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[μ-1-Benzyl-4-(4-*tert*-butylphenyl)-piperazine-κ^2N:N']bis[trimethylaluminium(III)]

Li-Chao Yang,[a] Qiang-Guo Xu,[b] Jia-Bao Ou,[b] Yi-Zhi Li[c]* and Lin Wu[a]

[a]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China, [b]Jiang Su Hengrui Medicine Co. Ltd, Lianyungang 222002, People's Republic of China, and [c]Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210093, People's Republic of China
Correspondence e-mail: shenyongmiao@nju.org.cn

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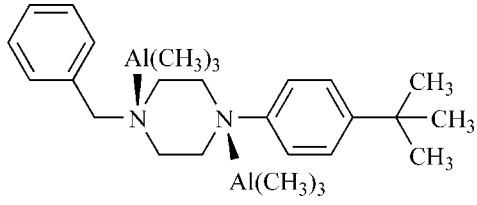
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.064; wR factor = 0.135; data-to-parameter ratio = 19.0.

In the title compound, $[Al_2(CH_3)_6(C_{21}H_{28}N_2)]$, the piperazine ring adopts a chair conformation. The Al—N bond lengths range from 2.089 (2) to 2.121 (2) Å. The four-coordinate environment of the Al atoms is defined by one piperazine N atom and three methyl ligands. The structure contains two independent molecules in the asymmetric unit. Both molecules have almost the same conformation, except for the benzyl groups which show different rotations in the two molecules. The independent molecules are related to one another by a pseudorotation in combination with a translation along the *a* axis. Intermolecular C—H$\cdots\pi$ contacts or stacking between the benzyl or phenyl rings are not observed.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Aguero *et al.*, (2005); Das & Shivashankar, (2007); Reier *et al.*, (1988). For information about Z' = 2 structures, see: Desiraju *et al.*, (1991); Brock & Dunitz, (1994); Steiner (2000).



Experimental

Crystal data

$[Al_2(CH_3)_6(C_{21}H_{28}N_2)]$
M_r = 452.62
Triclinic, $P\overline{1}$
a = 11.191 (3) Å
b = 12.809 (3) Å
c = 20.489 (5) Å
α = 101.419 (3)°
β = 96.138 (4)°
γ = 90.242 (4)°
V = 2861.5 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.892, T_{max} = 0.975
15540 measured reflections
10970 independent reflections
7250 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.135
S = 1.01
10970 reflections
577 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected torsion angles (°).

N1—C5—C6—C11	99.2 (3)	C13—C12—N2—Al2	−92.5 (3)
C2—C1—N1—C4	−53.5 (3)	C4—C3—N2—C2	60.2 (3)

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2027).

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supplementary materials

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[μ-1-Benzyl-4-(4-*tert*-butylphenyl)piperazine-κ^2N:N']bis[trimethylaluminium(III)]

L.-C. Yang, Q.-G. Xu, J.-B. Ou, Y.-Z. Li and L. Wu

Comment

MOCVD (metalorganic chemical vapour deposition) is a well known technique for growth of thin films of metals (Das *et al.*, 2007). The purity of metallorganic precursors plays an important role in the technique (Aguero *et al.*, 2005). Coordination is a good way to get the high purity of metallorganic precursors (Reier *et al.*, 1988). So, we synthesized the title compound and found two independent molecules (Z' = 2) in the asymmetric unit of the cell (Brock & Dunitz, 1994; Steiner, 2000) (Fig.1). Conformational differences of the molecules are distinguished by opposite rotation of their benzyl moieties: in molecule 1 the π system of the benzyl ring approaches H22C of a methyl of Al1, whereas in molecule 2, the benzyl ring rotates towards the opposite Al4 to approach H51B of a methyl group. The main part of the molecules (piperazine, both trimethylaluminum and *tert*-butylphenyl) have almost identical conformation. Intermolecular C—H···π contacts and stacking between benzyl or phenyl rings could not be observed. In a *b,c*-projection of the unit cell, the main part of the independent molecules seem to be related *via* a twofold symmetry, the axis running along *a* at 3/4*b* and *ca* 1/2*c*. In the *a,c*-projection of the unit cell (Fig. 2) however, one can imagine that after rotation around the pseudo-rotation axis at *c*/2, a translation of *ca* 0.65 along the *a* axis is necessary to find the molecules at identical positions, except of the benzyl moieties. The presented structure is found to agree well with the majority of triclinic structures with Z' = 2 in respect to symmetry relation between the independent molecules. Only few examples were found to have pseudoinversion centers between independent molecules (Desiraju *et al.*, 1991). In both molecules of the title compound, the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The four-coordinate environment of the Al atoms is completed by one N atom and three methyl ligands. The Al—N bond lengths range from 2.089 (2) Å to 2.121 (2) Å.

Experimental

In the absence of oxygen and under anhydrous conditions, to a solution of 1-benzyl-4-(4-*tert*-butylphenyl)piperazine (1 mmol) in petroleum ether (2 mL) was added the solution of trimethylaluminum (2 mol/*L*) in petroleum ether (1 mL) and heated to reflux. The resulting mixture was cooled to room temperature and white solid was obtained. It was solved in the petroleum ether and evaporated in the N_2 atmosphere. Then colourless block-shaped crystals suitable for X-ray diffraction were obtained after several days, these were filtered off and washed with petroleum ether (yield 73%).

Refinement

The H atoms were fixed geometrically and were treated as riding on their parent C atoms, with C—H distances in the range of 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(parent atom), or U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

Figures

Fig. 1. The independent molecules of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

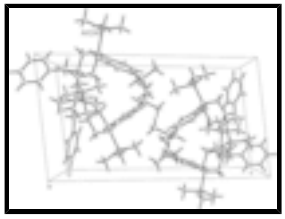


Fig. 2. The independent molecules of the title compound viewed along the **b**-axis of the unit cell.

[μ-1-Benzyl-4-(4-*tert*-butylphenyl)piperazine- $\kappa^2N:N'$]bis[trimethylaluminium(III)]

Crystal data

$[Al_2(CH_3)_6(C_{21}H_{28}N_2)]$	$Z = 4$
$M_r = 452.62$	$F_{000} = 992$
Triclinic, $P\overline{1}$	$D_x = 1.051$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 443 K
$a = 11.191$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 12.809$ (3) Å	Cell parameters from 4614 reflections
$c = 20.489$ (5) Å	$\theta = 2.5$–28.0º
$\alpha = 101.419$ (3)º	$\mu = 0.12$ mm^{-1}
$\beta = 96.138$ (4)º	$T = 291$ (2) K
$\gamma = 90.242$ (4)º	Block, colourless
$V = 2861.5$ (13) Å^3	0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	10970 independent reflections
Radiation source: sealed tube	7250 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
$T = 291(2)$ K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -7 \rightarrow 13$
$T_{min} = 0.892$, $T_{max} = 0.975$	$k = -15 \rightarrow 14$
15540 measured reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.135$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
10970 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
577 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Al1	0.64159 (7)	0.89507 (6)	0.14885 (4)	0.03113 (18)
Al2	1.21587 (7)	0.91358 (6)	0.30146 (4)	0.03029 (18)
Al3	0.27837 (7)	0.61368 (7)	0.85482 (4)	0.03272 (19)
Al4	0.79296 (7)	0.58930 (6)	0.70435 (4)	0.02890 (18)
C1	0.8858 (2)	0.8244 (2)	0.16797 (13)	0.0310 (6)
H1A	0.8803	0.7846	0.1222	0.037*
H1B	0.8436	0.7833	0.1938	0.037*
C2	1.0182 (2)	0.8382 (2)	0.19682 (12)	0.0320 (6)
H2A	1.0549	0.7690	0.1924	0.038*
H2B	1.0606	0.8806	0.1719	0.038*
C3	0.9768 (2)	1.0013 (2)	0.26989 (13)	0.0303 (6)
H3A	1.0241	1.0390	0.2444	0.036*
H3B	0.9819	1.0421	0.3154	0.036*
C4	0.8461 (2)	0.9936 (2)	0.23917 (13)	0.0335 (6)
H4A	0.7982	0.9618	0.2673	0.040*
H4B	0.8176	1.0650	0.2391	0.040*
C5	0.8775 (2)	0.9940 (2)	0.12317 (13)	0.0308 (6)
H5A	0.8343	1.0599	0.1258	0.037*
H5B	0.9608	1.0125	0.1400	0.037*
C6	0.8722 (2)	0.9393 (2)	0.05030 (13)	0.0325 (6)
C7	0.9613 (2)	0.8707 (2)	0.02695 (13)	0.0340 (6)
H7	1.0244	0.8566	0.0571	0.041*

C8	0.9583 (3)	0.8229 (2)	−0.03992 (13)	0.0397 (7)
H8	1.0170	0.7753	−0.0544	0.048*
C9	0.8659 (3)	0.8473 (2)	−0.08512 (14)	0.0412 (7)
H9	0.8636	0.8165	−0.1303	0.049*
C10	0.7781 (3)	0.9165 (2)	−0.06377 (14)	0.0398 (7)
H10	0.7171	0.9322	−0.0946	0.048*
C11	0.7800 (2)	0.9630 (2)	0.00359 (13)	0.0353 (6)
H11	0.7204	1.0098	0.0178	0.042*
C12	0.9765 (2)	0.8347 (2)	0.31560 (13)	0.0311 (6)
C13	0.9627 (3)	0.7213 (2)	0.30128 (13)	0.0340 (6)
H13	0.9852	0.6834	0.2611	0.041*
C14	0.9186 (3)	0.6675 (2)	0.34359 (13)	0.0354 (6)
H14	0.9113	0.5936	0.3319	0.043*
C15	0.8835 (2)	0.7196 (2)	0.40471 (13)	0.0305 (6)
C16	0.8951 (3)	0.8298 (2)	0.41933 (13)	0.0356 (6)
H16	0.8717	0.8667	0.4596	0.043*
C17	0.9407 (2)	0.8876 (2)	0.37573 (12)	0.0324 (6)
H17	0.9469	0.9615	0.3872	0.039*
C18	0.8331 (3)	0.6590 (2)	0.45344 (14)	0.0377 (6)
C19	0.8319 (3)	0.5369 (3)	0.42843 (18)	0.0562 (9)
H19A	0.8053	0.5024	0.4620	0.084*
H19B	0.9115	0.5147	0.4198	0.084*
H19C	0.7781	0.5179	0.3879	0.084*
C20	0.9149 (3)	0.6837 (3)	0.52033 (15)	0.0492 (8)
H20A	0.9312	0.7591	0.5329	0.074*
H20B	0.9891	0.6471	0.5153	0.074*
H20C	0.8753	0.6603	0.5544	0.074*
C21	0.7067 (3)	0.6965 (3)	0.46511 (19)	0.0615 (10)
H21A	0.7103	0.7703	0.4867	0.092*
H21B	0.6725	0.6551	0.4930	0.092*
H21C	0.6576	0.6878	0.4229	0.092*
C22	0.6199 (3)	0.7823 (2)	0.06713 (13)	0.0365 (6)
H22A	0.5357	0.7664	0.0546	0.055*
H22B	0.6597	0.7193	0.0757	0.055*
H22C	0.6538	0.8063	0.0314	0.055*
C23	0.5732 (3)	1.0357 (2)	0.14290 (15)	0.0402 (7)
H23A	0.5559	1.0404	0.0967	0.060*
H23B	0.6301	1.0911	0.1650	0.060*
H23C	0.5004	1.0436	0.1641	0.060*
C24	0.6038 (3)	0.8411 (2)	0.22921 (13)	0.0395 (7)
H24A	0.5213	0.8172	0.2232	0.059*
H24B	0.6172	0.8973	0.2681	0.059*
H24C	0.6549	0.7829	0.2351	0.059*
C25	1.2746 (2)	0.9738 (2)	0.22833 (14)	0.0351 (6)
H25A	1.3549	1.0023	0.2421	0.053*
H25B	1.2228	1.0296	0.2185	0.053*
H25C	1.2745	0.9188	0.1890	0.053*
C26	1.2214 (3)	1.0128 (2)	0.38873 (13)	0.0397 (7)
H26A	1.1903	0.9774	0.4207	0.060*

H26B	1.1735	1.0734	0.3839	0.060*
H26C	1.3031	1.0361	0.4041	0.060*
C27	1.2719 (2)	0.7689 (2)	0.30281 (14)	0.0361 (6)
H27A	1.3543	0.7724	0.3220	0.054*
H27B	1.2655	0.7280	0.2579	0.054*
H27C	1.2234	0.7356	0.3292	0.054*
C28	0.4553 (2)	0.5047 (2)	0.77416 (12)	0.0291 (6)
H28A	0.3941	0.5294	0.7439	0.035*
H28B	0.4312	0.4335	0.7778	0.035*
C29	0.5737 (2)	0.49806 (19)	0.74267 (12)	0.0259 (5)
H29A	0.6326	0.4633	0.7688	0.031*
H29B	0.5610	0.4550	0.6978	0.031*
C30	0.6428 (2)	0.6655 (2)	0.81280 (13)	0.0330 (6)
H30A	0.6974	0.6256	0.8380	0.040*
H30B	0.6794	0.7352	0.8153	0.040*
C31	0.5237 (2)	0.6781 (2)	0.84352 (13)	0.0334 (6)
H31A	0.5395	0.7153	0.8898	0.040*
H31B	0.4722	0.7224	0.8199	0.040*
C32	0.4999 (2)	0.5226 (2)	0.90057 (13)	0.0365 (7)
H32A	0.4906	0.5733	0.9416	0.044*
H32B	0.4455	0.4628	0.8989	0.044*
C33	0.6261 (2)	0.4825 (2)	0.90633 (13)	0.0301 (6)
C34	0.6475 (2)	0.3752 (2)	0.88124 (13)	0.0301 (6)
H34	0.5850	0.3300	0.8583	0.036*
C35	0.7626 (3)	0.3365 (2)	0.89078 (14)	0.0376 (6)
H35	0.7764	0.2653	0.8737	0.045*
C36	0.8557 (3)	0.4011 (3)	0.92486 (14)	0.0438 (7)
H36	0.9318	0.3736	0.9314	0.053*
C37	0.8367 (3)	0.5082 (3)	0.94981 (15)	0.0449 (7)
H37	0.9002	0.5529	0.9721	0.054*
C38	0.7214 (3)	0.5479 (2)	0.94111 (13)	0.0397 (7)
H38	0.7080	0.6189	0.9588	0.048*
C39	0.5475 (2)	0.6626 (2)	0.69475 (13)	0.0320 (6)
C40	0.5367 (3)	0.7738 (2)	0.70635 (14)	0.0364 (6)
H40	0.5732	0.8132	0.7467	0.044*
C41	0.4777 (2)	0.8268 (2)	0.66354 (13)	0.0328 (6)
H41	0.4755	0.9008	0.6743	0.039*
C42	0.4195 (2)	0.7718 (2)	0.60283 (14)	0.0344 (6)
C43	0.4286 (2)	0.6624 (2)	0.58951 (13)	0.0336 (6)
H43	0.3920	0.6241	0.5489	0.040*
C44	0.4894 (2)	0.6068 (2)	0.63361 (13)	0.0345 (6)
H44	0.4917	0.5329	0.6228	0.041*
C45	0.3507 (2)	0.8302 (2)	0.55320 (14)	0.0367 (6)
C46	0.2207 (3)	0.7874 (3)	0.53678 (17)	0.0520 (9)
H46A	0.2202	0.7129	0.5169	0.078*
H46B	0.1781	0.8253	0.5060	0.078*
H46C	0.1823	0.7971	0.5772	0.078*
C47	0.3529 (3)	0.9526 (3)	0.57814 (18)	0.0555 (9)
H47A	0.3151	0.9857	0.5434	0.083*

H47B	0.4347	0.9783	0.5895	0.083*
H47C	0.3104	0.9697	0.6170	0.083*
C48	0.4120 (3)	0.8086 (2)	0.48701 (14)	0.0425 (7)
H48A	0.4215	0.7334	0.4728	0.064*
H48B	0.4895	0.8441	0.4947	0.064*
H48C	0.3628	0.8352	0.4529	0.064*
C49	0.8475 (3)	0.7362 (2)	0.70366 (15)	0.0407 (7)
H49A	0.8504	0.7787	0.7480	0.061*
H49B	0.7924	0.7664	0.6737	0.061*
H49C	0.9262	0.7348	0.6889	0.061*
C50	0.7598 (3)	0.4889 (2)	0.61685 (13)	0.0381 (7)
H50A	0.8344	0.4679	0.5996	0.057*
H50B	0.7123	0.5233	0.5858	0.057*
H50C	0.7168	0.4271	0.6228	0.057*
C51	0.8883 (2)	0.5318 (2)	0.77515 (14)	0.0352 (6)
H51A	0.9667	0.5145	0.7620	0.053*
H51B	0.8487	0.4688	0.7819	0.053*
H51C	0.8958	0.5842	0.8161	0.053*
C52	0.2199 (3)	0.6759 (3)	0.77589 (16)	0.0478 (8)
H52A	0.1437	0.7079	0.7827	0.072*
H52B	0.2110	0.6206	0.7364	0.072*
H52C	0.2769	0.7290	0.7706	0.072*
C53	0.2949 (3)	0.7196 (2)	0.94034 (15)	0.0439 (7)
H53A	0.2176	0.7478	0.9491	0.066*
H53B	0.3489	0.7764	0.9372	0.066*
H53C	0.3263	0.6857	0.9761	0.066*
C54	0.2034 (3)	0.4745 (3)	0.85564 (17)	0.0492 (8)
H54A	0.2406	0.4472	0.8930	0.074*
H54B	0.2141	0.4257	0.8148	0.074*
H54C	0.1191	0.4829	0.8595	0.074*
N1	0.82603 (19)	0.92951 (17)	0.16896 (10)	0.0292 (5)
N2	1.02877 (19)	0.89295 (16)	0.27066 (10)	0.0294 (5)
N3	0.62219 (19)	0.60702 (17)	0.73935 (11)	0.0309 (5)
N4	0.45731 (19)	0.57570 (17)	0.84175 (10)	0.0304 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0286 (4)	0.0340 (4)	0.0311 (4)	0.0010 (3)	0.0052 (3)	0.0062 (3)
Al2	0.0318 (4)	0.0320 (4)	0.0277 (4)	0.0001 (3)	0.0005 (3)	0.0092 (3)
Al3	0.0294 (4)	0.0345 (4)	0.0383 (5)	0.0049 (3)	0.0066 (3)	0.0152 (4)
Al4	0.0282 (4)	0.0324 (4)	0.0294 (4)	0.0031 (3)	0.0115 (3)	0.0097 (3)
C1	0.0304 (14)	0.0297 (14)	0.0336 (14)	0.0013 (11)	0.0043 (11)	0.0076 (11)
C2	0.0317 (14)	0.0350 (15)	0.0283 (13)	0.0027 (11)	0.0027 (11)	0.0043 (11)
C3	0.0312 (14)	0.0307 (14)	0.0299 (13)	−0.0002 (11)	0.0007 (11)	0.0092 (11)
C4	0.0323 (15)	0.0317 (14)	0.0350 (14)	0.0006 (11)	0.0018 (11)	0.0037 (11)
C5	0.0328 (14)	0.0278 (14)	0.0348 (14)	−0.0021 (11)	0.0043 (11)	0.0134 (11)
C6	0.0352 (15)	0.0292 (14)	0.0337 (14)	−0.0047 (11)	0.0010 (11)	0.0095 (11)

C7	0.0297 (14)	0.0437 (16)	0.0316 (14)	−0.0017 (12)	0.0096 (11)	0.0118 (12)
C8	0.0371 (16)	0.0519 (18)	0.0319 (15)	−0.0052 (13)	0.0139 (12)	0.0074 (13)
C9	0.0426 (17)	0.0513 (18)	0.0299 (14)	−0.0241 (14)	0.0084 (12)	0.0070 (13)
C10	0.0356 (16)	0.0568 (19)	0.0301 (14)	−0.0108 (14)	−0.0035 (12)	0.0201 (13)
C11	0.0325 (15)	0.0473 (17)	0.0286 (14)	−0.0034 (12)	−0.0030 (11)	0.0172 (12)
C12	0.0305 (14)	0.0349 (14)	0.0303 (13)	−0.0002 (11)	0.0069 (11)	0.0107 (11)
C13	0.0419 (16)	0.0321 (14)	0.0299 (14)	0.0039 (12)	0.0141 (12)	0.0052 (11)
C14	0.0419 (16)	0.0343 (15)	0.0335 (14)	−0.0037 (12)	0.0118 (12)	0.0111 (12)
C15	0.0372 (15)	0.0304 (14)	0.0283 (13)	−0.0017 (11)	0.0106 (11)	0.0127 (11)
C16	0.0473 (17)	0.0315 (14)	0.0305 (14)	0.0020 (12)	0.0142 (12)	0.0066 (11)
C17	0.0373 (15)	0.0349 (15)	0.0280 (13)	0.0048 (12)	0.0131 (11)	0.0082 (11)
C18	0.0368 (15)	0.0436 (16)	0.0396 (15)	−0.0011 (12)	0.0189 (12)	0.0172 (13)
C19	0.055 (2)	0.050 (2)	0.066 (2)	−0.0124 (16)	0.0168 (17)	0.0138 (17)
C20	0.052 (2)	0.053 (2)	0.0437 (18)	−0.0154 (15)	0.0083 (15)	0.0115 (15)
C21	0.055 (2)	0.069 (2)	0.068 (2)	0.0145 (18)	0.0209 (18)	0.0229 (19)
C22	0.0335 (15)	0.0365 (15)	0.0358 (15)	−0.0101 (12)	0.0004 (11)	0.0003 (12)
C23	0.0302 (15)	0.0399 (16)	0.0534 (18)	0.0088 (12)	0.0123 (13)	0.0120 (14)
C24	0.0381 (16)	0.0514 (18)	0.0321 (15)	−0.0080 (13)	0.0124 (12)	0.0113 (13)
C25	0.0300 (14)	0.0392 (15)	0.0388 (15)	−0.0090 (12)	0.0033 (11)	0.0150 (12)
C26	0.0441 (17)	0.0393 (16)	0.0329 (15)	0.0024 (13)	−0.0039 (12)	0.0048 (12)
C27	0.0341 (15)	0.0330 (15)	0.0434 (16)	0.0041 (12)	−0.0005 (12)	0.0152 (12)
C28	0.0289 (14)	0.0270 (13)	0.0329 (14)	−0.0015 (11)	0.0115 (11)	0.0055 (11)
C29	0.0281 (13)	0.0238 (12)	0.0298 (13)	0.0027 (10)	0.0123 (10)	0.0097 (10)
C30	0.0310 (14)	0.0330 (14)	0.0346 (15)	0.0011 (11)	0.0042 (11)	0.0054 (11)
C31	0.0332 (15)	0.0330 (15)	0.0341 (14)	0.0043 (12)	0.0057 (11)	0.0057 (11)
C32	0.0344 (15)	0.0481 (17)	0.0356 (15)	0.0200 (13)	0.0148 (12)	0.0230 (13)
C33	0.0274 (13)	0.0343 (14)	0.0318 (14)	0.0044 (11)	0.0085 (11)	0.0113 (11)
C34	0.0325 (14)	0.0308 (14)	0.0311 (13)	0.0090 (11)	0.0075 (11)	0.0140 (11)
C35	0.0344 (15)	0.0390 (16)	0.0437 (16)	0.0103 (13)	0.0130 (13)	0.0136 (13)
C36	0.0387 (17)	0.060 (2)	0.0358 (16)	0.0147 (15)	0.0070 (13)	0.0154 (14)
C37	0.0368 (17)	0.0536 (19)	0.0422 (17)	0.0015 (14)	−0.0099 (13)	0.0121 (14)
C38	0.0446 (17)	0.0422 (17)	0.0302 (14)	0.0056 (13)	−0.0025 (12)	0.0056 (12)
C39	0.0327 (14)	0.0322 (14)	0.0320 (14)	0.0009 (11)	0.0056 (11)	0.0079 (11)
C40	0.0420 (16)	0.0312 (14)	0.0348 (15)	0.0011 (12)	−0.0004 (12)	0.0062 (12)
C41	0.0338 (15)	0.0294 (14)	0.0352 (14)	0.0023 (11)	0.0001 (11)	0.0085 (11)
C42	0.0336 (15)	0.0351 (15)	0.0366 (15)	0.0024 (12)	0.0029 (11)	0.0126 (12)
C43	0.0305 (14)	0.0349 (15)	0.0327 (14)	−0.0022 (11)	−0.0046 (11)	0.0046 (11)
C44	0.0346 (15)	0.0358 (15)	0.0301 (14)	−0.0004 (12)	−0.0043 (11)	0.0038 (11)
C45	0.0306 (15)	0.0443 (16)	0.0344 (15)	0.0038 (12)	−0.0084 (11)	0.0119 (12)
C46	0.051 (2)	0.051 (2)	0.0533 (19)	−0.0211 (15)	−0.0185 (15)	0.0215 (16)
C47	0.049 (2)	0.049 (2)	0.068 (2)	0.0183 (16)	−0.0039 (17)	0.0165 (17)
C48	0.0428 (17)	0.0464 (17)	0.0377 (16)	0.0100 (14)	−0.0105 (13)	0.0149 (13)
C49	0.0431 (17)	0.0312 (15)	0.0544 (18)	−0.0028 (13)	0.0220 (14)	0.0158 (13)
C50	0.0492 (18)	0.0377 (16)	0.0298 (14)	0.0044 (13)	0.0183 (12)	0.0054 (12)
C51	0.0267 (14)	0.0404 (16)	0.0383 (15)	0.0041 (12)	0.0041 (11)	0.0070 (12)
C52	0.0330 (16)	0.058 (2)	0.057 (2)	0.0065 (14)	−0.0002 (14)	0.0276 (16)
C53	0.0395 (17)	0.0460 (18)	0.0494 (18)	0.0131 (14)	0.0192 (14)	0.0095 (14)
C54	0.0364 (17)	0.0496 (19)	0.066 (2)	−0.0027 (14)	0.0051 (15)	0.0230 (16)
N1	0.0291 (11)	0.0277 (11)	0.0310 (11)	−0.0016 (9)	0.0054 (9)	0.0053 (9)

N2	0.0317 (12)	0.0261 (11)	0.0325 (12)	0.0028 (9)	0.0060 (9)	0.0091 (9)
N3	0.0308 (12)	0.0300 (12)	0.0337 (12)	0.0018 (9)	0.0089 (9)	0.0080 (9)
N4	0.0312 (12)	0.0334 (12)	0.0300 (11)	0.0042 (9)	0.0085 (9)	0.0118 (9)

Geometric parameters (Å, °)

Al1—C22	1.975 (3)	C25—H25B	0.9600
Al1—C23	1.980 (3)	C25—H25C	0.9600
Al1—C24	1.991 (3)	C26—H26A	0.9600
Al1—N1	2.089 (2)	C26—H26B	0.9600
Al2—C27	1.963 (3)	C26—H26C	0.9600
Al2—C26	1.973 (3)	C27—H27A	0.9600
Al2—C25	1.984 (3)	C27—H27B	0.9600
Al2—N2	2.121 (2)	C27—H27C	0.9600
Al3—C54	1.971 (3)	C28—N4	1.497 (3)
Al3—C53	1.983 (3)	C28—C29	1.530 (3)
Al3—C52	1.991 (3)	C28—H28A	0.9700
Al3—N4	2.095 (2)	C28—H28B	0.9700
Al4—C51	1.970 (3)	C29—N3	1.512 (3)
Al4—C49	1.979 (3)	C29—H29A	0.9700
Al4—C50	1.986 (3)	C29—H29B	0.9700
Al4—N3	2.109 (2)	C30—C31	1.530 (4)
C1—N1	1.504 (3)	C30—N3	1.535 (3)
C1—C2	1.531 (4)	C30—H30A	0.9700
C1—H1A	0.9700	C30—H30B	0.9700
C1—H1B	0.9700	C31—N4	1.497 (3)
C2—N2	1.528 (3)	C31—H31A	0.9700
C2—H2A	0.9700	C31—H31B	0.9700
C2—H2B	0.9700	C32—C33	1.505 (4)
C3—N2	1.509 (3)	C32—N4	1.532 (3)
C3—C4	1.524 (4)	C32—H32A	0.9700
C3—H3A	0.9700	C32—H32B	0.9700
C3—H3B	0.9700	C33—C38	1.393 (4)
C4—N1	1.502 (3)	C33—C34	1.401 (4)
C4—H4A	0.9700	C34—C35	1.389 (4)
C4—H4B	0.9700	C34—H34	0.9300
C5—C6	1.513 (4)	C35—C36	1.367 (4)
C5—N1	1.521 (3)	C35—H35	0.9300
C5—H5A	0.9700	C36—C37	1.391 (4)
C5—H5B	0.9700	C36—H36	0.9300
C6—C7	1.392 (4)	C37—C38	1.395 (4)
C6—C11	1.407 (4)	C37—H37	0.9300
C7—C8	1.382 (4)	C38—H38	0.9300
C7—H7	0.9300	C39—C44	1.404 (4)
C8—C9	1.392 (4)	C39—C40	1.404 (4)
C8—H8	0.9300	C39—N3	1.463 (3)
C9—C10	1.373 (4)	C40—C41	1.335 (4)
C9—H9	0.9300	C40—H40	0.9300
C10—C11	1.389 (4)	C41—C42	1.394 (4)

C10—H10	0.9300	C41—H41	0.9300
C11—H11	0.9300	C42—C43	1.381 (4)
C12—C17	1.384 (3)	C42—C45	1.525 (4)
C12—C13	1.428 (4)	C43—C44	1.383 (4)
C12—N2	1.460 (3)	C43—H43	0.9300
C13—C14	1.340 (4)	C44—H44	0.9300
C13—H13	0.9300	C45—C46	1.531 (4)
C14—C15	1.394 (4)	C45—C47	1.550 (4)
C14—H14	0.9300	C45—C48	1.562 (4)
C15—C16	1.387 (4)	C46—H46A	0.9600
C15—C18	1.530 (3)	C46—H46B	0.9600
C16—C17	1.401 (4)	C46—H46C	0.9600
C16—H16	0.9300	C47—H47A	0.9600
C17—H17	0.9300	C47—H47B	0.9600
C18—C21	1.525 (4)	C47—H47C	0.9600
C18—C20	1.541 (4)	C48—H48A	0.9600
C18—C19	1.546 (4)	C48—H48B	0.9600
C19—H19A	0.9600	C48—H48C	0.9600
C19—H19B	0.9600	C49—H49A	0.9600
C19—H19C	0.9600	C49—H49B	0.9600
C20—H20A	0.9600	C49—H49C	0.9600
C20—H20B	0.9600	C50—H50A	0.9600
C20—H20C	0.9600	C50—H50B	0.9600
C21—H21A	0.9600	C50—H50C	0.9600
C21—H21B	0.9600	C51—H51A	0.9600
C21—H21C	0.9600	C51—H51B	0.9600
C22—H22A	0.9600	C51—H51C	0.9600
C22—H22B	0.9600	C52—H52A	0.9600
C22—H22C	0.9600	C52—H52B	0.9600
C23—H23A	0.9600	C52—H52C	0.9600
C23—H23B	0.9600	C53—H53A	0.9600
C23—H23C	0.9600	C53—H53B	0.9600
C24—H24A	0.9600	C53—H53C	0.9600
C24—H24B	0.9600	C54—H54A	0.9600
C24—H24C	0.9600	C54—H54B	0.9600
C25—H25A	0.9600	C54—H54C	0.9600
C22—Al1—C23	117.28 (13)	N4—C28—C29	115.9 (2)
C22—Al1—C24	111.64 (13)	N4—C28—H28A	108.3
C23—Al1—C24	113.85 (13)	C29—C28—H28A	108.3
C22—Al1—N1	106.49 (11)	N4—C28—H28B	108.3
C23—Al1—N1	102.93 (11)	C29—C28—H28B	108.3
C24—Al1—N1	102.83 (11)	H28A—C28—H28B	107.4
C27—Al2—C26	116.72 (13)	N3—C29—C28	111.82 (19)
C27—Al2—C25	112.84 (13)	N3—C29—H29A	109.3
C26—Al2—C25	115.29 (13)	C28—C29—H29A	109.3
C27—Al2—N2	104.44 (11)	N3—C29—H29B	109.3
C26—Al2—N2	102.78 (11)	C28—C29—H29B	109.3
C25—Al2—N2	102.35 (10)	H29A—C29—H29B	107.9
C54—Al3—C53	116.88 (14)	C31—C30—N3	110.5 (2)

C54—Al3—C52	114.34 (14)	C31—C30—H30A	109.5
C53—Al3—C52	113.25 (14)	N3—C30—H30A	109.5
C54—Al3—N4	102.92 (12)	C31—C30—H30B	109.5
C53—Al3—N4	102.49 (11)	N3—C30—H30B	109.5
C52—Al3—N4	104.70 (11)	H30A—C30—H30B	108.1
C51—Al4—C49	110.99 (13)	N4—C31—C30	114.7 (2)
C51—Al4—C50	115.34 (12)	N4—C31—H31A	108.6
C49—Al4—C50	117.80 (13)	C30—C31—H31A	108.6
C51—Al4—N3	102.76 (10)	N4—C31—H31B	108.6
C49—Al4—N3	104.58 (11)	C30—C31—H31B	108.6
C50—Al4—N3	103.16 (11)	H31A—C31—H31B	107.6
N1—C1—C2	112.2 (2)	C33—C32—N4	119.1 (2)
N1—C1—H1A	109.2	C33—C32—H32A	107.6
C2—C1—H1A	109.2	N4—C32—H32A	107.6
N1—C1—H1B	109.2	C33—C32—H32B	107.6
C2—C1—H1B	109.2	N4—C32—H32B	107.6
H1A—C1—H1B	107.9	H32A—C32—H32B	107.0
N2—C2—C1	110.2 (2)	C38—C33—C34	118.7 (2)
N2—C2—H2A	109.6	C38—C33—C32	121.3 (3)
C1—C2—H2A	109.6	C34—C33—C32	119.8 (2)
N2—C2—H2B	109.6	C35—C34—C33	119.8 (3)
C1—C2—H2B	109.6	C35—C34—H34	120.1
H2A—C2—H2B	108.1	C33—C34—H34	120.1
N2—C3—C4	112.0 (2)	C36—C35—C34	121.2 (3)
N2—C3—H3A	109.2	C36—C35—H35	119.4
C4—C3—H3A	109.2	C34—C35—H35	119.4
N2—C3—H3B	109.2	C35—C36—C37	120.0 (3)
C4—C3—H3B	109.2	C35—C36—H36	120.0
H3A—C3—H3B	107.9	C37—C36—H36	120.0
N1—C4—C3	114.2 (2)	C36—C37—C38	119.4 (3)
N1—C4—H4A	108.7	C36—C37—H37	120.3
C3—C4—H4A	108.7	C38—C37—H37	120.3
N1—C4—H4B	108.7	C33—C38—C37	121.0 (3)
C3—C4—H4B	108.7	C33—C38—H38	119.5
H4A—C4—H4B	107.6	C37—C38—H38	119.5
C6—C5—N1	115.5 (2)	C44—C39—C40	115.4 (2)
C6—C5—H5A	108.4	C44—C39—N3	120.8 (2)
N1—C5—H5A	108.4	C40—C39—N3	123.6 (2)
C6—C5—H5B	108.4	C41—C40—C39	124.6 (3)
N1—C5—H5B	108.4	C41—C40—H40	117.7
H5A—C5—H5B	107.5	C39—C40—H40	117.7
C7—C6—C11	118.4 (3)	C40—C41—C42	120.3 (3)
C7—C6—C5	121.6 (2)	C40—C41—H41	119.9
C11—C6—C5	119.9 (2)	C42—C41—H41	119.9
C8—C7—C6	121.7 (3)	C43—C42—C41	116.8 (2)
C8—C7—H7	119.2	C43—C42—C45	121.7 (2)
C6—C7—H7	119.2	C41—C42—C45	121.5 (2)
C7—C8—C9	118.8 (3)	C42—C43—C44	123.2 (3)
C7—C8—H8	120.6	C42—C43—H43	118.4

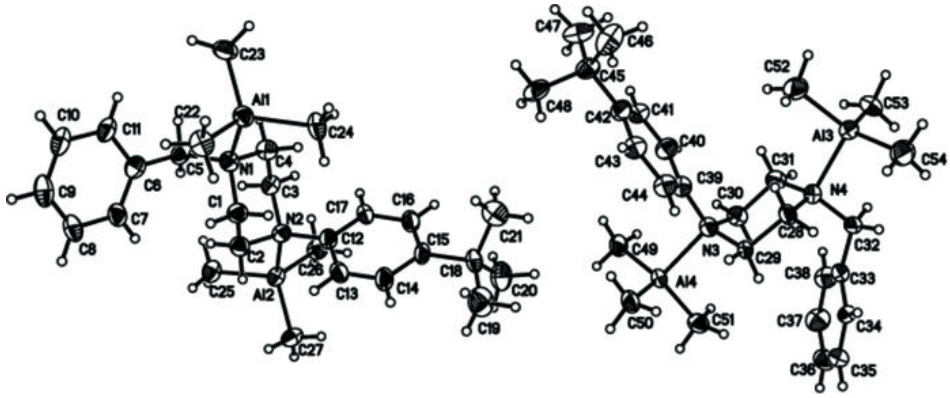
C9—C8—H8	120.6	C44—C43—H43	118.4
C10—C9—C8	120.8 (3)	C43—C44—C39	119.7 (3)
C10—C9—H9	119.6	C43—C44—H44	120.2
C8—C9—H9	119.6	C39—C44—H44	120.2
C9—C10—C11	120.4 (3)	C42—C45—C46	110.3 (2)
C9—C10—H10	119.8	C42—C45—C47	113.0 (2)
C11—C10—H10	119.8	C46—C45—C47	110.2 (2)
C10—C11—C6	119.9 (3)	C42—C45—C48	108.3 (2)
C10—C11—H11	120.0	C46—C45—C48	108.1 (2)
C6—C11—H11	120.0	C47—C45—C48	106.8 (3)
C17—C12—C13	116.6 (2)	C45—C46—H46A	109.5
C17—C12—N2	121.0 (2)	C45—C46—H46B	109.5
C13—C12—N2	122.4 (2)	H46A—C46—H46B	109.5
C14—C13—C12	122.5 (2)	C45—C46—H46C	109.5
C14—C13—H13	118.8	H46A—C46—H46C	109.5
C12—C13—H13	118.8	H46B—C46—H46C	109.5
C13—C14—C15	121.6 (3)	C45—C47—H47A	109.5
C13—C14—H14	119.2	C45—C47—H47B	109.5
C15—C14—H14	119.2	H47A—C47—H47B	109.5
C16—C15—C14	116.9 (2)	C45—C47—H47C	109.5
C16—C15—C18	121.1 (2)	H47A—C47—H47C	109.5
C14—C15—C18	122.1 (2)	H47B—C47—H47C	109.5
C15—C16—C17	122.4 (2)	C45—C48—H48A	109.5
C15—C16—H16	118.8	C45—C48—H48B	109.5
C17—C16—H16	118.8	H48A—C48—H48B	109.5
C12—C17—C16	120.0 (2)	C45—C48—H48C	109.5
C12—C17—H17	120.0	H48A—C48—H48C	109.5
C16—C17—H17	120.0	H48B—C48—H48C	109.5
C21—C18—C15	109.2 (2)	Al4—C49—H49A	109.5
C21—C18—C20	109.3 (3)	Al4—C49—H49B	109.5
C15—C18—C20	108.4 (2)	H49A—C49—H49B	109.5
C21—C18—C19	110.3 (3)	Al4—C49—H49C	109.5
C15—C18—C19	112.6 (2)	H49A—C49—H49C	109.5
C20—C18—C19	107.0 (3)	H49B—C49—H49C	109.5
C18—C19—H19A	109.5	Al4—C50—H50A	109.5
C18—C19—H19B	109.5	Al4—C50—H50B	109.5
H19A—C19—H19B	109.5	H50A—C50—H50B	109.5
C18—C19—H19C	109.5	Al4—C50—H50C	109.5
H19A—C19—H19C	109.5	H50A—C50—H50C	109.5
H19B—C19—H19C	109.5	H50B—C50—H50C	109.5
C18—C20—H20A	109.5	Al4—C51—H51A	109.5
C18—C20—H20B	109.5	Al4—C51—H51B	109.5
H20A—C20—H20B	109.5	H51A—C51—H51B	109.5
C18—C20—H20C	109.5	Al4—C51—H51C	109.5
H20A—C20—H20C	109.5	H51A—C51—H51C	109.5
H20B—C20—H20C	109.5	H51B—C51—H51C	109.5
C18—C21—H21A	109.5	Al3—C52—H52A	109.5
C18—C21—H21B	109.5	Al3—C52—H52B	109.5
H21A—C21—H21B	109.5	H52A—C52—H52B	109.5

C18—C21—H21C	109.5	Al3—C52—H52C	109.5
H21A—C21—H21C	109.5	H52A—C52—H52C	109.5
H21B—C21—H21C	109.5	H52B—C52—H52C	109.5
Al1—C22—H22A	109.5	Al3—C53—H53A	109.5
Al1—C22—H22B	109.5	Al3—C53—H53B	109.5
H22A—C22—H22B	109.5	H53A—C53—H53B	109.5
Al1—C22—H22C	109.5	Al3—C53—H53C	109.5
H22A—C22—H22C	109.5	H53A—C53—H53C	109.5
H22B—C22—H22C	109.5	H53B—C53—H53C	109.5
Al1—C23—H23A	109.5	Al3—C54—H54A	109.5
Al1—C23—H23B	109.5	Al3—C54—H54B	109.5
H23A—C23—H23B	109.5	H54A—C54—H54B	109.5
Al1—C23—H23C	109.5	Al3—C54—H54C	109.5
H23A—C23—H23C	109.5	H54A—C54—H54C	109.5
H23B—C23—H23C	109.5	H54B—C54—H54C	109.5
Al1—C24—H24A	109.5	C4—N1—C1	108.1 (2)
Al1—C24—H24B	109.5	C4—N1—C5	107.71 (19)
H24A—C24—H24B	109.5	C1—N1—C5	112.8 (2)
Al1—C24—H24C	109.5	C4—N1—Al1	106.49 (15)
H24A—C24—H24C	109.5	C1—N1—Al1	106.19 (15)
H24B—C24—H24C	109.5	C5—N1—Al1	115.23 (16)
Al2—C25—H25A	109.5	C12—N2—C3	114.3 (2)
Al2—C25—H25B	109.5	C12—N2—C2	116.1 (2)
H25A—C25—H25B	109.5	C3—N2—C2	104.13 (19)
Al2—C25—H25C	109.5	C12—N2—Al2	107.98 (16)
H25A—C25—H25C	109.5	C3—N2—Al2	108.25 (15)
H25B—C25—H25C	109.5	C2—N2—Al2	105.53 (15)
Al2—C26—H26A	109.5	C39—N3—C29	114.5 (2)
Al2—C26—H26B	109.5	C39—N3—C30	115.1 (2)
H26A—C26—H26B	109.5	C29—N3—C30	104.30 (19)
Al2—C26—H26C	109.5	C39—N3—Al4	107.48 (15)
H26A—C26—H26C	109.5	C29—N3—Al4	108.44 (15)
H26B—C26—H26C	109.5	C30—N3—Al4	106.70 (15)
Al2—C27—H27A	109.5	C28—N4—C31	110.38 (19)
Al2—C27—H27B	109.5	C28—N4—C32	114.7 (2)
H27A—C27—H27B	109.5	C31—N4—C32	113.1 (2)
Al2—C27—H27C	109.5	C28—N4—Al3	106.48 (15)
H27A—C27—H27C	109.5	C31—N4—Al3	106.98 (15)
H27B—C27—H27C	109.5	C32—N4—Al3	104.54 (15)
N1—C1—C2—N2	63.3 (3)	C24—Al1—N1—C4	−48.49 (18)
N2—C3—C4—N1	−57.4 (3)	C22—Al1—N1—C1	−50.98 (18)
N1—C5—C6—C7	−85.1 (3)	C23—Al1—N1—C1	−174.93 (17)
N1—C5—C6—C11	99.2 (3)	C24—Al1—N1—C1	66.53 (18)
C11—C6—C7—C8	−2.5 (4)	C22—Al1—N1—C5	74.66 (19)
C5—C6—C7—C8	−178.2 (2)	C23—Al1—N1—C5	−49.29 (19)
C6—C7—C8—C9	2.3 (4)	C24—Al1—N1—C5	−167.83 (17)
C7—C8—C9—C10	−0.9 (4)	C17—C12—N2—C3	−34.8 (3)
C8—C9—C10—C11	−0.2 (4)	C13—C12—N2—C3	147.0 (2)
C9—C10—C11—C6	0.0 (4)	C17—C12—N2—C2	−156.1 (2)

C7—C6—C11—C10	1.3 (4)	C13—C12—N2—C2	25.7 (3)
C5—C6—C11—C10	177.1 (2)	C17—C12—N2—Al2	85.7 (3)
C17—C12—C13—C14	−0.6 (4)	C13—C12—N2—Al2	−92.5 (3)
N2—C12—C13—C14	177.6 (3)	C4—C3—N2—C12	−67.5 (3)
C12—C13—C14—C15	−0.1 (5)	C4—C3—N2—C2	60.2 (3)
C13—C14—C15—C16	0.7 (4)	C4—C3—N2—Al2	172.11 (17)
C13—C14—C15—C18	−179.9 (3)	C1—C2—N2—C12	63.5 (3)
C14—C15—C16—C17	−0.5 (4)	C1—C2—N2—C3	−63.1 (2)
C18—C15—C16—C17	−179.9 (3)	C1—C2—N2—Al2	−177.02 (17)
C13—C12—C17—C16	0.8 (4)	C27—Al2—N2—C12	54.28 (18)
N2—C12—C17—C16	−177.5 (2)	C26—Al2—N2—C12	−68.03 (18)
C15—C16—C17—C12	−0.2 (4)	C25—Al2—N2—C12	172.10 (17)
C16—C15—C18—C21	59.0 (4)	C27—Al2—N2—C3	178.53 (16)
C14—C15—C18—C21	−120.3 (3)	C26—Al2—N2—C3	56.22 (18)
C16—C15—C18—C20	−60.0 (3)	C25—Al2—N2—C3	−63.65 (18)
C14—C15—C18—C20	120.7 (3)	C27—Al2—N2—C2	−70.47 (17)
C16—C15—C18—C19	−178.1 (3)	C26—Al2—N2—C2	167.22 (16)
C14—C15—C18—C19	2.5 (4)	C25—Al2—N2—C2	47.35 (18)
N4—C28—C29—N3	−54.3 (3)	C44—C39—N3—C29	−38.2 (3)
N3—C30—C31—N4	58.4 (3)	C40—C39—N3—C29	147.3 (3)
N4—C32—C33—C38	89.4 (3)	C44—C39—N3—C30	−159.0 (2)
N4—C32—C33—C34	−96.0 (3)	C40—C39—N3—C30	26.5 (3)
C38—C33—C34—C35	−0.7 (4)	C44—C39—N3—Al4	82.3 (3)
C32—C33—C34—C35	−175.4 (2)	C40—C39—N3—Al4	−92.2 (3)
C33—C34—C35—C36	0.6 (4)	C28—C29—N3—C39	−65.6 (3)
C34—C35—C36—C37	−1.0 (4)	C28—C29—N3—C30	61.0 (3)
C35—C36—C37—C38	1.6 (4)	C28—C29—N3—Al4	174.39 (16)
C34—C33—C38—C37	1.3 (4)	C31—C30—N3—C39	63.1 (3)
C32—C33—C38—C37	175.9 (3)	C31—C30—N3—C29	−63.1 (2)
C36—C37—C38—C33	−1.7 (4)	C31—C30—N3—Al4	−177.73 (17)
C44—C39—C40—C41	−0.9 (4)	C51—Al4—N3—C39	172.68 (17)
N3—C39—C40—C41	173.8 (3)	C49—Al4—N3—C39	56.67 (19)
C39—C40—C41—C42	1.1 (5)	C50—Al4—N3—C39	−67.08 (18)
C40—C41—C42—C43	−1.3 (4)	C51—Al4—N3—C29	−63.09 (18)
C40—C41—C42—C45	179.5 (3)	C49—Al4—N3—C29	−179.10 (17)
C41—C42—C43—C44	1.4 (4)	C50—Al4—N3—C29	57.15 (18)
C45—C42—C43—C44	−179.4 (3)	C51—Al4—N3—C30	48.73 (18)
C42—C43—C44—C39	−1.3 (4)	C49—Al4—N3—C30	−67.27 (18)
C40—C39—C44—C43	0.9 (4)	C50—Al4—N3—C30	168.97 (16)
N3—C39—C44—C43	−174.0 (2)	C29—C28—N4—C31	43.4 (3)
C43—C42—C45—C46	56.6 (4)	C29—C28—N4—C32	−85.8 (3)
C41—C42—C45—C46	−124.3 (3)	C29—C28—N4—Al3	159.12 (17)
C43—C42—C45—C47	−179.6 (3)	C30—C31—N4—C28	−45.6 (3)
C41—C42—C45—C47	−0.5 (4)	C30—C31—N4—C32	84.4 (3)
C43—C42—C45—C48	−61.5 (3)	C30—C31—N4—Al3	−161.01 (18)
C41—C42—C45—C48	117.6 (3)	C33—C32—N4—C28	62.6 (3)
C3—C4—N1—C1	50.7 (3)	C33—C32—N4—C31	−65.1 (3)
C3—C4—N1—C5	−71.4 (3)	C33—C32—N4—Al3	178.8 (2)
C3—C4—N1—Al1	164.42 (18)	C54—Al3—N4—C28	64.43 (18)

C2—C1—N1—C4	−53.5 (3)	C53—Al3—N4—C28	−173.84 (17)
C2—C1—N1—C5	65.4 (3)	C52—Al3—N4—C28	−55.40 (19)
C2—C1—N1—Al1	−167.47 (17)	C54—Al3—N4—C31	−177.54 (18)
C6—C5—N1—C4	176.5 (2)	C53—Al3—N4—C31	−55.81 (18)
C6—C5—N1—C1	57.4 (3)	C52—Al3—N4—C31	62.63 (19)
C6—C5—N1—Al1	−64.8 (3)	C54—Al3—N4—C32	−57.3 (2)
C22—Al1—N1—C4	−166.00 (17)	C53—Al3—N4—C32	64.4 (2)
C23—Al1—N1—C4	70.06 (18)	C52—Al3—N4—C32	−177.15 (19)

Fig. 1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C36
C35

Fig. 2