Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{2,2′-[Ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}(isopropanolato)-aluminium dichloromethane hemisolvate

Kirill V. Zaitsev,[a] Ekaterina A. Kuchuk,[a] Sergey S. Karlov,[a] Galina S. Zaitseva[a] and Andrei V. Churakov[b]*

[a]Department of Chemistry, M.V. Lomonosov Moscow State University, Leninskie Gory 1/3, Moscow 119991, Russian Federation, and [b]Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Leninskii prosp. 31, Moscow 119991, Russian Federation
Correspondence e-mail: churakov@igic.ras.ru

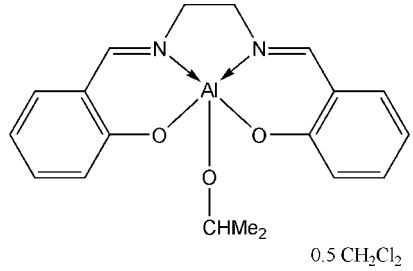
Received 18 October 2013; accepted 28 October 2013

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.081; data-to-parameter ratio = 16.8.

In the title compound, $[Al(C_{16}H_{14}N_2O_2)(C_3H_7O)]\cdot 0.5CH_2Cl_2$, the salen complex is monomeric and the dichlormethane solvent molecule lies on a crystallographic twofold axis. The central Al atom is fivefold coordinated and possesses a square-based pyramidal environment. The Al—OAlk(*i*propyl) bond [1.7404 (14) Å] is much shorter than the Al—OAr(salen) bond lengths [1.7974 (15) and 1.8094 (14) Å]. The isopropyloxo group forms an intramolecular C—H···N hydrogen bond. In the crystal, the complex molecules are linked by weak C—H···O interactions.

Related literature

For general background to the chemistry affording aluminium complexes based on salen-type ligands, see: Matsumoto *et al.* (2007); Gurian *et al.* (1991); Atwood *et al.* (1997); Muñoz-Hernandez *et al.* (2000). For our previous work on main group element complexes with polydentate *N*,*O*-ligands, see: Karlov & Zaitseva (2001). For structures of related monomeric Al-salen complexes, see: Darensburg & Billodeaux (2005); Gurian *et al.* (1991); Pang *et al.* (2008). For a description of the Cambridge Structural Database, see: Allen (2002).



0.5 CH_2Cl_2

Experimental

Crystal data

$[Al(C_{16}H_{14}N_2O_2)(C_3H_7O)]\cdot 0.5CH_2Cl_2$
M_r = 394.82
Orthorhombic, *Fdd*2
a = 24.427 (3) Å
b = 30.875 (4) Å
c = 10.0956 (13) Å
V = 7614.0 (16) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 173 K
0.25 × 0.15 × 0.04 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.936, T_{max} = 0.989
13794 measured reflections
4069 independent reflections
3687 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.081
S = 1.04
4069 reflections
242 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983), 1872 Friedel pairs
Absolute structure parameter: −0.09 (7)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···N1	1.00	2.64	3.204 (3)	116
C18—H18A···O3^{i}	0.99	2.55	3.508 (2)	163
C4—H4···O1^{ii}	0.96	2.33	3.2539 (18)	160

Symmetry codes: (i) $x+\frac{1}{4}, -y+\frac{3}{4}, z-\frac{1}{4}$; (ii) $-x+\frac{7}{4}, y+\frac{1}{4}, z-\frac{1}{4}$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was partially supported by the RFBR (12–03–00206_a) and a grant from the President of the Russian Federation to support the research of young Russian scientists and doctors (MD-3634.2012.3).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2075).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.

Atwood, D. A., Jegier, J. A. & Rutherford, D. (1997). *Bull. Chem. Soc. Jpn*, **70**, 2093–2100.

Bruker (2008). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Darensburg, D. J. & Billodeaux, D. R. (2005). *Inorg. Chem.* **44**, 1433–1442.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Gurian, P. L., Cheatham, L. K., Zillerb, J. W. & Barron, A. R. (1991). *J. Chem. Soc. Dalton Trans.* pp. 1449–1456.

Karlov, S. S. & Zaitseva, G. S. (2001). *Chem. Heterocycl. Compd*, **37**, 1325–1357.

Matsumoto, K., Saito, B. & Katsuki, T. (2007). *Chem. Commun.* pp. 3619–3627.

Muñoz-Hernandez, M.-A., Keizer, T. S., Parkin, S., Zhang, Y. & Atwood, D. A. (2000). *J. Chem. Crystallogr.* **30**, 219–222.

Pang, X., Du, H., Chen, X., Wand, X. & Jing, X. (2008). *Chem. Eur. J.* **14**, 3126–3136.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, m631–m632 [doi:10.1107/S1600536813029644]

{2,2′-[Ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}(isopropanolato)aluminium dichloromethane hemisolvate

Kirill V. Zaitsev, Ekaterina A. Kuchuk, Sergey S. Karlov, Galina S. Zaitseva and Andrei V. Churakov

S1. Comment

As a part of our investigation on chemistry of main group elements complexes based on tetradentate ligands (Karlov & Zaitseva, 2001) we obtained and studied the structure of the salen title compound [(salen)AlO-^{i}Pr]. The aluminium complex is monomeric (Fig. 1) with a fivefold coordinated Al centre. Its coordination geometry is close to square-based pyramidal with the salen ligand occupying the basal plane and the isopropyloxo group in axial position. It was shown, that the closely related methyloxo compound with an unsubstituted salen ligand $[(MeO)(salen)Al]_2$ is dimeric with two bridging μ_2-alkyloxo ligands (Gurian *et al.* (1991)). In contrast, a similar compound with bulky trimethylphenoxo substituent (2,4,6-$Me_3C_6H_2O$)(salen)Al exhibited monomeric nature (Atwood *et al.* (1997)). Also all Al compounds with substituted salen ligands, like widely studied complexes of bulky (^{t}Bu)$_4$salen, are monomeric according to CSD data (Allen, 2002), surely due to the steric hindrances. Thus, it may be assumed that the nuclearity of aluminium complexes with an unsubstituted salen ligand depends on the size of the additional alkyloxo group.

The central metal atom is displaced from the basal N,N,O,O plane by 0.4874 (9) Å. Unexpectedly, the Al-O(3)Alk distance (1.7404 (14) Å) is much shorter than Al-OAr bond lengths from the salen ligand (1.7974 (15) and 1.8094 (14) Å). On the other hand, the Al—O(3)—C(1) angle is quite large with 130.54 (12) °. These values indicate the noticeable degree of π- donation from the apical alkyloxo ligand towards the aluminium centre. The same features were previously found in the structure of the closely related monomeric ethyloxo complex (EtO)(salen(^{t}Bu)$_4$)Al (Muñoz-Hernandez *et al.* (2000)).

The isopropyloxo group forms an intramolecular hydrogen bond C1—H1A···N1 with H···N with 2.64 Å and C—H···N 116.0 (1)° that is connected with the mutual ecliptic arrangement of N1—Al1 and O3—C1 bonds.

In the crystal packing, the Al-complexes are linked by weak C18—H18A···O3 hydrogen bonds (C···O 3.508 (2) Å, C—H···O 162.9 (1)°). The asymmetric unit contains a solvent dichlormethane molecule that lies on a crystallographic 2-fold axis and forms C4—H4···O1 hydrogen bonds with C···O separations of 3.2539 (18) Å.

S2. Experimental

The title compound was obtained from reaction of equimolar amounts of Al(O-*i*Pr)$_3$ and salen in toluene at reflux as a solid.

^{1}H NMR ($CDCl_3$): δ 8.24 (s, 2H, N=CH), 7.40–7.33 (m, 2H, aromatic H atoms), 7.16–7.07 (m, 4H, aromatic H atoms), 6.73–6.67 (m, 2H, aromatic H atoms), 4.12–4.02 (m, 2H, NCH_2), 3.75 (sept, J = 6.1 Hz, 1H, OCH), 3.65–3.58 (m, 2H, NCH_2), 0.91 d (d, J = 6.1 Hz, 6H, OCH*Me*$_2$) p.p.m..

^{13}C NMR ($CDCl_3$): δ 168.97 (N=CH), 165.78, 135.46, 132.99, 122.26, 118.74, 116.55 (aromatic carbons), 62.80 (OCH), 54.44 (NCH_2), 27.33 (OCH*Me*$_2$) p.p.m..

S3. Refinement

All hydrogen atoms were placed in calculated positions and refined using a riding model with C—H = 1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) for methyne group; C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene groups; C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups; C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms.

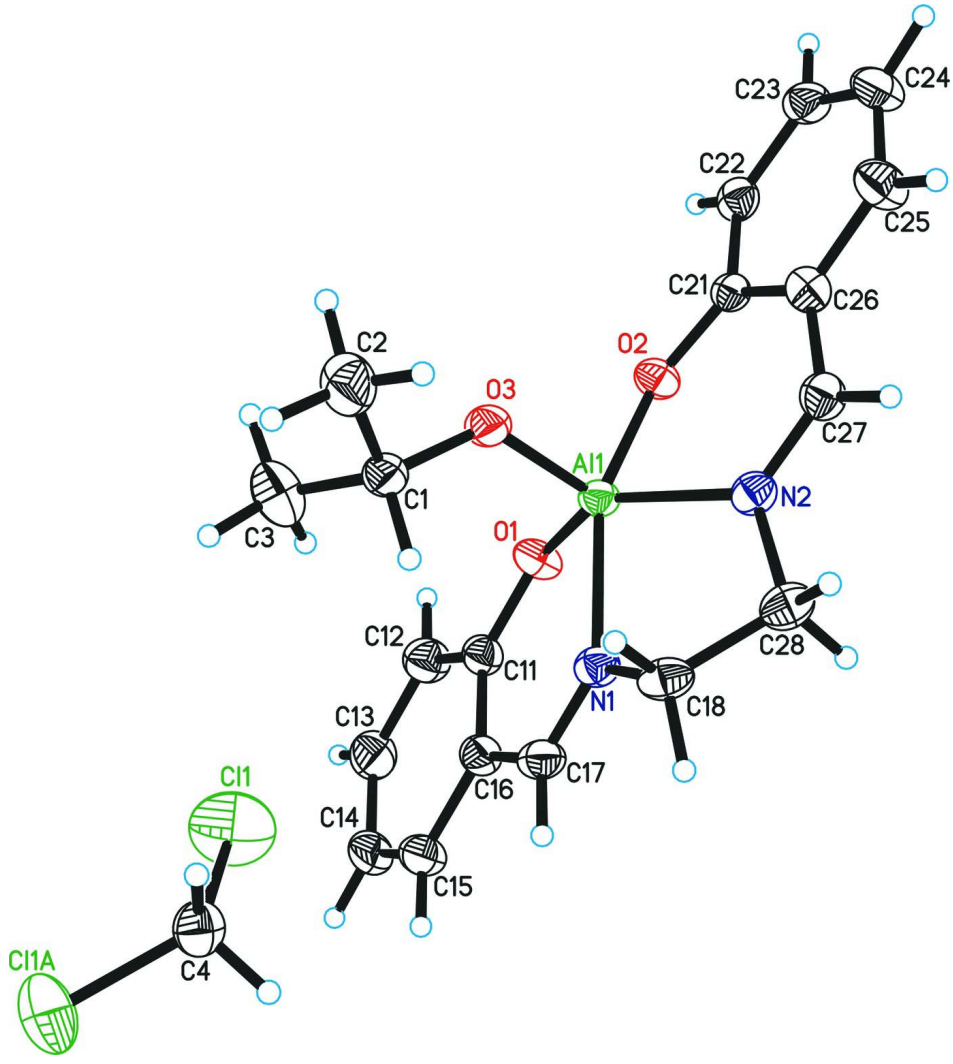


Figure 1

The molecular structure of the title compound. Anisotropic displacement ellipsoids are shown at the 50% probability level. [Symmetry code: (A) 2-x, 1-y, z]

{2,2′-[Ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}(isopropanolato)aluminium dichloromethane hemisolvate

Crystal data

$[Al(C_{16}H_{14}N_2O_2)(C_3H_7O)]\cdot 0.5CH_2Cl_2$
$M_r = 394.82$
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
$a = 24.427\ (3)$ Å
$b = 30.875\ (4)$ Å
$c = 10.0956\ (13)$ Å
$V = 7614.0\ (16)$ Å^3
$Z = 16$
$F(000) = 3312$
$D_x = 1.378$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4106 reflections
$\theta = 2.3–25.6°$
$\mu = 0.27$ mm^{-1}
$T = 173$ K
Plate, colourless
0.25 × 0.15 × 0.04 mm

Data collection

Bruker SMART APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.936$, $T_{max} = 0.989$
13794 measured reflections
4069 independent reflections
3687 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.3°$
$h = -31\rightarrow31$
$k = -39\rightarrow39$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.081$
$S = 1.04$
4069 reflections
242 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 4.145P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983), 1872 Friedel pairs
Absolute structure parameter: −0.09 (7)

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	0.80543 (2)	0.339391 (17)	0.48762 (6)	0.02073 (13)
O1	0.83307 (5)	0.32093 (4)	0.64267 (15)	0.0274 (3)

O2	0.74619 (5)	0.30520 (4)	0.51299 (14)	0.0244 (3)
O3	0.77795 (5)	0.39121 (4)	0.50117 (16)	0.0280 (3)
N1	0.88207 (6)	0.35385 (5)	0.42972 (17)	0.0233 (4)
N2	0.80155 (6)	0.32532 (5)	0.29380 (17)	0.0237 (4)
C1	0.80382 (8)	0.43157 (6)	0.5214 (2)	0.0265 (4)
H1A	0.8401	0.4311	0.4756	0.032*
C2	0.76904 (10)	0.46682 (7)	0.4601 (3)	0.0408 (6)
H2A	0.7647	0.4612	0.3651	0.061*
H2B	0.7869	0.4949	0.4730	0.061*
H2C	0.7330	0.4671	0.5025	0.061*
C3	0.81316 (11)	0.44040 (8)	0.6673 (3)	0.0438 (6)
H3A	0.8334	0.4162	0.7066	0.066*
H3B	0.7778	0.4435	0.7120	0.066*
H3C	0.8343	0.4672	0.6774	0.066*
C11	0.88005 (8)	0.32767 (6)	0.7048 (2)	0.0247 (4)
C12	0.88427 (9)	0.31743 (7)	0.8386 (2)	0.0332 (5)
H12	0.8533	0.3063	0.8842	0.040*
C13	0.93293 (9)	0.32316 (7)	0.9064 (3)	0.0366 (5)
H13	0.9349	0.3161	0.9978	0.044*
C14	0.97909 (9)	0.33922 (7)	0.8422 (3)	0.0350 (5)
H14	1.0125	0.3426	0.8890	0.042*
C15	0.97586 (9)	0.35001 (7)	0.7114 (3)	0.0328 (5)
H15	1.0073	0.3612	0.6678	0.039*
C16	0.92665 (8)	0.34479 (6)	0.6396 (2)	0.0261 (4)
C17	0.92542 (8)	0.35630 (6)	0.5013 (2)	0.0270 (4)
H17	0.9583	0.3662	0.4610	0.032*
C18	0.88543 (8)	0.36551 (7)	0.2887 (2)	0.0275 (5)
H18A	0.9239	0.3644	0.2578	0.033*
H18B	0.8711	0.3951	0.2742	0.033*
C21	0.70533 (7)	0.29526 (6)	0.4337 (2)	0.0212 (4)
C22	0.65738 (8)	0.27644 (6)	0.4864 (2)	0.0260 (4)
H22	0.6560	0.2686	0.5773	0.031*
C23	0.61261 (8)	0.26946 (6)	0.4067 (2)	0.0304 (5)
H23	0.5805	0.2571	0.4442	0.036*
C24	0.61294 (9)	0.27991 (7)	0.2725 (2)	0.0356 (5)
H24	0.5809	0.2767	0.2200	0.043*
C25	0.66070 (9)	0.29500 (7)	0.2186 (2)	0.0346 (5)
H25	0.6622	0.3008	0.1262	0.041*
C26	0.70752 (8)	0.30217 (6)	0.2965 (2)	0.0270 (4)
C27	0.75757 (8)	0.31427 (6)	0.2327 (2)	0.0269 (4)
H27	0.7583	0.3141	0.1387	0.032*
C28	0.85114 (8)	0.33286 (7)	0.2152 (2)	0.0293 (4)
H28A	0.8413	0.3441	0.1264	0.035*
H28B	0.8717	0.3055	0.2038	0.035*
Cl1	0.96134 (3)	0.46418 (3)	0.61765 (8)	0.0636 (2)
C4	1.0000	0.5000	0.5209 (3)	0.0304 (7)
H4	0.9758	0.5163	0.4650	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0173 (2)	0.0212 (3)	0.0238 (3)	−0.0013 (2)	0.0013 (2)	0.0001 (2)
O1	0.0219 (7)	0.0353 (8)	0.0249 (8)	−0.0063 (6)	−0.0031 (6)	0.0037 (6)
O2	0.0216 (6)	0.0264 (6)	0.0252 (8)	−0.0046 (5)	−0.0003 (6)	0.0029 (6)
O3	0.0210 (6)	0.0211 (6)	0.0418 (9)	−0.0013 (5)	0.0022 (7)	−0.0033 (7)
N1	0.0209 (8)	0.0223 (8)	0.0266 (9)	−0.0007 (6)	0.0031 (7)	0.0016 (7)
N2	0.0232 (8)	0.0241 (8)	0.0238 (9)	−0.0005 (6)	0.0037 (7)	0.0019 (7)
C1	0.0222 (9)	0.0229 (9)	0.0344 (12)	−0.0023 (7)	0.0027 (9)	−0.0023 (8)
C2	0.0459 (13)	0.0263 (10)	0.0502 (17)	0.0013 (9)	−0.0088 (12)	−0.0008 (10)
C3	0.0522 (15)	0.0374 (12)	0.0416 (15)	−0.0125 (11)	−0.0065 (12)	−0.0009 (11)
C11	0.0232 (9)	0.0233 (9)	0.0276 (12)	0.0007 (8)	−0.0031 (8)	−0.0012 (8)
C12	0.0300 (11)	0.0373 (12)	0.0321 (13)	−0.0002 (9)	−0.0016 (9)	0.0001 (10)
C13	0.0365 (12)	0.0431 (13)	0.0301 (13)	0.0050 (10)	−0.0075 (10)	−0.0040 (10)
C14	0.0272 (11)	0.0368 (12)	0.0409 (14)	0.0030 (9)	−0.0107 (10)	−0.0084 (10)
C15	0.0227 (9)	0.0293 (10)	0.0464 (15)	−0.0009 (8)	−0.0030 (9)	−0.0045 (10)
C16	0.0225 (9)	0.0226 (9)	0.0332 (12)	0.0004 (7)	−0.0024 (9)	−0.0028 (8)
C17	0.0200 (9)	0.0221 (9)	0.0390 (13)	−0.0003 (7)	0.0039 (9)	0.0003 (9)
C18	0.0214 (10)	0.0280 (10)	0.0330 (12)	−0.0003 (8)	0.0063 (9)	0.0068 (9)
C21	0.0205 (9)	0.0157 (8)	0.0275 (10)	0.0022 (7)	−0.0015 (8)	−0.0005 (7)
C22	0.0271 (10)	0.0207 (9)	0.0302 (11)	−0.0002 (7)	0.0022 (10)	−0.0006 (9)
C23	0.0222 (10)	0.0257 (10)	0.0433 (14)	−0.0029 (8)	0.0033 (10)	−0.0030 (9)
C24	0.0243 (10)	0.0413 (12)	0.0411 (14)	−0.0034 (9)	−0.0088 (10)	−0.0027 (10)
C25	0.0309 (11)	0.0429 (12)	0.0299 (12)	−0.0047 (9)	−0.0059 (10)	0.0020 (10)
C26	0.0268 (10)	0.0268 (10)	0.0273 (12)	−0.0015 (8)	−0.0016 (9)	−0.0002 (8)
C27	0.0280 (10)	0.0300 (10)	0.0228 (11)	−0.0008 (8)	0.0009 (9)	0.0001 (9)
C28	0.0272 (10)	0.0327 (10)	0.0280 (12)	0.0020 (8)	0.0064 (9)	0.0044 (9)
Cl1	0.0662 (4)	0.0686 (4)	0.0559 (5)	−0.0116 (4)	0.0136 (4)	0.0262 (4)
C4	0.0347 (16)	0.0328 (15)	0.0236 (16)	−0.0003 (12)	0.000	0.000

Geometric parameters (Å, º)

Al1—O3	1.7404 (14)	C14—C15	1.363 (4)
Al1—O1	1.7974 (15)	C14—H14	0.9500
Al1—O2	1.8094 (14)	C15—C16	1.413 (3)
Al1—N2	2.0066 (18)	C15—H15	0.9500
Al1—N1	2.0115 (17)	C16—C17	1.442 (3)
O1—C11	1.324 (2)	C17—H17	0.9500
O2—C21	1.315 (2)	C18—C28	1.506 (3)
O3—C1	1.412 (2)	C18—H18A	0.9900
N1—C17	1.284 (3)	C18—H18B	0.9900
N1—C18	1.471 (3)	C21—C26	1.403 (3)
N2—C27	1.285 (3)	C21—C22	1.412 (3)
N2—C28	1.467 (2)	C22—C23	1.375 (3)
C1—C2	1.513 (3)	C22—H22	0.9500
C1—C3	1.515 (3)	C23—C24	1.392 (3)
C1—H1A	1.0000	C23—H23	0.9500

C2—H2A	0.9800	C24—C25	1.369 (3)
C2—H2B	0.9800	C24—H24	0.9500
C2—H2C	0.9800	C25—C26	1.406 (3)
C3—H3A	0.9800	C25—H25	0.9500
C3—H3B	0.9800	C26—C27	1.431 (3)
C3—H3C	0.9800	C27—H27	0.9500
C11—C12	1.392 (3)	C28—H28A	0.9900
C11—C16	1.417 (3)	C28—H28B	0.9900
C12—C13	1.383 (3)	Cl1—C4	1.7521 (19)
C12—H12	0.9500	C4—Cl1^{i}	1.7520 (19)
C13—C14	1.392 (3)	C4—H4	0.9600
C13—H13	0.9500		

O3—Al1—O1	111.59 (8)	C15—C14—H14	120.3
O3—Al1—O2	102.52 (7)	C13—C14—H14	120.3
O1—Al1—O2	89.55 (7)	C14—C15—C16	121.2 (2)
O3—Al1—N2	104.92 (8)	C14—C15—H15	119.4
O1—Al1—N2	142.97 (7)	C16—C15—H15	119.4
O2—Al1—N2	88.51 (7)	C15—C16—C11	119.2 (2)
O3—Al1—N1	100.24 (7)	C15—C16—C17	119.13 (19)
O1—Al1—N1	88.50 (7)	C11—C16—C17	121.66 (18)
O2—Al1—N1	156.20 (7)	N1—C17—C16	123.21 (18)
N2—Al1—N1	78.96 (7)	N1—C17—H17	118.4
C11—O1—Al1	133.47 (13)	C16—C17—H17	118.4
C21—O2—Al1	131.06 (13)	N1—C18—C28	106.40 (16)
C1—O3—Al1	130.54 (12)	N1—C18—H18A	110.4
C17—N1—C18	118.95 (17)	C28—C18—H18A	110.4
C17—N1—Al1	128.11 (15)	N1—C18—H18B	110.4
C18—N1—Al1	112.80 (13)	C28—C18—H18B	110.4
C27—N2—C28	118.22 (18)	H18A—C18—H18B	108.6
C27—N2—Al1	124.39 (15)	O2—C21—C26	122.43 (17)
C28—N2—Al1	117.03 (13)	O2—C21—C22	119.78 (18)
O3—C1—C2	108.93 (17)	C26—C21—C22	117.78 (18)
O3—C1—C3	111.52 (18)	C23—C22—C21	120.3 (2)
C2—C1—C3	110.63 (19)	C23—C22—H22	119.9
O3—C1—H1A	108.6	C21—C22—H22	119.9
C2—C1—H1A	108.6	C22—C23—C24	121.9 (2)
C3—C1—H1A	108.6	C22—C23—H23	119.0
C1—C2—H2A	109.5	C24—C23—H23	119.0
C1—C2—H2B	109.5	C25—C24—C23	118.1 (2)
H2A—C2—H2B	109.5	C25—C24—H24	121.0
C1—C2—H2C	109.5	C23—C24—H24	121.0
H2A—C2—H2C	109.5	C24—C25—C26	121.6 (2)
H2B—C2—H2C	109.5	C24—C25—H25	119.2
C1—C3—H3A	109.5	C26—C25—H25	119.2
C1—C3—H3B	109.5	C21—C26—C25	119.85 (19)
H3A—C3—H3B	109.5	C21—C26—C27	121.08 (19)
C1—C3—H3C	109.5	C25—C26—C27	119.0 (2)

H3A—C3—H3C	109.5	N2—C27—C26	124.6 (2)
H3B—C3—H3C	109.5	N2—C27—H27	117.7
O1—C11—C12	119.22 (19)	C26—C27—H27	117.7
O1—C11—C16	122.36 (19)	N2—C28—C18	107.38 (17)
C12—C11—C16	118.41 (19)	N2—C28—H28A	110.2
C13—C12—C11	121.0 (2)	C18—C28—H28A	110.2
C13—C12—H12	119.5	N2—C28—H28B	110.2
C11—C12—H12	119.5	C18—C28—H28B	110.2
C12—C13—C14	120.8 (2)	H28A—C28—H28B	108.5
C12—C13—H13	119.6	Cl1^{i}—C4—Cl1	112.20 (18)
C14—C13—H13	119.6	Cl1^{i}—C4—H4	109.3
C15—C14—C13	119.4 (2)	Cl1—C4—H4	109.0

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···N1	1.00	2.64	3.204 (3)	116
C18—H18*A*···O3^{ii}	0.99	2.55	3.508 (2)	163
C4—H4···O1^{iii}	0.96	2.33	3.2539 (18)	160

Symmetry codes: (ii) $x+1/4, -y+3/4, z-1/4$; (iii) $-x+7/4, y+1/4, z-1/4$.