.2286 (3)	0.15255 (19)	0.15330 (9)	0.0702 (6)
H25A	0.3293	0.1184	0.1775	0.105*
H25B	0.1638	0.0912	0.1275	0.105*
H25C	0.1761	0.1832	0.1784	0.105*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0376 (3)	0.0463 (3)	0.0386 (3)	−0.0041 (3)	0.0135 (2)	0.0009 (3)
N1	0.0371 (8)	0.0443 (9)	0.0402 (9)	−0.0009 (7)	0.0156 (7)	−0.0046 (7)
N2	0.0405 (8)	0.0392 (9)	0.0421 (9)	−0.0055 (7)	0.0157 (7)	−0.0019 (7)
C1	0.0395 (10)	0.0405 (10)	0.0336 (10)	−0.0042 (9)	0.0101 (8)	0.0022 (8)
C2	0.0459 (12)	0.0568 (12)	0.0485 (12)	−0.0062 (10)	0.0189 (10)	−0.0105 (10)
C3	0.0451 (12)	0.0671 (14)	0.0543 (13)	−0.0140 (11)	0.0156 (10)	−0.0128 (11)
C4	0.0416 (11)	0.0752 (15)	0.0658 (14)	−0.0104 (11)	0.0230 (11)	−0.0070 (12)
C5	0.0461 (12)	0.0606 (13)	0.0611 (13)	−0.0036 (10)	0.0268 (10)	−0.0095 (11)
C6	0.0388 (10)	0.0452 (11)	0.0427 (11)	−0.0041 (9)	0.0194 (9)	−0.0028 (9)
C7	0.0516 (12)	0.0442 (11)	0.0501 (12)	−0.0008 (9)	0.0258 (10)	−0.0031 (9)
C8	0.0316 (10)	0.0481 (11)	0.0469 (12)	−0.0040 (9)	0.0100 (8)	−0.0101 (10)
C9	0.0418 (11)	0.0733 (14)	0.0497 (12)	−0.0071 (11)	0.0183 (10)	−0.0194 (12)
C10	0.0575 (15)	0.110 (2)	0.0721 (17)	−0.0199 (15)	0.0314 (13)	−0.0425 (16)
C11	0.0515 (15)	0.088 (2)	0.127 (3)	−0.0092 (14)	0.0383 (17)	−0.058 (2)
C12	0.0567 (15)	0.0547 (14)	0.116 (2)	0.0038 (11)	0.0168 (15)	−0.0218 (15)
C13	0.0479 (12)	0.0480 (12)	0.0686 (15)	−0.0024 (11)	0.0098 (11)	−0.0129 (11)
C14	0.0947 (18)	0.1040 (19)	0.0463 (14)	0.0072 (17)	0.0257 (13)	0.0064 (14)
C15	0.0993 (19)	0.0548 (14)	0.084 (2)	−0.0010 (14)	0.0152 (15)	0.0136 (13)
C16	0.0424 (11)	0.0557 (12)	0.0487 (12)	−0.0046 (10)	0.0183 (9)	−0.0144 (10)
C17	0.0647 (14)	0.0544 (14)	0.0845 (18)	−0.0083 (12)	0.0317 (13)	−0.0254 (13)
C18	0.0756 (19)	0.0850 (19)	0.116 (2)	−0.0164 (16)	0.0305 (19)	−0.054 (2)
C19	0.0681 (18)	0.157 (3)	0.083 (2)	−0.012 (2)	0.0155 (16)	−0.073 (2)

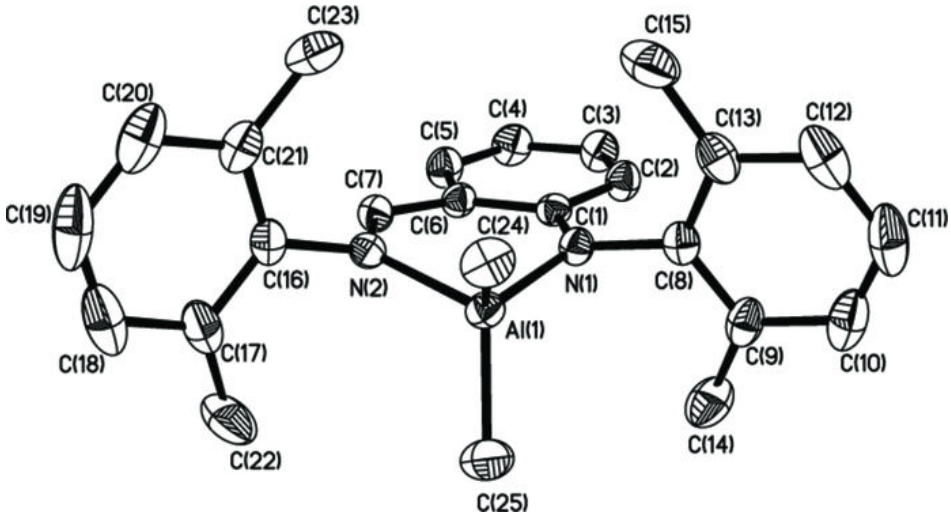
C20	0.0721 (17)	0.138 (3)	0.0485 (15)	0.0066 (18)	0.0157 (12)	−0.0192 (17)
C21	0.0583 (13)	0.0787 (16)	0.0478 (13)	0.0008 (12)	0.0228 (10)	−0.0080 (11)
C22	0.137 (3)	0.0426 (14)	0.138 (3)	−0.0030 (16)	0.062 (2)	−0.0014 (16)
C23	0.118 (2)	0.0892 (19)	0.0665 (17)	0.0023 (17)	0.0486 (16)	0.0222 (14)
C24	0.0433 (11)	0.0760 (15)	0.0568 (13)	0.0023 (11)	0.0134 (10)	0.0072 (11)
C25	0.0751 (16)	0.0721 (15)	0.0663 (16)	−0.0134 (13)	0.0292 (12)	0.0093 (12)

Geometric parameters (Å, °)

Al1—N1	1.8783 (15)	C13—C15	1.496 (3)
Al1—C25	1.943 (2)	C14—H14A	0.9600
Al1—N2	1.9453 (15)	C14—H14B	0.9600
Al1—C24	1.948 (2)	C14—H14C	0.9600
N1—C1	1.365 (2)	C15—H15A	0.9600
N1—C8	1.441 (2)	C15—H15B	0.9600
N2—C7	1.295 (2)	C15—H15C	0.9600
N2—C16	1.441 (2)	C16—C17	1.384 (3)
C1—C2	1.402 (2)	C16—C21	1.387 (3)
C1—C6	1.422 (2)	C17—C18	1.384 (3)
C2—C3	1.360 (3)	C17—C22	1.490 (3)
C2—H2	0.9300	C18—C19	1.346 (4)
C3—C4	1.388 (3)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.369 (4)
C4—C5	1.342 (3)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.371 (3)
C5—C6	1.410 (2)	C20—H20	0.9300
C5—H5	0.9300	C21—C23	1.506 (3)
C6—C7	1.408 (2)	C22—H22A	0.9600
C7—H7	0.9300	C22—H22B	0.9600
C8—C13	1.387 (3)	C22—H22C	0.9600
C8—C9	1.393 (3)	C23—H23A	0.9600
C9—C10	1.388 (3)	C23—H23B	0.9600
C9—C14	1.488 (3)	C23—H23C	0.9600
C10—C11	1.369 (3)	C24—H24A	0.9600
C10—H10	0.9300	C24—H24B	0.9600
C11—C12	1.364 (4)	C24—H24C	0.9600
C11—H11	0.9300	C25—H25A	0.9600
C12—C13	1.389 (3)	C25—H25B	0.9600
C12—H12	0.9300	C25—H25C	0.9600
N1—Al1—C25	112.62 (8)	H14A—C14—H14B	109.5
N1—Al1—N2	93.86 (6)	C9—C14—H14C	109.5
C25—Al1—N2	111.81 (8)	H14A—C14—H14C	109.5
N1—Al1—C24	115.96 (8)	H14B—C14—H14C	109.5
C25—Al1—C24	112.67 (10)	C13—C15—H15A	109.5
N2—Al1—C24	108.36 (8)	C13—C15—H15B	109.5
C1—N1—C8	117.81 (14)	H15A—C15—H15B	109.5
C1—N1—Al1	127.06 (12)	C13—C15—H15C	109.5
C8—N1—Al1	115.10 (10)	H15A—C15—H15C	109.5
C7—N2—C16	117.44 (15)	H15B—C15—H15C	109.5

C7—N2—Al1	122.85 (12)	C17—C16—C21	122.3 (2)
C16—N2—Al1	119.52 (11)	C17—C16—N2	119.67 (19)
N1—C1—C2	122.15 (16)	C21—C16—N2	118.02 (18)
N1—C1—C6	121.20 (15)	C18—C17—C16	117.0 (2)
C2—C1—C6	116.63 (16)	C18—C17—C22	120.8 (2)
C3—C2—C1	121.57 (18)	C16—C17—C22	122.1 (2)
C3—C2—H2	119.2	C19—C18—C17	121.4 (3)
C1—C2—H2	119.2	C19—C18—H18	119.3
C2—C3—C4	121.76 (19)	C17—C18—H18	119.3
C2—C3—H3	119.1	C18—C19—C20	120.8 (3)
C4—C3—H3	119.1	C18—C19—H19	119.6
C5—C4—C3	118.37 (18)	C20—C19—H19	119.6
C5—C4—H4	120.8	C19—C20—C21	120.5 (3)
C3—C4—H4	120.8	C19—C20—H20	119.7
C4—C5—C6	122.28 (19)	C21—C20—H20	119.7
C4—C5—H5	118.9	C20—C21—C16	117.9 (2)
C6—C5—H5	118.9	C20—C21—C23	120.2 (2)
C7—C6—C5	116.65 (17)	C16—C21—C23	121.9 (2)
C7—C6—C1	123.64 (16)	C17—C22—H22A	109.5
C5—C6—C1	119.34 (16)	C17—C22—H22B	109.5
N2—C7—C6	127.61 (17)	H22A—C22—H22B	109.5
N2—C7—H7	116.2	C17—C22—H22C	109.5
C6—C7—H7	116.2	H22A—C22—H22C	109.5
C13—C8—C9	121.40 (18)	H22B—C22—H22C	109.5
C13—C8—N1	118.19 (17)	C21—C23—H23A	109.5
C9—C8—N1	120.39 (17)	C21—C23—H23B	109.5
C10—C9—C8	118.2 (2)	H23A—C23—H23B	109.5
C10—C9—C14	119.6 (2)	C21—C23—H23C	109.5
C8—C9—C14	122.25 (18)	H23A—C23—H23C	109.5
C11—C10—C9	120.5 (2)	H23B—C23—H23C	109.5
C11—C10—H10	119.7	Al1—C24—H24A	109.5
C9—C10—H10	119.7	Al1—C24—H24B	109.5
C12—C11—C10	120.9 (2)	H24A—C24—H24B	109.5
C12—C11—H11	119.5	Al1—C24—H24C	109.5
C10—C11—H11	119.5	H24A—C24—H24C	109.5
C11—C12—C13	120.5 (2)	H24B—C24—H24C	109.5
C11—C12—H12	119.7	Al1—C25—H25A	109.5
C13—C12—H12	119.7	Al1—C25—H25B	109.5
C8—C13—C12	118.4 (2)	H25A—C25—H25B	109.5
C8—C13—C15	121.89 (19)	Al1—C25—H25C	109.5
C12—C13—C15	119.7 (2)	H25A—C25—H25C	109.5
C9—C14—H14A	109.5	H25B—C25—H25C	109.5
C9—C14—H14B	109.5		

Fig. 1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