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Tris[3,6-di-*tert*-butyl-1-(isoquinolin-1-yl)naphthalen-2-olato-κ^2N,O]-aluminium(III) toluene sesquisolvate

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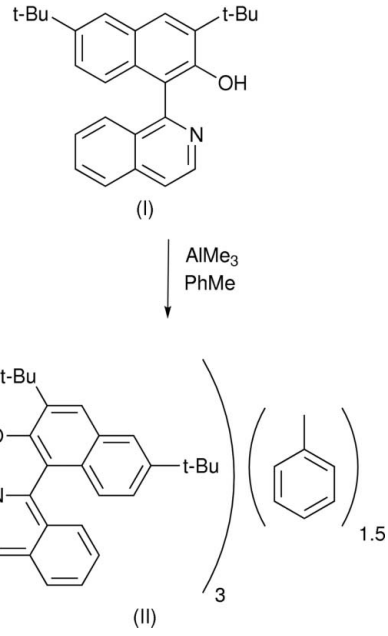
The central Al^{III} atom of the title compound, $[Al(C_{27}H_{28}NO)_3]\cdot 1.5C_7H_8$, has octahedral geometry in which the three N atoms are arranged in a meridional fashion. One of the toluene solvent molecules is located on a general position, while the second is disordered around a centre of inversion. The ligand molecule has axial chirality, and two of the three ligands in the complex exhibit the same stereochemistry. The three independent chelate rings exhibit significantly different bite angles at the metal atom, with one [83.72 (8)°] notably smaller than the other two [87.22 (8) and 87.13 (8)°]. Calculation of the solid angle covered by the ligands at the metal atom reveals that coverage is greatest for the ligand group with the shortest Al—O bond distance.

Comment

The formation of polyesters continues to be a focus of research as a means of producing bioresourced and biodegradable polymers that can replace polyolefins in many applications. One particularly attractive route is the synthesis of such polyesters by the ring-opening polymerization of lactones catalysed by metal complexes, and in particular the polymerization of lactide. Polylactide can exist as a number of stereoisomers (Amgoune *et al.*, 2007; Dechy-Cabaret *et al.*, 2004; Stanford & Dove, 2010; Thomas, 2010). Complexes of aluminium bearing a variety of chiral chelating ligands have been investigated as catalysts of choice over several years (Spassky *et al.*, 1996; Ovitt & Coates, 1999, 2002; Zhong *et al.*, 2003; Du *et al.*, 2009). Whereas many of these complexes show good activity in lactide polymerization, there is no clear correlation between ligand chirality and the ability of the resulting complexes to control stereoselectivity in the resulting polylactide, and new ligand types continue to be explored.

We have recently reported the synthesis and structural characterization of 3,6-di-*tert*-butyl-1-(isoquinolin-1-yl)-2-naphthol (*L*H), (I), which reacts with bis(silyl)amide complexes of magnesium, calcium and zinc to give complexes containing the ligand as *N*,*O*-chelates (Howard *et al.*, 2009). We report here the reaction of (I) with trimethylaluminium. Although the molar ratio was adjusted to result in a mixed-ligand complex L_2AlMe, in all cases complete substitution of all three methyl ligands was observed, and [AlL_3] was the only isolable product. In reactions with ε-caprolactone or *rac*-lactide in tetrahydrofuran at 323 K, this complex produced only traces of polymers. Recrystallization from toluene afforded the title compound, (II), as yellow blocks which were suitable for X-ray crystallography.



Compound (II) (Fig. 1) crystallizes as the toluene sesquisolvate in the space group $P\overline{1}$ with no symmetry relationship between the three ligand groups on the Al^{III} centre. Two of the three ligands show the same stereochemistry and the third the opposite, so the complex is a 1:1 mixture of the *R*,*R*,*S* and *S*,*S*,*R* isomers. The arrangement of the three ligands results in meridional coordination geometry for both the N and the O atoms. A search of the Cambridge Structural Database (CSD, Version 5.33; Allen, 2002) shows that three structures have previously been reported containing pyridinyl–phenolate chelates on Al^{III} [CSD refcodes ACEJOH and ACEJUN (Liu *et al.*, 2000), and HALXEY (Steinhauser *et al.*, 2004)]. ACEJOH and ACEJUN feature two *N*,*O*-chelating ligands, while HALXEY contains two bis(phenolate)pyridinyl groups. In these structures, the N—Al—O angles fall in the range 86.63 (8)–89.89 (9)°. In (II), the two ligands with the same sense of chirality have angles which fall within this range, while the N1—Al1—O1 angle is significantly smaller. This may reflect the steric demand of accommodating three *N*,*O*-chelating ligands around the Al^{III} atom, with the requirements of three separate ligands at the metal centre forcing one ligand to adopt a sub-optimal bite angle.

Examination of the geometric parameters of the metal coordination sphere (Table 1) shows that the three ligands have statistically different bond lengths to the metal. The

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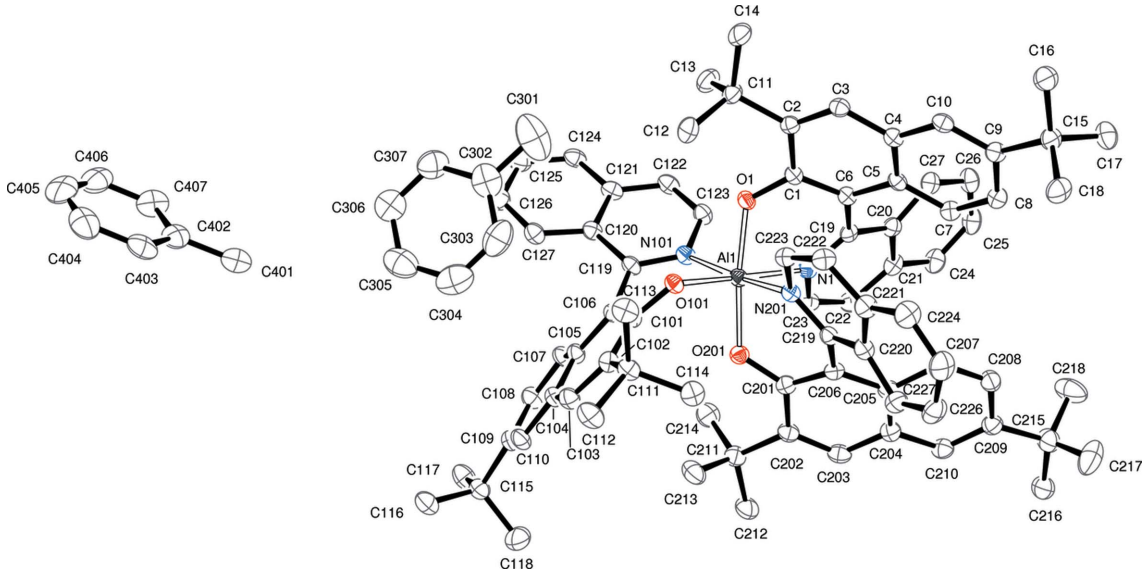

Figure 1
The structure of (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. For the disordered toluene molecule (C401–C407), only one disorder component is shown.

previously reported structures have Al—N bond lengths in the range 2.088 (2)–2.197 (4) Å and Al—O bond lengths in the range 1.741 (2)–1.8823 (17) Å; the values observed for (II) fall within these ranges. Using the *Solid-G* program (Guzei & Wendt, 2006), it is possible to calculate solid-angle and equivalent cone-angle data for the three ligands around the metal atom (Table 2). The largest cone angle is found for the N101/O101 ligand, which features the shortest Al—O vector and longest Al—N distance. This can be rationalized as the presence of the O atom close to the metal atom requiring that the *tert*-butyl group also be closer, increasing the steric crowding caused by the N101/O101 ligand compared with the other two ligand groups. The coordination of the N101-pyridine ring to the Al atom is distinct from the other two ligand groups; the six-membered ring is bent significantly relative to the Al—N bond. The angle subtended by Al1—N101···C121 (C121 is the 4-position relative to the N atom) is 156.71 (11)°, compared with 176.10 (11) and 175.71 (11)° for the other two pyridine rings. A search of the CSD shows that the range previously reported for this angle is 147.5–179.8° for the 304 structures containing a pyridine-ligated Al^{III} atom. There are a total of 528 distinct angles reported, of which only 31 are smaller than that seen in (II). This again seems most likely to be due to the steric constraints of packing three bulky ligands around the Al centre.

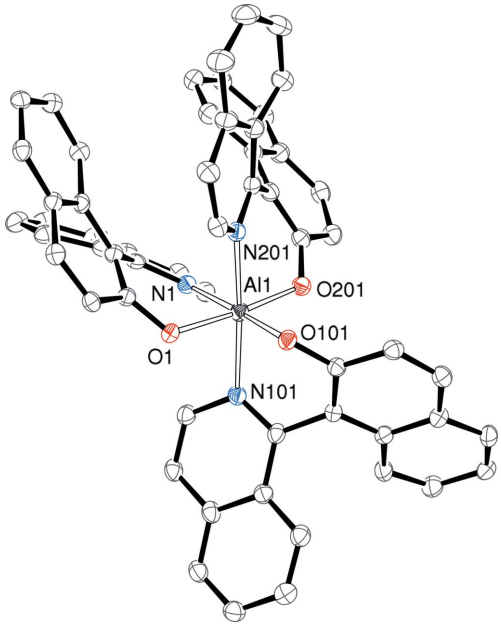

Figure 2
A view of the metal coordination geometry in (II). Displacement ellipsoids are drawn at the 50% probability level. H atoms, toluene solvent molecules and *tert*-butyl groups have been omitted for clarity.

Overall, compound (II) is very crowded, and we suspect that this high degree of steric hindrance prevents the association of a cyclic ester monomer and the initiation of the subsequent ring-opening step.

Experimental

A solution of 3,6-di-*tert*-butyl-1-(isoquinolin-1-yl)naphthalen-2-ol (0.15 g, 0.40 mmol) in toluene (20 ml) was added to a solution of 2.0 *M* $AlMe_3$ in toluene (0.1 ml, 0.2 mmol). The mixture was stirred for 4 h. Removal of the volatiles gave a yellow solid. Extraction with toluene (5 ml), concentration to 3 ml and cooling to 278 K yielded small yellow crystals of (II) (0.18 mmol, 0.22 g, 90%). Analysis calculated for $C_{81}H_{84}AlN_3O_3$: C 80.56, H 7.01, N 3.48%; found: C 80.67, H 7.08, N 3.33%. ^{1}H NMR (300 MHz, 300 K, C_6D_6): δ 8.18 (*s*, 3H, aromatic CH), 7.98 (*d*, 3H, ^3J = 6.0 Hz, 3H, aromatic CH), 7.93 (*d*, 3H, ^3J = 1.9 Hz, aromatic CH), 7.62 (*d*, 3H, ^3J = 8.4 Hz, aromatic CH), 7.30–7.09 (*m*, 9H, aromatic CH), 7.04 (*d*, 3H, ^3J = 6.0 Hz, aromatic CH), 6.91 (*d*, 3H, ^3J = 9.0 Hz, aromatic CH), 6.7 (*m*, 3H, aromatic CH), 1.94 (*s*, 27H, CMe_3), 1.42 (*s*, 27H, CMe_3); ^{13}C NMR (75 MHz, 300 K, C_6D_6): δ 162.3–114.8 (57 C, C_{arom}), 36.5, 34.4 (CMe_3), 31.1, 30.4 (CMe_3).

Table 1
Selected geometric parameters (Å, °).

Al1—N1	2.077 (2)	Al1—O1	1.8485 (17)
Al1—N101	2.110 (2)	Al1—O101	1.8338 (18)
Al1—N201	2.035 (2)	Al1—O201	1.8573 (17)
N1—Al1—O1	83.72 (8)	N201—Al1—O201	87.13 (8)
N101—Al1—O101	87.22 (8)		

Table 2
Metal ligand coverage.

Values calculated using *Solid-G* (Guzei & Wendt, 2006).

Ligand	Solid angle (steradians)	Equivalent cone angle (°)
N1—O1	4.77	152.0
N101—O101	4.93	155.1
N201—O201	4.79	152.6

Crystal data

$[Al(C_{27}H_{28}NO)_3]\cdot 1.5C_7H_8$
M_r = 1312.70
Triclinic, $P\overline{1}$
a = 13.0728 (2) Å
b = 15.9452 (3) Å
c = 19.4565 (4) Å
α = 75.217 (1)°
β = 75.262 (1)°
γ = 74.200 (1)°
V = 3697.98 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 120 K
0.10 × 0.08 × 0.04 mm

Data collection

Bruker–Nonius APEXII CCD area-detector diffractometer on κ-goniostat
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.850, T_{max} = 0.997
70540 measured reflections
16846 independent reflections
11372 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.155
S = 1.05
16846 reflections
915 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

All C-bound H atoms were refined using a riding model, with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH groups or 1.5U_{eq}(C) for methyl groups. The two toluene solvent molecules were constrained such that the aromatic rings were regular hexagons in which the C···C bond length was 1.39 Å.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *WinGX* (Farrugia, 1999) and *publCIF* (Westrip, 2010).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GZ3214). Services for accessing these data are described at the back of the journal.

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supplementary materials

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Crystal data

$[Al(C_{27}H_{28}NO)_3]\cdot 1.5C_7H_8$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 13.0728$ (2) Å
$b = 15.9452$ (3) Å
$c = 19.4565$ (4) Å
$\alpha = 75.217$ (1)°
$\beta = 75.262$ (1)°
$\gamma = 74.200$ (1)°
$V = 3697.98$ (12) Å^3
$Z = 2$
$F(000) = 1406$
$D_x = 1.179$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 60331 reflections
$\theta = 2.9$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 120$ K
Block, yellow
0.10 × 0.08 × 0.04 mm

Data collection

Bruker Nonius APEXII CCD area-detector diffractometer on κ-goniostat
Radiation source: Bruker Nonius FR591 rotating anode
10cm confocal mirrors monochromator
Detector resolution: 8.25 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.850$, $T_{max} = 0.997$
70540 measured reflections
16846 independent reflections
11372 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -16\rightarrow16$
$k = -20\rightarrow20$
$l = -25\rightarrow25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.155$
$S = 1.05$
16846 reflections
915 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
$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 5.7694P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.79485 (6)	0.07498 (5)	0.21542 (4)	0.01929 (16)	
N1	0.81350 (15)	−0.05136 (13)	0.19670 (11)	0.0207 (4)	
O1	0.92325 (12)	0.07448 (11)	0.14798 (9)	0.0208 (4)	
C1	1.01245 (18)	0.01249 (16)	0.15404 (13)	0.0192 (5)	
C2	1.11511 (18)	0.03910 (16)	0.13199 (13)	0.0194 (5)	
C3	1.20268 (19)	−0.01984 (16)	0.15560 (13)	0.0209 (5)	
H3	1.2707	−0.0033	0.1418	0.025*	
C4	1.19593 (18)	−0.10524 (16)	0.20013 (13)	0.0205 (5)	
C5	1.09940 (18)	−0.13577 (16)	0.21254 (13)	0.0199 (5)	
C6	1.00881 (18)	−0.07736 (16)	0.18268 (13)	0.0191 (5)	
C7	1.09617 (19)	−0.21937 (16)	0.25994 (13)	0.0211 (5)	
H7	1.0324	−0.2418	0.2703	0.025*	
C8	1.18206 (19)	−0.26857 (17)	0.29106 (14)	0.0233 (5)	
H8	1.1758	−0.3237	0.3232	0.028*	
C9	1.28040 (19)	−0.23986 (17)	0.27690 (13)	0.0215 (5)	
C10	1.28441 (19)	−0.15867 (16)	0.23168 (13)	0.0215 (5)	
H10	1.3491	−0.1376	0.2212	0.026*	
C11	1.1228 (2)	0.13147 (17)	0.08573 (14)	0.0245 (5)	
C12	1.0645 (2)	0.20481 (18)	0.12922 (16)	0.0334 (6)	
H12A	0.9872	0.2043	0.1444	0.050*	
H12B	1.0732	0.2628	0.0989	0.050*	
H12C	1.0959	0.1942	0.1722	0.050*	
C13	1.0733 (2)	0.14716 (19)	0.01887 (15)	0.0333 (6)	
H13A	1.1106	0.1001	−0.0086	0.050*	
H13B	1.0817	0.2050	−0.0118	0.050*	
H13C	0.9961	0.1464	0.0343	0.050*	
C14	1.2414 (2)	0.1394 (2)	0.05839 (18)	0.0384 (7)	
H14A	1.2733	0.1365	0.0996	0.058*	
H14B	1.2444	0.1962	0.0244	0.058*	
H14C	1.2821	0.0904	0.0337	0.058*	
C15	1.3740 (2)	−0.29659 (17)	0.31433 (14)	0.0249 (5)	
C16	1.4797 (2)	−0.2645 (2)	0.28092 (16)	0.0325 (6)	
H16A	1.5378	−0.3036	0.3050	0.049*	
H16B	1.4696	−0.2035	0.2873	0.049*	
H16C	1.4993	−0.2658	0.2291	0.049*	
C17	1.3947 (2)	−0.39425 (18)	0.30809 (17)	0.0333 (6)	
H17A	1.4564	−0.4293	0.3304	0.050*	

H17B	1.4110	−0.3981	0.2568	0.050*
H17C	1.3300	−0.4177	0.3330	0.050*
C18	1.3420 (2)	−0.2897 (2)	0.39478 (15)	0.0320 (6)
H18A	1.2745	−0.3099	0.4169	0.048*
H18B	1.3315	−0.2277	0.3987	0.048*
H18C	1.3998	−0.3270	0.4200	0.048*
C19	0.91083 (18)	−0.10708 (16)	0.18354 (13)	0.0191 (5)
C20	0.91842 (19)	−0.19168 (16)	0.16552 (13)	0.0216 (5)
C21	0.8218 (2)	−0.21953 (17)	0.17246 (14)	0.0240 (5)
C22	0.7216 (2)	−0.15938 (18)	0.18843 (14)	0.0265 (6)
H22	0.6552	−0.1762	0.1936	0.032*
C23	0.72148 (19)	−0.07725 (17)	0.19630 (13)	0.0235 (5)
H23	0.6541	−0.0353	0.2018	0.028*
C24	0.8274 (2)	−0.30369 (18)	0.15812 (16)	0.0312 (6)
H24	0.7627	−0.3238	0.1653	0.037*
C25	0.9251 (2)	−0.35588 (18)	0.13415 (16)	0.0313 (6)
H25	0.9284	−0.4127	0.1255	0.038*
C26	1.0211 (2)	−0.32579 (18)	0.12214 (15)	0.0296 (6)
H26	1.0886	−0.3613	0.1034	0.036*
C27	1.0181 (2)	−0.24578 (17)	0.13731 (14)	0.0239 (5)
H27	1.0836	−0.2263	0.1288	0.029*
N101	0.72309 (16)	0.13318 (14)	0.12381 (11)	0.0214 (4)
O101	0.77769 (12)	0.18817 (11)	0.22871 (9)	0.0206 (4)
C101	0.67893 (18)	0.24122 (16)	0.23548 (13)	0.0196 (5)
C102	0.63538 (19)	0.28567 (16)	0.29604 (13)	0.0220 (5)
C103	0.5306 (2)	0.33407 (17)	0.30276 (14)	0.0248 (5)
H103	0.5027	0.3658	0.3412	0.030*
C104	0.46135 (19)	0.33949 (16)	0.25545 (14)	0.0233 (5)
C105	0.50497 (19)	0.29927 (16)	0.19428 (13)	0.0217 (5)
C106	0.61676 (19)	0.25441 (16)	0.18303 (13)	0.0206 (5)
C107	0.4311 (2)	0.30089 (17)	0.15120 (14)	0.0263 (6)
H107	0.4571	0.2745	0.1096	0.032*
C108	0.3232 (2)	0.33963 (18)	0.16842 (15)	0.0277 (6)
H108	0.2766	0.3391	0.1383	0.033*
C109	0.2784 (2)	0.38022 (17)	0.22903 (14)	0.0256 (6)
C110	0.3497 (2)	0.37995 (17)	0.27075 (14)	0.0259 (6)
H110	0.3227	0.4081	0.3113	0.031*
C111	0.7017 (2)	0.27560 (17)	0.35351 (14)	0.0243 (5)
C112	0.6438 (2)	0.33767 (19)	0.40696 (15)	0.0326 (6)
H11A	0.6297	0.3993	0.3802	0.049*
H11B	0.6898	0.3315	0.4414	0.049*
H11C	0.5749	0.3219	0.4334	0.049*
C113	0.8134 (2)	0.29730 (19)	0.31891 (15)	0.0297 (6)
H11D	0.8532	0.2580	0.2849	0.045*
H11E	0.8543	0.2885	0.3569	0.045*
H11F	0.8039	0.3593	0.2928	0.045*
C114	0.7137 (2)	0.17949 (18)	0.39829 (15)	0.0293 (6)
H11G	0.6416	0.1670	0.4197	0.044*
H11H	0.7525	0.1729	0.4370	0.044*

H11I	0.7545	0.1376	0.3666	0.044*
C115	0.1562 (2)	0.41759 (18)	0.25217 (15)	0.0289 (6)
C116	0.1348 (2)	0.50850 (19)	0.27167 (16)	0.0347 (7)
H11J	0.1681	0.5026	0.3130	0.052*
H11K	0.0565	0.5318	0.2846	0.052*
H11L	0.1663	0.5495	0.2300	0.052*
C117	0.0946 (2)	0.4268 (2)	0.19240 (17)	0.0374 (7)
H11M	0.1246	0.4654	0.1482	0.056*
H11N	0.0177	0.4530	0.2083	0.056*
H11O	0.1021	0.3680	0.1824	0.056*
C118	0.1121 (2)	0.3517 (2)	0.31856 (18)	0.0463 (8)
H11P	0.1251	0.2936	0.3057	0.069*
H11Q	0.0340	0.3739	0.3343	0.069*
H11R	0.1491	0.3456	0.3581	0.069*
C119	0.66822 (18)	0.21822 (16)	0.11672 (13)	0.0211 (5)
C120	0.66441 (19)	0.27431 (17)	0.04623 (13)	0.0220 (5)
C121	0.70587 (19)	0.23521 (17)	−0.01592 (14)	0.0241 (5)
C122	0.75517 (19)	0.14361 (17)	−0.00517 (14)	0.0246 (5)
H122	0.7808	0.1144	−0.0452	0.030*
C123	0.76568 (19)	0.09768 (17)	0.06243 (14)	0.0236 (5)
H123	0.8047	0.0375	0.0678	0.028*
C124	0.69999 (19)	0.28941 (18)	−0.08573 (14)	0.0263 (6)
H124	0.7232	0.2631	−0.1273	0.032*
C125	0.6611 (2)	0.37942 (19)	−0.09331 (15)	0.0292 (6)
H125	0.6578	0.4153	−0.1402	0.035*
C126	0.6257 (2)	0.41927 (18)	−0.03197 (15)	0.0293 (6)
H126	0.6017	0.4821	−0.0381	0.035*
C127	0.6257 (2)	0.36827 (17)	0.03626 (14)	0.0256 (5)
H127	0.5997	0.3957	0.0772	0.031*
N201	0.87696 (15)	0.02216 (13)	0.29806 (11)	0.0197 (4)
O201	0.66937 (12)	0.06040 (11)	0.28366 (9)	0.0211 (4)
C201	0.65997 (19)	−0.01451 (16)	0.33083 (13)	0.0212 (5)
C202	0.55507 (19)	−0.03863 (17)	0.35514 (14)	0.0242 (5)
C203	0.5533 (2)	−0.12470 (18)	0.38974 (14)	0.0259 (6)
H203	0.4852	−0.1409	0.4070	0.031*
C204	0.6492 (2)	−0.19119 (17)	0.40101 (14)	0.0248 (5)
C205	0.74845 (19)	−0.16462 (17)	0.38483 (13)	0.0228 (5)
C206	0.74977 (19)	−0.07238 (16)	0.35701 (13)	0.0214 (5)
C207	0.8439 (2)	−0.23242 (17)	0.39125 (14)	0.0255 (6)
H207	0.9122	−0.2165	0.3796	0.031*
C208	0.8395 (2)	−0.31968 (17)	0.41372 (14)	0.0266 (6)
H208	0.9051	−0.3634	0.4164	0.032*
C209	0.7397 (2)	−0.34748 (17)	0.43326 (14)	0.0260 (6)
C210	0.6469 (2)	−0.28247 (17)	0.42666 (14)	0.0260 (6)
H210	0.5790	−0.2992	0.4397	0.031*
C211	0.45107 (19)	0.03134 (18)	0.34228 (15)	0.0276 (6)
C212	0.3490 (2)	−0.00548 (19)	0.37958 (17)	0.0353 (7)
H21A	0.3481	−0.0259	0.4317	0.053*
H21B	0.3496	−0.0555	0.3587	0.053*

H21C	0.2842	0.0414	0.3721	0.053*
C213	0.4435 (2)	0.11224 (19)	0.37420 (17)	0.0353 (7)
H21D	0.4419	0.0933	0.4264	0.053*
H21E	0.3772	0.1568	0.3659	0.053*
H21F	0.5068	0.1381	0.3506	0.053*
C214	0.4480 (2)	0.0616 (2)	0.26081 (16)	0.0346 (7)
H21G	0.3802	0.1052	0.2545	0.052*
H21H	0.4523	0.0101	0.2407	0.052*
H21I	0.5097	0.0889	0.2355	0.052*
C215	0.7421 (2)	−0.44679 (19)	0.45816 (17)	0.0342 (7)
C216	0.6292 (2)	−0.46525 (19)	0.48021 (17)	0.0371 (7)
H21J	0.5874	−0.4354	0.5202	0.056*
H21K	0.6345	−0.5295	0.4960	0.056*
H21L	0.5928	−0.4428	0.4388	0.056*
C217	0.7983 (3)	−0.4841 (2)	0.5235 (2)	0.0549 (10)
H21M	0.7567	−0.4545	0.5637	0.082*
H21N	0.8718	−0.4733	0.5099	0.082*
H21O	0.8021	−0.5482	0.5387	0.082*
C218	0.8066 (3)	−0.4944 (2)	0.3963 (2)	0.0572 (11)
H21P	0.8117	−0.5586	0.4128	0.086*
H21Q	0.8796	−0.4826	0.3815	0.086*
H21R	0.7698	−0.4726	0.3551	0.086*
C219	0.84518 (18)	−0.03871 (16)	0.35493 (13)	0.0200 (5)
C220	0.90097 (19)	−0.06855 (17)	0.41487 (14)	0.0238 (5)
C221	1.0023 (2)	−0.04704 (17)	0.40523 (14)	0.0255 (5)
C222	1.0337 (2)	0.01675 (17)	0.34309 (14)	0.0251 (5)
H222	1.1005	0.0340	0.3353	0.030*
C223	0.96720 (19)	0.05262 (17)	0.29521 (14)	0.0219 (5)
H223	0.9834	0.1013	0.2577	0.026*
C224	1.0654 (2)	−0.08487 (19)	0.45984 (16)	0.0331 (6)
H224	1.1360	−0.0745	0.4521	0.040*
C225	1.0249 (2)	−0.1359 (2)	0.52305 (16)	0.0358 (7)
H225	1.0682	−0.1624	0.5588	0.043*
C226	0.9194 (2)	−0.14977 (19)	0.53581 (15)	0.0330 (6)
H226	0.8901	−0.1823	0.5814	0.040*
C227	0.8586 (2)	−0.11699 (17)	0.48338 (14)	0.0265 (6)
H227	0.7873	−0.1267	0.4928	0.032*
C301	0.9026 (4)	0.4213 (3)	0.0501 (3)	0.0852 (15)
H30A	0.8855	0.3663	0.0474	0.128*
H30B	0.9487	0.4082	0.0859	0.128*
H30C	0.9409	0.4471	0.0025	0.128*
C302	0.80085 (15)	0.48543 (14)	0.07232 (12)	0.0497 (9)
C303	0.7367 (2)	0.46572 (13)	0.14065 (11)	0.0562 (10)
H303	0.7594	0.4122	0.1734	0.067*
C304	0.63942 (19)	0.52424 (17)	0.16104 (10)	0.0629 (11)
H304	0.5956	0.5108	0.2077	0.075*
C305	0.60623 (15)	0.60248 (15)	0.11309 (13)	0.0566 (10)
H305	0.5397	0.6425	0.1270	0.068*
C306	0.67035 (18)	0.62220 (12)	0.04476 (12)	0.0510 (9)

H306	0.6477	0.6757	0.0120	0.061*	
C307	0.76766 (16)	0.56367 (15)	0.02438 (9)	0.0480 (8)	
H307	0.8115	0.5771	−0.0223	0.058*	
C401	0.4916 (8)	0.8509 (8)	0.0559 (6)	0.045 (2)	0.50
H40A	0.5536	0.8234	0.0799	0.068*	0.50
H40B	0.4948	0.8185	0.0187	0.068*	0.50
H40C	0.4240	0.8490	0.0919	0.068*	0.50
C402	0.4953 (4)	0.9453 (3)	0.0215 (3)	0.0356 (14)	0.50
C403	0.5125 (4)	0.9987 (4)	0.0619 (2)	0.038 (2)	0.50
H403	0.5198	0.9754	0.1109	0.046*	0.50
C404	0.5189 (4)	1.0863 (4)	0.0306 (4)	0.0517 (19)	0.50
H404	0.5306	1.1229	0.0583	0.062*	0.50
C405	0.5081 (4)	1.1205 (3)	−0.0411 (4)	0.063 (4)	0.50
H405	0.5125	1.1803	−0.0624	0.075*	0.50
C406	0.4910 (4)	1.0670 (5)	−0.0815 (2)	0.053 (2)	0.50
H406	0.4836	1.0903	−0.1305	0.064*	0.50
C407	0.4845 (4)	0.9794 (5)	−0.0502 (3)	0.041 (2)	0.50
H407	0.4728	0.9428	−0.0778	0.049*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0171 (3)	0.0206 (4)	0.0199 (4)	−0.0027 (3)	−0.0043 (3)	−0.0046 (3)
N1	0.0188 (10)	0.0231 (11)	0.0195 (11)	−0.0034 (8)	−0.0049 (8)	−0.0034 (9)
O1	0.0188 (8)	0.0202 (9)	0.0212 (9)	−0.0001 (6)	−0.0040 (7)	−0.0046 (7)
C1	0.0191 (11)	0.0211 (12)	0.0178 (12)	−0.0017 (9)	−0.0056 (9)	−0.0056 (10)
C2	0.0216 (12)	0.0205 (12)	0.0174 (12)	−0.0052 (9)	−0.0024 (9)	−0.0070 (10)
C3	0.0184 (11)	0.0231 (13)	0.0228 (13)	−0.0067 (9)	−0.0029 (9)	−0.0065 (10)
C4	0.0192 (11)	0.0226 (13)	0.0204 (13)	−0.0031 (9)	−0.0045 (9)	−0.0065 (10)
C5	0.0198 (11)	0.0208 (12)	0.0195 (12)	−0.0015 (9)	−0.0028 (9)	−0.0090 (10)
C6	0.0187 (11)	0.0212 (12)	0.0188 (12)	−0.0034 (9)	−0.0053 (9)	−0.0058 (10)
C7	0.0209 (12)	0.0231 (13)	0.0217 (13)	−0.0070 (9)	−0.0051 (9)	−0.0056 (10)
C8	0.0256 (13)	0.0222 (13)	0.0224 (13)	−0.0057 (10)	−0.0059 (10)	−0.0035 (10)
C9	0.0198 (12)	0.0266 (13)	0.0187 (12)	−0.0037 (10)	−0.0070 (9)	−0.0042 (10)
C10	0.0170 (11)	0.0258 (13)	0.0231 (13)	−0.0046 (9)	−0.0033 (9)	−0.0082 (11)
C11	0.0232 (12)	0.0224 (13)	0.0268 (14)	−0.0080 (10)	−0.0050 (10)	0.0002 (11)
C12	0.0382 (16)	0.0221 (14)	0.0385 (17)	−0.0088 (11)	−0.0068 (13)	−0.0023 (12)
C13	0.0366 (15)	0.0323 (16)	0.0275 (15)	−0.0098 (12)	−0.0078 (12)	0.0040 (12)
C14	0.0271 (14)	0.0313 (16)	0.0480 (19)	−0.0107 (12)	−0.0031 (13)	0.0079 (14)
C15	0.0229 (12)	0.0271 (14)	0.0249 (14)	−0.0049 (10)	−0.0084 (10)	−0.0024 (11)
C16	0.0247 (13)	0.0373 (16)	0.0327 (16)	−0.0052 (11)	−0.0099 (11)	0.0004 (13)
C17	0.0294 (14)	0.0295 (15)	0.0410 (17)	−0.0008 (11)	−0.0142 (12)	−0.0060 (13)
C18	0.0341 (15)	0.0376 (16)	0.0248 (14)	−0.0090 (12)	−0.0121 (11)	0.0002 (12)
C19	0.0212 (12)	0.0216 (12)	0.0147 (12)	−0.0044 (9)	−0.0071 (9)	−0.0008 (10)
C20	0.0251 (12)	0.0227 (13)	0.0173 (12)	−0.0052 (10)	−0.0065 (10)	−0.0028 (10)
C21	0.0286 (13)	0.0238 (13)	0.0228 (13)	−0.0095 (10)	−0.0098 (10)	−0.0017 (11)
C22	0.0229 (13)	0.0311 (15)	0.0289 (14)	−0.0109 (10)	−0.0054 (10)	−0.0064 (12)
C23	0.0185 (12)	0.0308 (14)	0.0223 (13)	−0.0057 (10)	−0.0052 (10)	−0.0059 (11)
C24	0.0338 (15)	0.0272 (15)	0.0369 (16)	−0.0113 (11)	−0.0130 (12)	−0.0031 (12)

C25	0.0436 (16)	0.0189 (13)	0.0387 (17)	−0.0074 (11)	−0.0184 (13)	−0.0076 (12)
C26	0.0334 (14)	0.0255 (14)	0.0318 (15)	−0.0014 (11)	−0.0136 (12)	−0.0077 (12)
C27	0.0261 (13)	0.0238 (13)	0.0239 (14)	−0.0051 (10)	−0.0099 (10)	−0.0038 (11)
N101	0.0205 (10)	0.0249 (11)	0.0193 (11)	−0.0023 (8)	−0.0055 (8)	−0.0067 (9)
O101	0.0180 (8)	0.0221 (9)	0.0214 (9)	−0.0013 (6)	−0.0053 (7)	−0.0059 (7)
C101	0.0207 (12)	0.0181 (12)	0.0195 (12)	−0.0038 (9)	−0.0031 (9)	−0.0041 (10)
C102	0.0242 (12)	0.0217 (13)	0.0215 (13)	−0.0050 (10)	−0.0071 (10)	−0.0044 (10)
C103	0.0277 (13)	0.0260 (14)	0.0218 (13)	−0.0035 (10)	−0.0054 (10)	−0.0087 (11)
C104	0.0210 (12)	0.0220 (13)	0.0250 (14)	−0.0013 (10)	−0.0044 (10)	−0.0051 (11)
C105	0.0230 (12)	0.0209 (13)	0.0204 (13)	−0.0009 (9)	−0.0063 (10)	−0.0050 (10)
C106	0.0211 (12)	0.0193 (12)	0.0196 (12)	−0.0012 (9)	−0.0030 (9)	−0.0052 (10)
C107	0.0258 (13)	0.0300 (14)	0.0226 (14)	0.0001 (10)	−0.0053 (10)	−0.0103 (11)
C108	0.0236 (13)	0.0315 (15)	0.0283 (14)	−0.0015 (10)	−0.0095 (11)	−0.0074 (12)
C109	0.0223 (12)	0.0219 (13)	0.0275 (14)	0.0013 (10)	−0.0046 (10)	−0.0031 (11)
C110	0.0268 (13)	0.0252 (14)	0.0244 (14)	0.0012 (10)	−0.0040 (10)	−0.0111 (11)
C111	0.0240 (12)	0.0291 (14)	0.0227 (13)	−0.0039 (10)	−0.0064 (10)	−0.0105 (11)
C112	0.0361 (15)	0.0382 (16)	0.0285 (15)	−0.0023 (12)	−0.0093 (12)	−0.0186 (13)
C113	0.0276 (14)	0.0369 (16)	0.0302 (15)	−0.0088 (11)	−0.0097 (11)	−0.0110 (12)
C114	0.0321 (14)	0.0317 (15)	0.0267 (15)	−0.0054 (11)	−0.0107 (11)	−0.0072 (12)
C115	0.0231 (13)	0.0295 (15)	0.0310 (15)	−0.0018 (10)	−0.0038 (11)	−0.0066 (12)
C116	0.0283 (14)	0.0363 (16)	0.0366 (17)	0.0015 (12)	−0.0057 (12)	−0.0122 (13)
C117	0.0258 (14)	0.0400 (17)	0.0471 (19)	0.0027 (12)	−0.0124 (13)	−0.0157 (14)
C118	0.0327 (16)	0.0441 (19)	0.049 (2)	−0.0078 (13)	−0.0006 (14)	0.0052 (16)
C119	0.0173 (11)	0.0240 (13)	0.0228 (13)	−0.0008 (9)	−0.0059 (9)	−0.0082 (10)
C120	0.0188 (12)	0.0261 (13)	0.0211 (13)	−0.0025 (10)	−0.0061 (9)	−0.0054 (10)
C121	0.0204 (12)	0.0313 (14)	0.0223 (13)	−0.0041 (10)	−0.0045 (10)	−0.0097 (11)
C122	0.0231 (12)	0.0313 (14)	0.0219 (13)	−0.0023 (10)	−0.0056 (10)	−0.0126 (11)
C123	0.0242 (12)	0.0233 (13)	0.0234 (13)	−0.0005 (10)	−0.0067 (10)	−0.0081 (11)
C124	0.0217 (12)	0.0361 (15)	0.0202 (13)	−0.0027 (11)	−0.0040 (10)	−0.0082 (11)
C125	0.0241 (13)	0.0349 (15)	0.0236 (14)	−0.0037 (11)	−0.0047 (10)	−0.0004 (12)
C126	0.0291 (14)	0.0271 (14)	0.0296 (15)	−0.0025 (11)	−0.0077 (11)	−0.0042 (12)
C127	0.0252 (13)	0.0274 (14)	0.0248 (14)	−0.0014 (10)	−0.0072 (10)	−0.0088 (11)
N201	0.0180 (10)	0.0214 (11)	0.0195 (11)	−0.0029 (8)	−0.0034 (8)	−0.0055 (9)
O201	0.0186 (8)	0.0229 (9)	0.0212 (9)	−0.0039 (7)	−0.0042 (7)	−0.0035 (7)
C201	0.0234 (12)	0.0226 (13)	0.0195 (13)	−0.0067 (10)	−0.0038 (10)	−0.0062 (10)
C202	0.0193 (12)	0.0287 (14)	0.0255 (14)	−0.0057 (10)	−0.0042 (10)	−0.0068 (11)
C203	0.0212 (12)	0.0335 (15)	0.0260 (14)	−0.0101 (10)	−0.0011 (10)	−0.0105 (12)
C204	0.0258 (13)	0.0254 (14)	0.0242 (14)	−0.0063 (10)	−0.0048 (10)	−0.0059 (11)
C205	0.0233 (12)	0.0276 (14)	0.0181 (13)	−0.0059 (10)	−0.0038 (10)	−0.0057 (10)
C206	0.0201 (12)	0.0247 (13)	0.0189 (13)	−0.0064 (10)	−0.0022 (9)	−0.0038 (10)
C207	0.0226 (12)	0.0288 (14)	0.0256 (14)	−0.0072 (10)	−0.0038 (10)	−0.0054 (11)
C208	0.0267 (13)	0.0249 (14)	0.0269 (14)	−0.0026 (10)	−0.0056 (11)	−0.0059 (11)
C209	0.0295 (13)	0.0247 (14)	0.0239 (14)	−0.0077 (10)	−0.0022 (10)	−0.0062 (11)
C210	0.0257 (13)	0.0269 (14)	0.0280 (14)	−0.0112 (10)	−0.0018 (10)	−0.0075 (11)
C211	0.0182 (12)	0.0295 (14)	0.0340 (15)	−0.0054 (10)	−0.0050 (10)	−0.0046 (12)
C212	0.0222 (13)	0.0344 (16)	0.0462 (18)	−0.0056 (11)	−0.0012 (12)	−0.0088 (14)
C213	0.0241 (14)	0.0324 (16)	0.0488 (19)	−0.0038 (11)	−0.0020 (12)	−0.0148 (14)
C214	0.0239 (13)	0.0395 (17)	0.0396 (17)	−0.0036 (12)	−0.0117 (12)	−0.0050 (13)
C215	0.0328 (15)	0.0263 (15)	0.0431 (18)	−0.0081 (11)	−0.0029 (13)	−0.0091 (13)

C216	0.0378 (16)	0.0250 (15)	0.0455 (18)	−0.0098 (12)	0.0018 (13)	−0.0087 (13)
C217	0.059 (2)	0.0387 (19)	0.066 (2)	−0.0211 (16)	−0.0258 (18)	0.0149 (17)
C218	0.051 (2)	0.0401 (19)	0.079 (3)	−0.0191 (16)	0.0224 (18)	−0.0340 (19)
C219	0.0198 (11)	0.0203 (12)	0.0193 (12)	−0.0012 (9)	−0.0040 (9)	−0.0064 (10)
C220	0.0235 (12)	0.0235 (13)	0.0242 (14)	−0.0020 (10)	−0.0059 (10)	−0.0069 (11)
C221	0.0265 (13)	0.0290 (14)	0.0232 (13)	−0.0051 (10)	−0.0096 (10)	−0.0055 (11)
C222	0.0231 (12)	0.0313 (14)	0.0235 (14)	−0.0088 (10)	−0.0058 (10)	−0.0060 (11)
C223	0.0221 (12)	0.0234 (13)	0.0215 (13)	−0.0071 (10)	−0.0025 (10)	−0.0062 (10)
C224	0.0305 (14)	0.0392 (17)	0.0331 (16)	−0.0084 (12)	−0.0143 (12)	−0.0047 (13)
C225	0.0381 (16)	0.0393 (17)	0.0313 (16)	−0.0040 (13)	−0.0191 (13)	−0.0018 (13)
C226	0.0450 (17)	0.0325 (16)	0.0210 (14)	−0.0100 (12)	−0.0086 (12)	−0.0009 (12)
C227	0.0287 (13)	0.0270 (14)	0.0234 (14)	−0.0076 (11)	−0.0042 (10)	−0.0039 (11)
C301	0.089 (3)	0.076 (3)	0.098 (4)	0.015 (2)	−0.043 (3)	−0.043 (3)
C302	0.056 (2)	0.052 (2)	0.052 (2)	−0.0086 (16)	−0.0236 (17)	−0.0192 (18)
C303	0.078 (3)	0.048 (2)	0.052 (2)	−0.0260 (19)	−0.029 (2)	0.0012 (18)
C304	0.065 (3)	0.075 (3)	0.054 (2)	−0.033 (2)	−0.0050 (19)	−0.012 (2)
C305	0.0426 (19)	0.068 (3)	0.068 (3)	−0.0147 (17)	−0.0050 (18)	−0.031 (2)
C306	0.053 (2)	0.055 (2)	0.051 (2)	−0.0148 (17)	−0.0163 (17)	−0.0106 (18)
C307	0.052 (2)	0.059 (2)	0.0331 (18)	−0.0140 (17)	−0.0123 (15)	−0.0035 (16)
C401	0.038 (5)	0.052 (6)	0.041 (4)	−0.008 (3)	0.001 (3)	−0.014 (5)
C402	0.021 (3)	0.044 (4)	0.041 (4)	−0.006 (3)	−0.008 (2)	−0.006 (3)
C403	0.017 (4)	0.052 (6)	0.043 (5)	0.002 (3)	−0.009 (3)	−0.013 (4)
C404	0.026 (3)	0.050 (4)	0.086 (6)	−0.009 (3)	−0.010 (3)	−0.026 (4)
C405	0.019 (4)	0.057 (9)	0.096 (10)	−0.015 (4)	−0.002 (4)	0.010 (6)
C406	0.027 (3)	0.059 (5)	0.059 (5)	−0.009 (3)	−0.006 (3)	0.011 (4)
C407	0.034 (5)	0.059 (6)	0.036 (4)	−0.013 (4)	−0.015 (4)	−0.007 (4)

Geometric parameters (Å, º)

Al1—N1	2.077 (2)	C118—H11P	0.9800
Al1—N101	2.110 (2)	C118—H11Q	0.9800
Al1—N201	2.035 (2)	C118—H11R	0.9800
Al1—O1	1.8485 (17)	C119—C120	1.438 (3)
Al1—O101	1.8338 (18)	C120—C121	1.419 (3)
Al1—O201	1.8573 (17)	C120—C127	1.424 (4)
N1—C19	1.345 (3)	C121—C122	1.412 (4)
N1—C23	1.376 (3)	C121—C124	1.420 (4)
O1—C1	1.317 (3)	C122—C123	1.353 (4)
C1—C6	1.408 (3)	C122—H122	0.9500
C1—C2	1.445 (3)	C123—H123	0.9500
C2—C3	1.366 (3)	C124—C125	1.369 (4)
C2—C11	1.532 (3)	C124—H124	0.9500
C3—C4	1.427 (3)	C125—C126	1.410 (4)
C3—H3	0.9500	C125—H125	0.9500
C4—C10	1.414 (3)	C126—C127	1.368 (4)
C4—C5	1.417 (3)	C126—H126	0.9500
C5—C7	1.419 (3)	C127—H127	0.9500
C5—C6	1.442 (3)	N201—C219	1.333 (3)
C6—C19	1.477 (3)	N201—C223	1.377 (3)
C7—C8	1.366 (3)	O201—C201	1.322 (3)

C7—H7	0.9500	C201—C206	1.401 (3)
C8—C9	1.419 (3)	C201—C202	1.455 (3)
C8—H8	0.9500	C202—C203	1.369 (4)
C9—C10	1.373 (3)	C202—C211	1.536 (3)
C9—C15	1.536 (3)	C203—C204	1.429 (4)
C10—H10	0.9500	C203—H203	0.9500
C11—C13	1.532 (4)	C204—C205	1.409 (3)
C11—C14	1.535 (3)	C204—C210	1.419 (4)
C11—C12	1.535 (4)	C205—C207	1.421 (3)
C12—H12A	0.9800	C205—C206	1.435 (3)
C12—H12B	0.9800	C206—C219	1.474 (3)
C12—H12C	0.9800	C207—C208	1.361 (4)
C13—H13A	0.9800	C207—H207	0.9500
C13—H13B	0.9800	C208—C209	1.421 (4)
C13—H13C	0.9800	C208—H208	0.9500
C14—H14A	0.9800	C209—C210	1.375 (4)
C14—H14B	0.9800	C209—C215	1.527 (4)
C14—H14C	0.9800	C210—H210	0.9500
C15—C16	1.534 (4)	C211—C213	1.539 (4)
C15—C17	1.537 (4)	C211—C212	1.539 (3)
C15—C18	1.539 (4)	C211—C214	1.542 (4)
C16—H16A	0.9800	C212—H21A	0.9800
C16—H16B	0.9800	C212—H21B	0.9800
C16—H16C	0.9800	C212—H21C	0.9800
C17—H17A	0.9800	C213—H21D	0.9800
C17—H17B	0.9800	C213—H21E	0.9800
C17—H17C	0.9800	C213—H21F	0.9800
C18—H18A	0.9800	C214—H21G	0.9800
C18—H18B	0.9800	C214—H21H	0.9800
C18—H18C	0.9800	C214—H21I	0.9800
C19—C20	1.450 (3)	C215—C216	1.515 (4)
C20—C21	1.414 (3)	C215—C218	1.528 (4)
C20—C27	1.418 (3)	C215—C217	1.537 (4)
C21—C22	1.412 (4)	C216—H21J	0.9800
C21—C24	1.418 (4)	C216—H21K	0.9800
C22—C23	1.356 (4)	C216—H21L	0.9800
C22—H22	0.9500	C217—H21M	0.9800
C23—H23	0.9500	C217—H21N	0.9800
C24—C25	1.362 (4)	C217—H21O	0.9800
C24—H24	0.9500	C218—H21P	0.9800
C25—C26	1.409 (4)	C218—H21Q	0.9800
C25—H25	0.9500	C218—H21R	0.9800
C26—C27	1.369 (4)	C219—C220	1.442 (3)
C26—H26	0.9500	C220—C221	1.413 (3)
C27—H27	0.9500	C220—C227	1.419 (4)
N101—C119	1.341 (3)	C221—C222	1.418 (4)
N101—C123	1.375 (3)	C221—C224	1.421 (4)
O101—C101	1.332 (3)	C222—C223	1.349 (3)
C101—C106	1.402 (3)	C222—H222	0.9500

C101—C102	1.442 (3)	C223—H223	0.9500
C102—C103	1.369 (3)	C224—C225	1.359 (4)
C102—C111	1.534 (3)	C224—H224	0.9500
C103—C104	1.420 (3)	C225—C226	1.407 (4)
C103—H103	0.9500	C225—H225	0.9500
C104—C105	1.413 (3)	C226—C227	1.364 (4)
C104—C110	1.414 (3)	C226—H226	0.9500
C105—C107	1.423 (3)	C227—H227	0.9500
C105—C106	1.429 (3)	C301—C302	1.481 (4)
C106—C119	1.475 (3)	C301—H30A	0.9800
C107—C108	1.369 (3)	C301—H30B	0.9800
C107—H107	0.9500	C301—H30C	0.9800
C108—C109	1.409 (4)	C302—C303	1.3900
C108—H108	0.9500	C302—C307	1.3900
C109—C110	1.382 (4)	C303—C304	1.3900
C109—C115	1.537 (3)	C303—H303	0.9500
C110—H110	0.9500	C304—C305	1.3900
C111—C112	1.533 (4)	C304—H304	0.9500
C111—C113	1.537 (3)	C305—C306	1.3900
C111—C114	1.546 (4)	C305—H305	0.9500
C112—H11A	0.9800	C306—C307	1.3900
C112—H11B	0.9800	C306—H306	0.9500
C112—H11C	0.9800	C307—H307	0.9500
C113—H11D	0.9800	C401—C402	1.491 (12)
C113—H11E	0.9800	C401—H40A	0.9800
C113—H11F	0.9800	C401—H40B	0.9800
C114—H11G	0.9800	C401—H40C	0.9800
C114—H11H	0.9800	C402—C403	1.3900
C114—H11I	0.9800	C402—C407	1.3900
C115—C116	1.526 (4)	C403—C404	1.3900
C115—C117	1.531 (4)	C403—H403	0.9500
C115—C118	1.537 (4)	C404—C405	1.3900
C116—H11J	0.9800	C404—H404	0.9500
C116—H11K	0.9800	C405—C406	1.3900
C116—H11L	0.9800	C405—H405	0.9500
C117—H11M	0.9800	C406—C407	1.3900
C117—H11N	0.9800	C406—H406	0.9500
C117—H11O	0.9800	C407—H407	0.9500

O101—Al1—O1	95.49 (8)	H11J—C116—H11L	109.5
O101—Al1—O201	91.48 (8)	H11K—C116—H11L	109.5
O1—Al1—O201	172.89 (9)	C115—C117—H11M	109.5
O101—Al1—N201	91.57 (8)	C115—C117—H11N	109.5
O1—Al1—N201	91.24 (8)	H11M—C117—H11N	109.5
O101—Al1—N1	178.01 (9)	C115—C117—H11O	109.5
N1—Al1—O1	83.72 (8)	H11M—C117—H11O	109.5
O201—Al1—N1	89.37 (8)	H11N—C117—H11O	109.5
N201—Al1—N1	90.27 (8)	C115—C118—H11P	109.5
N101—Al1—O101	87.22 (8)	C115—C118—H11Q	109.5

N201—Al1—O201	87.13 (8)	H11P—C118—H11Q	109.5
O1—Al1—N101	83.70 (8)	C115—C118—H11R	109.5
O201—Al1—N101	98.09 (8)	H11P—C118—H11R	109.5
N201—Al1—N101	174.66 (9)	H11Q—C118—H11R	109.5
N1—Al1—N101	90.88 (8)	N101—C119—C120	120.9 (2)
C19—N1—C23	119.4 (2)	N101—C119—C106	118.4 (2)
C19—N1—Al1	122.90 (16)	C120—C119—C106	120.6 (2)
C23—N1—Al1	117.66 (16)	C121—C120—C127	118.7 (2)
C1—O1—Al1	123.63 (15)	C121—C120—C119	118.8 (2)
O1—C1—C6	121.4 (2)	C127—C120—C119	122.4 (2)
O1—C1—C2	118.3 (2)	C122—C121—C120	117.7 (2)
C6—C1—C2	120.3 (2)	C122—C121—C124	122.9 (2)
C3—C2—C1	117.6 (2)	C120—C121—C124	119.4 (2)
C3—C2—C11	122.1 (2)	C123—C122—C121	119.6 (2)
C1—C2—C11	120.3 (2)	C123—C122—H122	120.2
C2—C3—C4	122.6 (2)	C121—C122—H122	120.2
C2—C3—H3	118.7	C122—C123—N101	123.8 (2)
C4—C3—H3	118.7	C122—C123—H123	118.1
C10—C4—C5	120.4 (2)	N101—C123—H123	118.1
C10—C4—C3	120.4 (2)	C125—C124—C121	120.3 (2)
C5—C4—C3	119.3 (2)	C125—C124—H124	119.9
C4—C5—C7	116.4 (2)	C121—C124—H124	119.9
C4—C5—C6	118.7 (2)	C124—C125—C126	120.5 (2)
C7—C5—C6	124.6 (2)	C124—C125—H125	119.8
C1—C6—C5	118.5 (2)	C126—C125—H125	119.8
C1—C6—C19	118.7 (2)	C127—C126—C125	120.6 (3)
C5—C6—C19	122.7 (2)	C127—C126—H126	119.7
C8—C7—C5	121.9 (2)	C125—C126—H126	119.7
C8—C7—H7	119.0	C126—C127—C120	120.4 (2)
C5—C7—H7	119.0	C126—C127—H127	119.8
C7—C8—C9	122.0 (2)	C120—C127—H127	119.8
C7—C8—H8	119.0	C219—N201—C223	119.4 (2)
C9—C8—H8	119.0	C219—N201—Al1	122.53 (16)
C10—C9—C8	116.7 (2)	C223—N201—Al1	118.06 (16)
C10—C9—C15	123.0 (2)	C201—O201—Al1	123.51 (15)
C8—C9—C15	120.1 (2)	O201—C201—C206	121.3 (2)
C9—C10—C4	122.5 (2)	O201—C201—C202	119.7 (2)
C9—C10—H10	118.7	C206—C201—C202	119.1 (2)
C4—C10—H10	118.7	C203—C202—C201	117.6 (2)
C13—C11—C2	109.7 (2)	C203—C202—C211	122.1 (2)
C13—C11—C14	107.2 (2)	C201—C202—C211	120.2 (2)
C2—C11—C14	111.1 (2)	C202—C203—C204	123.0 (2)
C13—C11—C12	109.8 (2)	C202—C203—H203	118.5
C2—C11—C12	111.4 (2)	C204—C203—H203	118.5
C14—C11—C12	107.6 (2)	C205—C204—C210	119.8 (2)
C11—C12—H12A	109.5	C205—C204—C203	118.5 (2)
C11—C12—H12B	109.5	C210—C204—C203	121.8 (2)
H12A—C12—H12B	109.5	C204—C205—C207	117.6 (2)
C11—C12—H12C	109.5	C204—C205—C206	119.0 (2)

H12A—C12—H12C	109.5	C207—C205—C206	123.2 (2)
H12B—C12—H12C	109.5	C201—C206—C205	119.4 (2)
C11—C13—H13A	109.5	C201—C206—C219	120.1 (2)
C11—C13—H13B	109.5	C205—C206—C219	120.5 (2)
H13A—C13—H13B	109.5	C208—C207—C205	121.2 (2)
C11—C13—H13C	109.5	C208—C207—H207	119.4
H13A—C13—H13C	109.5	C205—C207—H207	119.4
H13B—C13—H13C	109.5	C207—C208—C209	122.0 (2)
C11—C14—H14A	109.5	C207—C208—H208	119.0
C11—C14—H14B	109.5	C209—C208—H208	119.0
H14A—C14—H14B	109.5	C210—C209—C208	117.2 (2)
C11—C14—H14C	109.5	C210—C209—C215	124.2 (2)
H14A—C14—H14C	109.5	C208—C209—C215	118.6 (2)
H14B—C14—H14C	109.5	C209—C210—C204	122.1 (2)
C16—C15—C9	112.0 (2)	C209—C210—H210	118.9
C16—C15—C17	108.2 (2)	C204—C210—H210	118.9
C9—C15—C17	110.3 (2)	C202—C211—C213	109.7 (2)
C16—C15—C18	108.5 (2)	C202—C211—C212	111.5 (2)
C9—C15—C18	108.2 (2)	C213—C211—C212	107.5 (2)
C17—C15—C18	109.6 (2)	C202—C211—C214	111.5 (2)
C15—C16—H16A	109.5	C213—C211—C214	109.6 (2)
C15—C16—H16B	109.5	C212—C211—C214	106.9 (2)
H16A—C16—H16B	109.5	C211—C212—H21A	109.5
C15—C16—H16C	109.5	C211—C212—H21B	109.5
H16A—C16—H16C	109.5	H21A—C212—H21B	109.5
H16B—C16—H16C	109.5	C211—C212—H21C	109.5
C15—C17—H17A	109.5	H21A—C212—H21C	109.5
C15—C17—H17B	109.5	H21B—C212—H21C	109.5
H17A—C17—H17B	109.5	C211—C213—H21D	109.5
C15—C17—H17C	109.5	C211—C213—H21E	109.5
H17A—C17—H17C	109.5	H21D—C213—H21E	109.5
H17B—C17—H17C	109.5	C211—C213—H21F	109.5
C15—C18—H18A	109.5	H21D—C213—H21F	109.5
C15—C18—H18B	109.5	H21E—C213—H21F	109.5
H18A—C18—H18B	109.5	C211—C214—H21G	109.5
C15—C18—H18C	109.5	C211—C214—H21H	109.5
H18A—C18—H18C	109.5	H21G—C214—H21H	109.5
H18B—C18—H18C	109.5	C211—C214—H21I	109.5
N1—C19—C20	119.9 (2)	H21G—C214—H21I	109.5
N1—C19—C6	118.6 (2)	H21H—C214—H21I	109.5
C20—C19—C6	121.4 (2)	C216—C215—C209	112.2 (2)
C21—C20—C27	118.1 (2)	C216—C215—C218	108.9 (3)
C21—C20—C19	118.8 (2)	C209—C215—C218	109.1 (2)
C27—C20—C19	123.0 (2)	C216—C215—C217	108.5 (3)
C22—C21—C20	118.5 (2)	C209—C215—C217	109.2 (2)
C22—C21—C24	121.6 (2)	C218—C215—C217	109.0 (3)
C20—C21—C24	119.8 (2)	C215—C216—H21J	109.5
C23—C22—C21	119.0 (2)	C215—C216—H21K	109.5
C23—C22—H22	120.5	H21J—C216—H21K	109.5

C21—C22—H22	120.5	C215—C216—H21L	109.5
C22—C23—N1	123.7 (2)	H21J—C216—H21L	109.5
C22—C23—H23	118.2	H21K—C216—H21L	109.5
N1—C23—H23	118.2	C215—C217—H21M	109.5
C25—C24—C21	120.4 (2)	C215—C217—H21N	109.5
C25—C24—H24	119.8	H21M—C217—H21N	109.5
C21—C24—H24	119.8	C215—C217—H21O	109.5
C24—C25—C26	120.1 (3)	H21M—C217—H21O	109.5
C24—C25—H25	119.9	H21N—C217—H21O	109.5
C26—C25—H25	119.9	C215—C218—H21P	109.5
C27—C26—C25	120.6 (3)	C215—C218—H21Q	109.5
C27—C26—H26	119.7	H21P—C218—H21Q	109.5
C25—C26—H26	119.7	C215—C218—H21R	109.5
C26—C27—C20	120.8 (2)	H21P—C218—H21R	109.5
C26—C27—H27	119.6	H21Q—C218—H21R	109.5
C20—C27—H27	119.6	N201—C219—C220	120.3 (2)
C119—N101—C123	118.5 (2)	N201—C219—C206	119.2 (2)
C119—N101—Al1	118.71 (16)	C220—C219—C206	120.5 (2)
C123—N101—Al1	118.25 (16)	C221—C220—C227	118.3 (2)
C101—O101—Al1	119.10 (15)	C221—C220—C219	118.2 (2)
O101—C101—C106	119.7 (2)	C227—C220—C219	123.4 (2)
O101—C101—C102	120.7 (2)	C220—C221—C222	118.1 (2)
C106—C101—C102	119.5 (2)	C220—C221—C224	119.4 (2)
C103—C102—C101	117.9 (2)	C222—C221—C224	122.4 (2)
C103—C102—C111	120.6 (2)	C223—C222—C221	118.9 (2)
C101—C102—C111	121.4 (2)	C223—C222—H222	120.5
C102—C103—C104	123.6 (2)	C221—C222—H222	120.5
C102—C103—H103	118.2	C222—C223—N201	123.3 (2)
C104—C103—H103	118.2	C222—C223—H223	118.4
C105—C104—C110	120.2 (2)	N201—C223—H223	118.4
C105—C104—C103	118.6 (2)	C225—C224—C221	120.2 (3)
C110—C104—C103	121.1 (2)	C225—C224—H224	119.9
C104—C105—C107	116.7 (2)	C221—C224—H224	119.9
C104—C105—C106	118.5 (2)	C224—C225—C226	120.4 (3)
C107—C105—C106	124.6 (2)	C224—C225—H225	119.8
C101—C106—C105	121.0 (2)	C226—C225—H225	119.8
C101—C106—C119	118.5 (2)	C227—C226—C225	120.7 (3)
C105—C106—C119	120.4 (2)	C227—C226—H226	119.7
C108—C107—C105	121.4 (2)	C225—C226—H226	119.7
C108—C107—H107	119.3	C226—C227—C220	120.5 (2)
C105—C107—H107	119.3	C226—C227—H227	119.8
C107—C108—C109	122.7 (2)	C220—C227—H227	119.8
C107—C108—H108	118.6	C302—C301—H30A	109.5
C109—C108—H108	118.6	C302—C301—H30B	109.5
C110—C109—C108	116.4 (2)	H30A—C301—H30B	109.5
C110—C109—C115	120.4 (2)	C302—C301—H30C	109.5
C108—C109—C115	123.1 (2)	H30A—C301—H30C	109.5
C109—C110—C104	122.6 (2)	H30B—C301—H30C	109.5
C109—C110—H110	118.7	C303—C302—C307	120.0

C104—C110—H110	118.7	C303—C302—C301	119.6 (3)
C112—C111—C102	111.7 (2)	C307—C302—C301	120.3 (3)
C112—C111—C113	107.3 (2)	C304—C303—C302	120.0
C102—C111—C113	111.6 (2)	C304—C303—H303	120.0
C112—C111—C114	106.8 (2)	C302—C303—H303	120.0
C102—C111—C114	108.5 (2)	C303—C304—C305	120.0
C113—C111—C114	110.8 (2)	C303—C304—H304	120.0
C111—C112—H11A	109.5	C305—C304—H304	120.0
C111—C112—H11B	109.5	C306—C305—C304	120.0
H11A—C112—H11B	109.5	C306—C305—H305	120.0
C111—C112—H11C	109.5	C304—C305—H305	120.0
H11A—C112—H11C	109.5	C307—C306—C305	120.0
H11B—C112—H11C	109.5	C307—C306—H306	120.0
C111—C113—H11D	109.5	C305—C306—H306	120.0
C111—C113—H11E	109.5	C306—C307—C302	120.0
H11D—C113—H11E	109.5	C306—C307—H307	120.0
C111—C113—H11F	109.5	C302—C307—H307	120.0
H11D—C113—H11F	109.5	C403—C402—C407	120.0
H11E—C113—H11F	109.5	C403—C402—C401	118.8 (6)
C111—C114—H11G	109.5	C407—C402—C401	121.2 (6)
C111—C114—H11H	109.5	C404—C403—C402	120.0
H11G—C114—H11H	109.5	C404—C403—H403	120.0
C111—C114—H11I	109.5	C402—C403—H403	120.0
H11G—C114—H11I	109.5	C403—C404—C405	120.0
H11H—C114—H11I	109.5	C403—C404—H404	120.0
C116—C115—C117	108.5 (2)	C405—C404—H404	120.0
C116—C115—C118	109.7 (2)	C406—C405—C404	120.0
C117—C115—C118	107.8 (2)	C406—C405—H405	120.0
C116—C115—C109	111.0 (2)	C404—C405—H405	120.0
C117—C115—C109	111.8 (2)	C405—C406—C407	120.0
C118—C115—C109	107.8 (2)	C405—C406—H406	120.0
C115—C116—H11J	109.5	C407—C406—H406	120.0
C115—C116—H11K	109.5	C406—C407—C402	120.0
H11J—C116—H11K	109.5	C406—C407—H407	120.0
C115—C116—H11L	109.5	C402—C407—H407	120.0

O1—Al1—N1—C19	35.64 (19)	C108—C109—C115—C116	−135.8 (3)
O201—Al1—N1—C19	−142.71 (19)	C110—C109—C115—C117	169.9 (2)
N201—Al1—N1—C19	−55.58 (19)	C108—C109—C115—C117	−14.4 (4)
N101—Al1—N1—C19	119.20 (19)	C110—C109—C115—C118	−71.7 (3)
O1—Al1—N1—C23	−142.82 (18)	C108—C109—C115—C118	103.9 (3)
O201—Al1—N1—C23	38.83 (18)	C123—N101—C119—C120	−7.1 (3)
N201—Al1—N1—C23	125.96 (18)	Al1—N101—C119—C120	148.66 (18)
N101—Al1—N1—C23	−59.25 (18)	C123—N101—C119—C106	176.2 (2)
O101—Al1—O1—C1	126.65 (18)	Al1—N101—C119—C106	−28.0 (3)
N201—Al1—O1—C1	34.96 (19)	C101—C106—C119—N101	49.2 (3)
N1—Al1—O1—C1	−55.18 (19)	C105—C106—C119—N101	−128.7 (2)
N101—Al1—O1—C1	−146.76 (19)	C101—C106—C119—C120	−127.5 (2)
Al1—O1—C1—C6	37.3 (3)	C105—C106—C119—C120	54.6 (3)

Al1—O1—C1—C2	−141.33 (18)	N101—C119—C120—C121	9.3 (3)
O1—C1—C2—C3	163.1 (2)	C106—C119—C120—C121	−174.2 (2)
C6—C1—C2—C3	−15.5 (3)	N101—C119—C120—C127	−167.4 (2)
O1—C1—C2—C11	−15.1 (3)	C106—C119—C120—C127	9.2 (4)
C6—C1—C2—C11	166.3 (2)	C127—C120—C121—C122	172.8 (2)
C1—C2—C3—C4	0.3 (4)	C119—C120—C121—C122	−4.0 (3)
C11—C2—C3—C4	178.5 (2)	C127—C120—C121—C124	−4.9 (3)
C2—C3—C4—C10	−170.9 (2)	C119—C120—C121—C124	178.3 (2)
C2—C3—C4—C5	8.9 (4)	C120—C121—C122—C123	−3.0 (4)
C10—C4—C5—C7	2.6 (3)	C124—C121—C122—C123	174.6 (2)
C3—C4—C5—C7	−177.2 (2)	C121—C122—C123—N101	5.4 (4)
C10—C4—C5—C6	176.6 (2)	C119—N101—C123—C122	−0.2 (4)
C3—C4—C5—C6	−3.2 (3)	Al1—N101—C123—C122	−156.1 (2)
O1—C1—C6—C5	−157.6 (2)	C122—C121—C124—C125	−173.4 (2)
C2—C1—C6—C5	21.0 (3)	C120—C121—C124—C125	4.2 (4)
O1—C1—C6—C19	20.1 (3)	C121—C124—C125—C126	−0.4 (4)
C2—C1—C6—C19	−161.4 (2)	C124—C125—C126—C127	−2.6 (4)
C4—C5—C6—C1	−11.4 (3)	C125—C126—C127—C120	1.8 (4)
C7—C5—C6—C1	162.1 (2)	C121—C120—C127—C126	1.9 (4)
C4—C5—C6—C19	171.1 (2)	C119—C120—C127—C126	178.6 (2)
C7—C5—C6—C19	−15.4 (4)	O101—Al1—N201—C219	123.14 (19)
C4—C5—C7—C8	−1.0 (4)	O1—Al1—N201—C219	−141.33 (19)
C6—C5—C7—C8	−174.7 (2)	O201—Al1—N201—C219	31.74 (19)
C5—C7—C8—C9	−1.1 (4)	N1—Al1—N201—C219	−57.61 (19)
C7—C8—C9—C10	1.7 (4)	O101—Al1—N201—C223	−55.32 (18)
C7—C8—C9—C15	178.8 (2)	O1—Al1—N201—C223	40.21 (18)
C8—C9—C10—C4	−0.1 (4)	O201—Al1—N201—C223	−146.71 (18)
C15—C9—C10—C4	−177.1 (2)	N1—Al1—N201—C223	123.93 (18)
C5—C4—C10—C9	−2.1 (4)	O101—Al1—O201—C201	−140.57 (18)
C3—C4—C10—C9	177.7 (2)	N201—Al1—O201—C201	−49.07 (19)
C3—C2—C11—C13	129.8 (3)	N1—Al1—O201—C201	41.22 (19)
C1—C2—C11—C13	−52.1 (3)	N101—Al1—O201—C201	132.02 (18)
C3—C2—C11—C14	11.4 (3)	Al1—O201—C201—C206	30.3 (3)
C1—C2—C11—C14	−170.5 (2)	Al1—O201—C201—C202	−148.44 (19)
C3—C2—C11—C12	−108.5 (3)	O201—C201—C202—C203	164.8 (2)
C1—C2—C11—C12	69.6 (3)	C206—C201—C202—C203	−13.9 (4)
C10—C9—C15—C16	−14.5 (4)	O201—C201—C202—C211	−15.6 (4)
C8—C9—C15—C16	168.5 (2)	C206—C201—C202—C211	165.7 (2)
C10—C9—C15—C17	−135.1 (3)	C201—C202—C203—C204	−1.7 (4)
C8—C9—C15—C17	48.0 (3)	C211—C202—C203—C204	178.8 (2)
C10—C9—C15—C18	105.0 (3)	C202—C203—C204—C205	8.9 (4)
C8—C9—C15—C18	−71.9 (3)	C202—C203—C204—C210	−170.0 (3)
C23—N1—C19—C20	3.1 (3)	C210—C204—C205—C207	3.5 (4)
Al1—N1—C19—C20	−175.34 (16)	C203—C204—C205—C207	−175.4 (2)
C23—N1—C19—C6	178.7 (2)	C210—C204—C205—C206	178.3 (2)
Al1—N1—C19—C6	0.3 (3)	C203—C204—C205—C206	−0.7 (4)
C1—C6—C19—N1	−36.5 (3)	O201—C201—C206—C205	−156.6 (2)
C5—C6—C19—N1	141.1 (2)	C202—C201—C206—C205	22.1 (4)
C1—C6—C19—C20	139.1 (2)	O201—C201—C206—C219	22.5 (4)

C5—C6—C19—C20	−43.4 (3)	C202—C201—C206—C219	−158.8 (2)
N1—C19—C20—C21	−9.1 (3)	C204—C205—C206—C201	−14.7 (4)
C6—C19—C20—C21	175.4 (2)	C207—C205—C206—C201	159.7 (2)
N1—C19—C20—C27	167.2 (2)	C204—C205—C206—C219	166.2 (2)
C6—C19—C20—C27	−8.3 (4)	C207—C205—C206—C219	−19.4 (4)
C27—C20—C21—C22	−169.2 (2)	C204—C205—C207—C208	−1.4 (4)
C19—C20—C21—C22	7.3 (4)	C206—C205—C207—C208	−175.9 (2)
C27—C20—C21—C24	6.1 (4)	C205—C207—C208—C209	−1.3 (4)
C19—C20—C21—C24	−177.3 (2)	C207—C208—C209—C210	1.8 (4)
C20—C21—C22—C23	0.2 (4)	C207—C208—C209—C215	−179.8 (3)
C24—C21—C22—C23	−175.1 (3)	C208—C209—C210—C204	0.5 (4)
C21—C22—C23—N1	−6.6 (4)	C215—C209—C210—C204	−177.9 (3)
C19—N1—C23—C22	5.0 (4)	C205—C204—C210—C209	−3.1 (4)
Al1—N1—C23—C22	−176.5 (2)	C203—C204—C210—C209	175.8 (3)
C22—C21—C24—C25	171.9 (3)	C203—C202—C211—C213	124.9 (3)
C20—C21—C24—C25	−3.4 (4)	C201—C202—C211—C213	−54.7 (3)
C21—C24—C25—C26	−1.2 (4)	C203—C202—C211—C212	5.9 (4)
C24—C25—C26—C27	2.8 (4)	C201—C202—C211—C212	−173.7 (2)
C25—C26—C27—C20	0.1 (4)	C203—C202—C211—C214	−113.6 (3)
C21—C20—C27—C26	−4.6 (4)	C201—C202—C211—C214	66.9 (3)
C19—C20—C27—C26	179.0 (2)	C210—C209—C215—C216	−4.2 (4)
O101—Al1—N101—C119	−16.36 (18)	C208—C209—C215—C216	177.4 (3)
O1—Al1—N101—C119	−112.20 (18)	C210—C209—C215—C218	116.4 (3)
O201—Al1—N101—C119	74.73 (18)	C208—C209—C215—C218	−61.9 (4)
N1—Al1—N101—C119	164.22 (18)	C210—C209—C215—C217	−124.6 (3)
O101—Al1—N101—C123	139.50 (18)	C208—C209—C215—C217	57.1 (3)
O1—Al1—N101—C123	43.67 (18)	C223—N201—C219—C220	3.6 (3)
O201—Al1—N101—C123	−129.40 (18)	Al1—N201—C219—C220	−174.82 (17)
N1—Al1—N101—C123	−39.91 (19)	C223—N201—C219—C206	−178.8 (2)
O1—Al1—O101—C101	139.92 (17)	Al1—N201—C219—C206	2.8 (3)
O201—Al1—O101—C101	−41.51 (17)	C201—C206—C219—N201	−38.0 (3)
N201—Al1—O101—C101	−128.68 (17)	C205—C206—C219—N201	141.1 (2)
N101—Al1—O101—C101	56.52 (17)	C201—C206—C219—C220	139.6 (2)
Al1—O101—C101—C106	−52.6 (3)	C205—C206—C219—C220	−41.3 (3)
Al1—O101—C101—C102	127.7 (2)	N201—C219—C220—C221	−13.5 (4)
O101—C101—C102—C103	−175.3 (2)	C206—C219—C220—C221	168.9 (2)
C106—C101—C102—C103	5.0 (4)	N201—C219—C220—C227	165.3 (2)
O101—C101—C102—C111	1.6 (4)	C206—C219—C220—C227	−12.2 (4)
C106—C101—C102—C111	−178.1 (2)	C227—C220—C221—C222	−166.7 (2)
C101—C102—C103—C104	3.0 (4)	C219—C220—C221—C222	12.2 (4)
C111—C102—C103—C104	−174.0 (2)	C227—C220—C221—C224	9.0 (4)
C102—C103—C104—C105	−5.7 (4)	C219—C220—C221—C224	−172.1 (2)
C102—C103—C104—C110	171.0 (2)	C220—C221—C222—C223	−1.5 (4)
C110—C104—C105—C107	−1.0 (4)	C224—C221—C222—C223	−177.1 (3)
C103—C104—C105—C107	175.7 (2)	C221—C222—C223—N201	−9.0 (4)
C110—C104—C105—C106	−176.3 (2)	C219—N201—C223—C222	8.0 (4)
C103—C104—C105—C106	0.4 (4)	Al1—N201—C223—C222	−173.5 (2)
O101—C101—C106—C105	170.1 (2)	C220—C221—C224—C225	−4.9 (4)
C102—C101—C106—C105	−10.2 (4)	C222—C221—C224—C225	170.7 (3)

O101—C101—C106—C119	−7.8 (3)	C221—C224—C225—C226	−1.7 (5)
C102—C101—C106—C119	171.9 (2)	C224—C225—C226—C227	4.1 (5)
C104—C105—C106—C101	7.4 (4)	C225—C226—C227—C220	0.2 (4)
C107—C105—C106—C101	−167.5 (2)	C221—C220—C227—C226	−6.7 (4)
C104—C105—C106—C119	−174.7 (2)	C219—C220—C227—C226	174.4 (3)
C107—C105—C106—C119	10.4 (4)	C307—C302—C303—C304	0.0
C104—C105—C107—C108	0.0 (4)	C301—C302—C303—C304	−178.0 (3)
C106—C105—C107—C108	175.1 (3)	C302—C303—C304—C305	0.0
C105—C107—C108—C109	0.1 (4)	C303—C304—C305—C306	0.0
C107—C108—C109—C110	0.6 (4)	C304—C305—C306—C307	0.0
C107—C108—C109—C115	−175.2 (3)	C305—C306—C307—C302	0.0
C108—C109—C110—C104	−1.6 (4)	C303—C302—C307—C306	0.0
C115—C109—C110—C104	174.3 (2)	C301—C302—C307—C306	178.0 (3)
C105—C104—C110—C109	1.8 (4)	C407—C402—C403—C404	0.0
C103—C104—C110—C109	−174.8 (3)	C401—C402—C403—C404	178.5 (7)
C103—C102—C111—C112	−10.0 (3)	C402—C403—C404—C405	0.0
C101—C102—C111—C112	173.1 (2)	C403—C404—C405—C406	0.0
C103—C102—C111—C113	−130.2 (3)	C404—C405—C406—C407	0.0
C101—C102—C111—C113	52.9 (3)	C405—C406—C407—C402	0.0
C103—C102—C111—C114	107.4 (3)	C403—C402—C407—C406	0.0
C101—C102—C111—C114	−69.5 (3)	C401—C402—C407—C406	−178.4 (8)
C110—C109—C115—C116	48.5 (3)		

Metal ligand coverage

Ligand	Solid angle (steradians)	Equivalent cone angle (°)
N1—O1	4.77	152.0
N101—O101	4.93	155.1
N201—O201	4.79	152.6

Values calculated using Solid-G (Guzei & Wendt, 2006).