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# Bis($\mu$-9-anthracenemethanolato)bis-[dimethylaluminium(III)]

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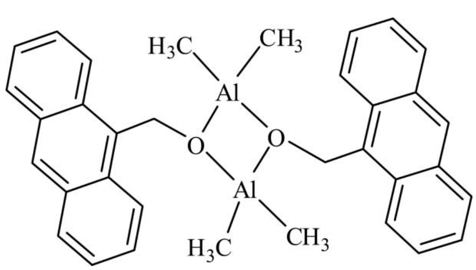
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.058; $wR$ factor = 0.234; data-to-parameter ratio = 21.3.

The title complex, $[Al_2(CH_3)_4(C_{15}H_{11}O)_2]$, is dimeric bridged through the O atoms of the 9-anthracenemethanolate anions. Each Al atom is tetracoordinated by two bridging O atoms from two different 9-anthracenemethanolate ligands and by two C atoms from two methyl groups, forming a distorted tetrahedral environment. The average Al—O bond distance in the $Al_2O_2$ core is 1.845 Å.

## Related literature

For background to metal complex-catalysed ring-opening polymerization of lactones/lactides, see: Liu *et al.* (2001); Wu *et al.* (2006). For related structures, see: Lin *et al.* (1999); Lou *et al.* (2002).



## Experimental

*Crystal data*

$[Al_2(CH_3)_4(C_{15}H_{11}O)_2]$
$M_r$ = 528.57
Triclinic, $P\overline{1}$
$a$ = 7.7852 (3) Å
$b$ = 11.3804 (4) Å
$c$ = 17.6749 (6) Å
$\alpha$ = 85.683 (2)°
$\beta$ = 79.883 (2)°
$\gamma$ = 74.617 (2)°
$V$ = 1485.72 (9) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K
0.45 × 0.38 × 0.32 mm

*Data collection*

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008) $T_{min}$ = 0.945, $T_{max}$ = 0.960
31484 measured reflections
7298 independent reflections
4944 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.234
$S$ = 1.01
7298 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.27 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2172).

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# supporting information

*Acta Cryst.* (2009). E**65**, m1320 [https://doi.org/10.1107/S1600536809040161]

## Bis($\mu$-9-anthracenemethanolato)bis[dimethylaluminium(III)]

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### S1. Comment

During the last decade, it has been of great interest to develop new catalytic/initiating systems for the preparation of aliphatic polyesters, such as *poly*($\varepsilon$-caprolactone) and *poly*(lactide). Metal complex-catalyzed ring-opening polymerization (*ROP*) of lactones/lactides has been proven to be the most promising method to synthesize these polymers (Wu *et al.*, 2006). Among them, a variety of main group metal complexes, such as magnesium, zinc and lithium as well as aluminium complexes have been reported to be efficient initiators/catalysts. In particular, Liu *et al.* (2001) have reported the aluminium benzylalkoxide complexes supported by the bulky bisphenolate ligand and these complexes have been demonstrated as efficient initiators to catalyze *ROP* of cyclic esters. Recently, our group is interested in the synthesis and preparation of aluminium complexes derived from the 9-anthracenemethanolate ligands. The compound, 9-anthracene-methanol has been proven as a useful initiator to initiate living cationic polymerization of $\delta$-valerolactone in the presence of HCl·$Et_2$O (Lou *et al.*, 2002). We report herein the synthesis and crystal structure of the 9-anthracenemethanolate ligand incorporated $Al^{III}$ complex, **I**, a potential initiator for the *ROP* of $\varepsilon$-caprolactone (Fig. 2).

The solid structure of **I** reveals a dimeric $Al^{III}$ complex (Fig. 1), doubly bridged through the O atoms of the 9-anthracenemethanolate anions. The geometry around each Al atom is four-coordinated with a distorted tetrahedral environment in which two bridging O atoms come from two different 9-anthracenemethanolate ligands and two C atoms are from two methyl groups. The average bond distance of Al-O in the $Al_2O_2$ core of 1.8453 (14)Å is within a normal range for an $Al_2O_2$ ring of four-coordinated aluminium complexes (Lin *et al.*, 1999).

### S2. Experimental

The title compound **I** was synthesized by the following procedures (Fig. 2): to a rapidly stirred solution of 9-anthracene-methanol (0.21 g, 1.0 mmol) in 1,2-dichloroethane (20 ml) was slowly added Al$Me_3$ (0.6 ml, 2.0 *M* in toluene, 1.2 mmol). The mixture was further stirred at room temperature for 4 h and then dried under vacuum. The residue was extracted with 1,2-dichloroethane (10 ml), and the saturated solution was cooled to 273 K, yielding colourless crystals. Yield: 0.22 g (83%). $^1$H NMR ($CDCl_3$, p.p.m.): $\delta$ 7.43-8.47 (18*H*, m, *Ar*H), 5.67 (4*H*, s, $CH_2$), -1.39 (12*H*, s, $AlCH_3$).

### S3. Refinement

The H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H = 0.93 Å with $U_{iso}$(H) = 1.2 $U_{eq}$(C) for phenyl hydrogen; 0.96 Å with $U_{iso}$(H) = 1.5 $U_{eq}$(C) for $CH_3$ group; 0.97 Å with $U_{iso}$(H) = 1.2 $U_{eq}$(C) for $CH_2$ group.

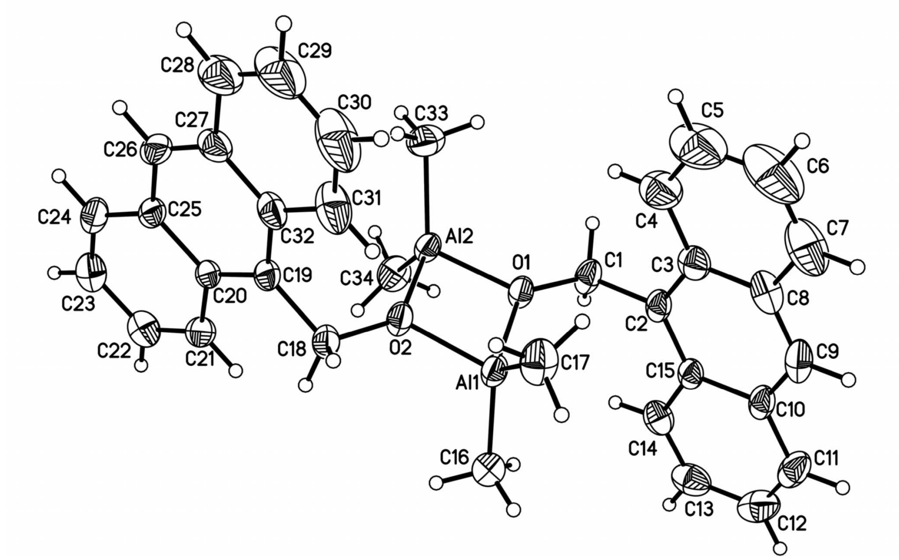


**Figure 1**

A view of the molecular structure of **I** with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as a small spheres of arbitrary radius.

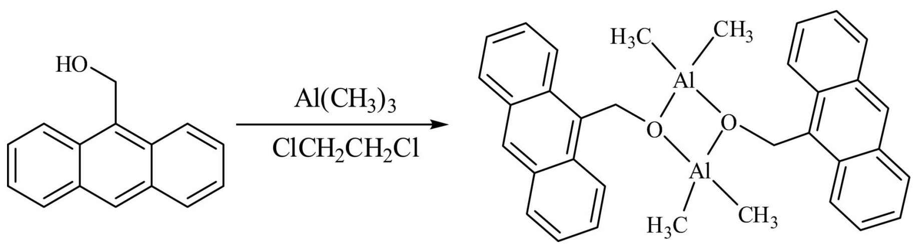


**Figure 2**

The title compound, **I**, (reaction path scheme).

**Bis($\mu$-9-anthracenemethanolato)bis[dimethylaluminium(III)]**

*Crystal data*

$[Al_2(CH_3)_4(C_{15}H_{11}O)_2]$
$M_r = 528.57$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.7852$ (3) Å
$b = 11.3804$ (4) Å
$c = 17.6749$ (6) Å
$\alpha = 85.683$ (2)°
$\beta = 79.883$ (2)°
$\gamma = 74.617$ (2)°
$V = 1485.72$ (9) Å$^3$
$Z = 2$
$F(000) = 560$
$D_x = 1.181$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9970 reflections
$\theta = 2.2$–28.2°
$\mu = 0.13$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.45 × 0.38 × 0.32 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)

$T_{min}$ = 0.945, $T_{max}$ = 0.960
31484 measured reflections
7298 independent reflections
4944 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 28.4°, $\theta_{min}$ = 1.9°
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 15$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.234$
$S = 1.01$
7298 reflections
343 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
$w = 1/[\sigma^2(F_o^2) + (0.17P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.27$ 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 $F^2 > \sigma(F^2)$ 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 | 0.71289 (7) | 0.62997 (5) | 0.30278 (4) | 0.0483 (2) |
| Al2 | 0.36490 (7) | 0.76614 (5) | 0.27971 (3) | 0.0449 (2) |
| O1 | 0.50638 (17) | 0.60755 (11) | 0.27575 (8) | 0.0466 (3) |
| O2 | 0.57693 (17) | 0.79058 (12) | 0.29925 (9) | 0.0501 (4) |
| C1 | 0.4531 (3) | 0.50037 (18) | 0.26509 (14) | 0.0550 (5) |
| H1A | 0.3752 | 0.5170 | 0.2262 | 0.066* |
| H1B | 0.3847 | 0.4779 | 0.3128 | 0.066* |
| C2 | 0.6143 (2) | 0.39518 (17) | 0.24061 (12) | 0.0460 (4) |
| C3 | 0.6999 (3) | 0.3874 (2) | 0.16343 (13) | 0.0571 (5) |
| C4 | 0.6426 (5) | 0.4791 (3) | 0.10646 (17) | 0.0878 (9) |
| H4A | 0.5446 | 0.5454 | 0.1197 | 0.105* |
| C5 | 0.7327 (7) | 0.4689 (5) | 0.0324 (2) | 0.1269 (16) |
| H5A | 0.6961 | 0.5290 | −0.0043 | 0.152* |
| C6 | 0.8791 (8) | 0.3689 (5) | 0.0114 (2) | 0.143 (2) |
| H6A | 0.9359 | 0.3626 | −0.0396 | 0.171* |
| C7 | 0.9404 (5) | 0.2806 (4) | 0.06366 (19) | 0.1063 (12) |
| H7A | 1.0406 | 0.2165 | 0.0487 | 0.128* |
| C8 | 0.8509 (3) | 0.2866 (2) | 0.14130 (14) | 0.0662 (7) |
| C9 | 0.9068 (3) | 0.1975 (2) | 0.19499 (16) | 0.0651 (6) |
| H9A | 1.0028 | 0.1310 | 0.1794 | 0.078* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.8260 (3) | 0.20243 (18) | 0.27155 (13) | 0.0509 (5) |
| C11 | 0.8872 (3) | 0.1102 (2) | 0.32601 (19) | 0.0709 (7) |
| H11A | 0.9810 | 0.0429 | 0.3098 | 0.085* |
| C12 | 0.8137 (4) | 0.1174 (3) | 0.40009 (19) | 0.0814 (8) |
| H12A | 0.8572 | 0.0564 | 0.4351 | 0.098* |
| C13 | 0.6709 (4) | 0.2172 (3) | 0.42484 (15) | 0.0720 (7) |
| H13A | 0.6209 | 0.2218 | 0.4767 | 0.086* |
| C14 | 0.6036 (3) | 0.3072 (2) | 0.37536 (13) | 0.0580 (6) |
| H14A | 0.5074 | 0.3718 | 0.3938 | 0.070* |
| C15 | 0.6778 (2) | 0.30507 (17) | 0.29495 (11) | 0.0435 (4) |
| C16 | 0.7421 (4) | 0.5780 (2) | 0.40803 (15) | 0.0778 (8) |
| H16A | 0.8646 | 0.5327 | 0.4093 | 0.117* |
| H16B | 0.6624 | 0.5273 | 0.4276 | 0.117* |
| H16C | 0.7136 | 0.6482 | 0.4392 | 0.117* |
| C17 | 0.9212 (3) | 0.6023 (2) | 0.22087 (17) | 0.0745 (7) |
| H17A | 1.0257 | 0.5541 | 0.2408 | 0.112* |
| H17B | 0.9420 | 0.6792 | 0.2013 | 0.112* |
| H17C | 0.8986 | 0.5600 | 0.1802 | 0.112* |
| C18 | 0.6307 (3) | 0.89486 (18) | 0.31628 (13) | 0.0550 (5) |
| H18A | 0.7572 | 0.8851 | 0.2951 | 0.066* |
| H18B | 0.6175 | 0.9003 | 0.3716 | 0.066* |
| C19 | 0.5213 (3) | 1.01085 (17) | 0.28411 (11) | 0.0450 (4) |
| C20 | 0.3866 (2) | 1.09329 (17) | 0.33176 (10) | 0.0401 (4) |
| C21 | 0.3403 (3) | 1.0730 (2) | 0.41330 (12) | 0.0514 (5) |
| H21A | 0.3966 | 1.0001 | 0.4364 | 0.062* |
| C22 | 0.2155 (3) | 1.1591 (2) | 0.45698 (14) | 0.0625 (6) |
| H22A | 0.1897 | 1.1442 | 0.5097 | 0.075* |
| C23 | 0.1249 (3) | 1.2691 (2) | 0.42521 (15) | 0.0659 (6) |
| H23A | 0.0414 | 1.3271 | 0.4565 | 0.079* |
| C24 | 0.1592 (3) | 1.2906 (2) | 0.34909 (15) | 0.0601 (6) |
| H24A | 0.0965 | 1.3632 | 0.3279 | 0.072* |
| C25 | 0.2891 (3) | 1.20518 (18) | 0.30016 (12) | 0.0460 (4) |
| C26 | 0.3239 (3) | 1.2290 (2) | 0.22149 (13) | 0.0574 (6) |
| H26A | 0.2579 | 1.3008 | 0.2007 | 0.069* |
| C27 | 0.4547 (4) | 1.1484 (2) | 0.17324 (13) | 0.0614 (6) |
| C28 | 0.4924 (5) | 1.1736 (3) | 0.09214 (15) | 0.0921 (10) |
| H28A | 0.4240 | 1.2435 | 0.0705 | 0.110* |
| C29 | 0.6261 (7) | 1.0967 (4) | 0.04722 (17) | 0.1195 (15) |
| H29A | 0.6502 | 1.1150 | −0.0051 | 0.143* |
| C30 | 0.7283 (6) | 0.9909 (4) | 0.0774 (2) | 0.1214 (15) |
| H30A | 0.8206 | 0.9396 | 0.0452 | 0.146* |
| C31 | 0.6957 (4) | 0.9609 (3) | 0.15368 (16) | 0.0860 (9) |
| H31A | 0.7643 | 0.8886 | 0.1728 | 0.103* |
| C32 | 0.5583 (3) | 1.0386 (2) | 0.20398 (12) | 0.0560 (5) |
| C33 | 0.3002 (4) | 0.8271 (3) | 0.17994 (14) | 0.0738 (7) |
| H33A | 0.1750 | 0.8706 | 0.1863 | 0.111* |
| H33B | 0.3209 | 0.7599 | 0.1469 | 0.111* |
| H33C | 0.3728 | 0.8810 | 0.1574 | 0.111* |

| | | | | |
|---|---|---|---|---|
| C34 | 0.1772 (3) | 0.7840 (2) | 0.37059 (14) | 0.0673 (6) |
| H34A | 0.0645 | 0.8314 | 0.3570 | 0.101* |
| H34B | 0.2097 | 0.8245 | 0.4095 | 0.101* |
| H34C | 0.1652 | 0.7049 | 0.3898 | 0.101* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Al1 | 0.0401 (3) | 0.0352 (3) | 0.0677 (4) | −0.0034 (2) | −0.0115 (3) | −0.0059 (3) |
| Al2 | 0.0410 (3) | 0.0354 (3) | 0.0551 (4) | −0.0032 (2) | −0.0095 (2) | −0.0001 (2) |
| O1 | 0.0405 (7) | 0.0330 (7) | 0.0656 (8) | −0.0061 (5) | −0.0100 (6) | −0.0060 (6) |
| O2 | 0.0437 (7) | 0.0330 (7) | 0.0742 (9) | −0.0088 (5) | −0.0121 (6) | −0.0041 (6) |
| C1 | 0.0448 (10) | 0.0343 (11) | 0.0875 (15) | −0.0110 (8) | −0.0136 (10) | −0.0016 (10) |
| C2 | 0.0431 (9) | 0.0333 (10) | 0.0643 (12) | −0.0127 (7) | −0.0097 (8) | −0.0056 (8) |
| C3 | 0.0709 (14) | 0.0490 (12) | 0.0601 (12) | −0.0285 (10) | −0.0148 (10) | 0.0017 (10) |
| C4 | 0.124 (3) | 0.080 (2) | 0.0741 (17) | −0.0458 (18) | −0.0311 (16) | 0.0150 (14) |
| C5 | 0.195 (5) | 0.136 (4) | 0.071 (2) | −0.085 (4) | −0.028 (3) | 0.032 (2) |
| C6 | 0.201 (5) | 0.191 (6) | 0.059 (2) | −0.112 (5) | 0.021 (2) | −0.015 (3) |
| C7 | 0.121 (3) | 0.120 (3) | 0.077 (2) | −0.050 (2) | 0.0299 (19) | −0.036 (2) |
| C8 | 0.0713 (15) | 0.0648 (16) | 0.0659 (14) | −0.0290 (12) | 0.0059 (11) | −0.0211 (12) |
| C9 | 0.0531 (12) | 0.0468 (13) | 0.0918 (17) | −0.0092 (10) | 0.0008 (11) | −0.0232 (12) |
| C10 | 0.0446 (10) | 0.0341 (10) | 0.0768 (14) | −0.0114 (8) | −0.0125 (9) | −0.0082 (9) |
| C11 | 0.0621 (14) | 0.0389 (13) | 0.119 (2) | −0.0142 (10) | −0.0352 (14) | 0.0051 (13) |
| C12 | 0.092 (2) | 0.0694 (19) | 0.102 (2) | −0.0431 (16) | −0.0486 (17) | 0.0321 (16) |
| C13 | 0.0897 (18) | 0.082 (2) | 0.0616 (14) | −0.0488 (16) | −0.0242 (13) | 0.0115 (13) |
| C14 | 0.0592 (12) | 0.0580 (14) | 0.0635 (13) | −0.0270 (10) | −0.0065 (10) | −0.0096 (10) |
| C15 | 0.0408 (9) | 0.0344 (10) | 0.0598 (11) | −0.0147 (7) | −0.0107 (8) | −0.0057 (8) |
| C16 | 0.0953 (19) | 0.0590 (16) | 0.0813 (17) | −0.0070 (14) | −0.0378 (15) | −0.0061 (13) |
| C17 | 0.0463 (12) | 0.0707 (18) | 0.1021 (19) | −0.0134 (11) | 0.0024 (12) | −0.0149 (14) |
| C18 | 0.0538 (11) | 0.0385 (11) | 0.0758 (14) | −0.0087 (9) | −0.0203 (10) | −0.0096 (10) |
| C19 | 0.0500 (10) | 0.0348 (10) | 0.0559 (11) | −0.0174 (8) | −0.0141 (8) | −0.0006 (8) |
| C20 | 0.0446 (9) | 0.0337 (9) | 0.0489 (10) | −0.0186 (7) | −0.0141 (7) | 0.0017 (7) |
| C21 | 0.0567 (11) | 0.0488 (12) | 0.0544 (11) | −0.0226 (9) | −0.0135 (9) | 0.0064 (9) |
| C22 | 0.0649 (13) | 0.0680 (16) | 0.0582 (12) | −0.0289 (12) | 0.0008 (10) | −0.0070 (11) |
| C23 | 0.0548 (13) | 0.0591 (15) | 0.0837 (17) | −0.0167 (11) | −0.0018 (11) | −0.0162 (12) |
| C24 | 0.0520 (12) | 0.0388 (12) | 0.0912 (17) | −0.0103 (9) | −0.0188 (11) | −0.0012 (11) |
| C25 | 0.0467 (10) | 0.0377 (10) | 0.0603 (11) | −0.0193 (8) | −0.0165 (8) | 0.0055 (8) |
| C26 | 0.0707 (14) | 0.0456 (12) | 0.0670 (13) | −0.0274 (10) | −0.0292 (11) | 0.0166 (10) |
| C27 | 0.0900 (17) | 0.0613 (15) | 0.0494 (11) | −0.0433 (13) | −0.0216 (11) | 0.0061 (10) |
| C28 | 0.144 (3) | 0.096 (2) | 0.0536 (14) | −0.060 (2) | −0.0243 (16) | 0.0117 (15) |
| C29 | 0.201 (4) | 0.131 (4) | 0.0437 (14) | −0.086 (3) | 0.003 (2) | −0.0071 (18) |
| C30 | 0.177 (4) | 0.118 (3) | 0.073 (2) | −0.070 (3) | 0.036 (2) | −0.038 (2) |
| C31 | 0.106 (2) | 0.0741 (19) | 0.0757 (17) | −0.0322 (16) | 0.0162 (15) | −0.0268 (14) |
| C32 | 0.0733 (14) | 0.0493 (13) | 0.0544 (11) | −0.0314 (11) | −0.0076 (10) | −0.0090 (9) |
| C33 | 0.0879 (18) | 0.0706 (18) | 0.0672 (15) | −0.0211 (14) | −0.0297 (13) | 0.0142 (12) |
| C34 | 0.0529 (12) | 0.0675 (16) | 0.0729 (15) | −0.0059 (11) | −0.0001 (10) | −0.0059 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Al1—O1 | 1.8396 (13) | C16—H16B | 0.9600 |
| Al1—O2 | 1.8560 (14) | C16—H16C | 0.9600 |
| Al1—C16 | 1.943 (3) | C17—H17A | 0.9600 |
| Al1—C17 | 1.949 (2) | C17—H17B | 0.9600 |
| Al1—Al2 | 2.8236 (8) | C17—H17C | 0.9600 |
| Al2—O2 | 1.8384 (14) | C18—C19 | 1.501 (3) |
| Al2—O1 | 1.8473 (14) | C18—H18A | 0.9700 |
| Al2—C33 | 1.946 (2) | C18—H18B | 0.9700 |
| Al2—C34 | 1.956 (2) | C19—C20 | 1.406 (3) |
| O1—C1 | 1.424 (2) | C19—C32 | 1.424 (3) |
| O2—C18 | 1.427 (2) | C20—C25 | 1.428 (3) |
| C1—C2 | 1.512 (3) | C20—C21 | 1.439 (3) |
| C1—H1A | 0.9700 | C21—C22 | 1.359 (3) |
| C1—H1B | 0.9700 | C21—H21A | 0.9300 |
| C2—C15 | 1.403 (3) | C22—C23 | 1.395 (4) |
| C2—C3 | 1.407 (3) | C22—H22A | 0.9300 |
| C3—C8 | 1.429 (3) | C23—C24 | 1.342 (3) |
| C3—C4 | 1.433 (4) | C23—H23A | 0.9300 |
| C4—C5 | 1.369 (5) | C24—C25 | 1.419 (3) |
| C4—H4A | 0.9300 | C24—H24A | 0.9300 |
| C5—C6 | 1.400 (6) | C25—C26 | 1.389 (3) |
| C5—H5A | 0.9300 | C26—C27 | 1.387 (4) |
| C6—C7 | 1.360 (6) | C26—H26A | 0.9300 |
| C6—H6A | 0.9300 | C27—C32 | 1.422 (4) |
| C7—C8 | 1.423 (4) | C27—C28 | 1.435 (3) |
| C7—H7A | 0.9300 | C28—C29 | 1.345 (5) |
| C8—C9 | 1.373 (4) | C28—H28A | 0.9300 |
| C9—C10 | 1.387 (3) | C29—C30 | 1.382 (6) |
| C9—H9A | 0.9300 | C29—H29A | 0.9300 |
| C10—C11 | 1.414 (3) | C30—C31 | 1.362 (4) |
| C10—C15 | 1.434 (3) | C30—H30A | 0.9300 |
| C11—C12 | 1.333 (4) | C31—C32 | 1.414 (3) |
| C11—H11A | 0.9300 | C31—H31A | 0.9300 |
| C12—C13 | 1.396 (4) | C33—H33A | 0.9600 |
| C12—H12A | 0.9300 | C33—H33B | 0.9600 |
| C13—C14 | 1.353 (4) | C33—H33C | 0.9600 |
| C13—H13A | 0.9300 | C34—H34A | 0.9600 |
| C14—C15 | 1.437 (3) | C34—H34B | 0.9600 |
| C14—H14A | 0.9300 | C34—H34C | 0.9600 |
| C16—H16A | 0.9600 | | |
| | | | |
| O1—Al1—O2 | 79.89 (6) | C10—C15—C14 | 115.7 (2) |
| O1—Al1—C16 | 113.50 (10) | Al1—C16—H16A | 109.5 |
| O2—Al1—C16 | 110.32 (9) | Al1—C16—H16B | 109.5 |
| O1—Al1—C17 | 114.72 (10) | H16A—C16—H16B | 109.5 |
| O2—Al1—C17 | 110.62 (10) | Al1—C16—H16C | 109.5 |

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| C16—Al1—C17 | 120.46 (13) | H16A—C16—H16C | 109.5 |
| O1—Al1—Al2 | 40.12 (4) | H16B—C16—H16C | 109.5 |
| O2—Al1—Al2 | 39.93 (4) | Al1—C17—H17A | 109.5 |
| C16—Al1—Al2 | 116.40 (9) | Al1—C17—H17B | 109.5 |
| C17—Al1—Al2 | 122.85 (9) | H17A—C17—H17B | 109.5 |
| O2—Al2—O1 | 80.15 (6) | Al1—C17—H17C | 109.5 |
| O2—Al2—C33 | 115.53 (10) | H17A—C17—H17C | 109.5 |
| O1—Al2—C33 | 111.86 (10) | H17B—C17—H17C | 109.5 |
| O2—Al2—C34 | 112.98 (9) | O2—C18—C19 | 112.21 (16) |
| O1—Al2—C34 | 109.75 (9) | O2—C18—H18A | 109.2 |
| C33—Al2—C34 | 119.67 (12) | C19—C18—H18A | 109.2 |
| O2—Al2—Al1 | 40.39 (4) | O2—C18—H18B | 109.2 |
| O1—Al2—Al1 | 39.92 (4) | C19—C18—H18B | 109.2 |
| C33—Al2—Al1 | 124.36 (9) | H18A—C18—H18B | 107.9 |
| C34—Al2—Al1 | 115.69 (8) | C20—C19—C32 | 119.69 (19) |
| C1—O1—Al1 | 132.01 (11) | C20—C19—C18 | 121.31 (18) |
| C1—O1—Al2 | 127.49 (11) | C32—C19—C18 | 118.98 (19) |
| Al1—O1—Al2 | 99.97 (6) | C19—C20—C25 | 120.19 (18) |
| C18—O2—Al2 | 134.10 (12) | C19—C20—C21 | 123.53 (19) |
| C18—O2—Al1 | 125.88 (11) | C25—C20—C21 | 116.28 (18) |
| Al2—O2—Al1 | 99.69 (6) | C22—C21—C20 | 120.8 (2) |
| O1—C1—C2 | 111.61 (15) | C22—C21—H21A | 119.6 |
| O1—C1—H1A | 109.3 | C20—C21—H21A | 119.6 |
| C2—C1—H1A | 109.3 | C21—C22—C23 | 122.0 (2) |
| O1—C1—H1B | 109.3 | C21—C22—H22A | 119.0 |
| C2—C1—H1B | 109.3 | C23—C22—H22A | 119.0 |
| H1A—C1—H1B | 108.0 | C24—C23—C22 | 119.4 (2) |
| C15—C2—C3 | 120.10 (19) | C24—C23—H23A | 120.3 |
| C15—C2—C1 | 119.84 (19) | C22—C23—H23A | 120.3 |
| C3—C2—C1 | 120.1 (2) | C23—C24—C25 | 121.5 (2) |
| C2—C3—C8 | 119.2 (2) | C23—C24—H24A | 119.2 |
| C2—C3—C4 | 122.0 (2) | C25—C24—H24A | 119.2 |
| C8—C3—C4 | 118.8 (2) | C26—C25—C24 | 120.9 (2) |
| C5—C4—C3 | 119.8 (4) | C26—C25—C20 | 119.19 (19) |
| C5—C4—H4A | 120.1 | C24—C25—C20 | 119.94 (19) |
| C3—C4—H4A | 120.1 | C27—C26—C25 | 121.6 (2) |
| C4—C5—C6 | 120.7 (4) | C27—C26—H26A | 119.2 |
| C4—C5—H5A | 119.7 | C25—C26—H26A | 119.2 |
| C6—C5—H5A | 119.7 | C26—C27—C32 | 120.1 (2) |
| C7—C6—C5 | 121.6 (3) | C26—C27—C28 | 121.7 (3) |
| C7—C6—H6A | 119.2 | C32—C27—C28 | 118.2 (3) |
| C5—C6—H6A | 119.2 | C29—C28—C27 | 120.4 (3) |
| C6—C7—C8 | 119.9 (4) | C29—C28—H28A | 119.8 |
| C6—C7—H7A | 120.1 | C27—C28—H28A | 119.8 |
| C8—C7—H7A | 120.1 | C28—C29—C30 | 121.2 (3) |
| C9—C8—C7 | 121.3 (3) | C28—C29—H29A | 119.4 |
| C9—C8—C3 | 119.6 (2) | C30—C29—H29A | 119.4 |
| C7—C8—C3 | 119.1 (3) | C31—C30—C29 | 120.9 (3) |

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| C8—C9—C10 | 122.7 (2) | C31—C30—H30A | 119.6 |
| C8—C9—H9A | 118.7 | C29—C30—H30A | 119.6 |
| C10—C9—H9A | 118.7 | C30—C31—C32 | 120.6 (3) |
| C9—C10—C11 | 121.7 (2) | C30—C31—H31A | 119.7 |
| C9—C10—C15 | 118.2 (2) | C32—C31—H31A | 119.7 |
| C11—C10—C15 | 120.1 (2) | C31—C32—C27 | 118.7 (2) |
| C12—C11—C10 | 121.5 (3) | C31—C32—C19 | 122.2 (2) |
| C12—C11—H11A | 119.2 | C27—C32—C19 | 119.2 (2) |
| C10—C11—H11A | 119.2 | Al2—C33—H33A | 109.5 |
| C11—C12—C13 | 119.7 (2) | Al2—C33—H33B | 109.5 |
| C11—C12—H12A | 120.2 | H33A—C33—H33B | 109.5 |
| C13—C12—H12A | 120.2 | Al2—C33—H33C | 109.5 |
| C14—C13—C12 | 121.7 (3) | H33A—C33—H33C | 109.5 |
| C14—C13—H13A | 119.1 | H33B—C33—H33C | 109.5 |
| C12—C13—H13A | 119.1 | Al2—C34—H34A | 109.5 |
| C13—C14—C15 | 121.3 (2) | Al2—C34—H34B | 109.5 |
| C13—C14—H14A | 119.4 | H34A—C34—H34B | 109.5 |
| C15—C14—H14A | 119.4 | Al2—C34—H34C | 109.5 |
| C2—C15—C10 | 120.14 (19) | H34A—C34—H34C | 109.5 |
| C2—C15—C14 | 124.20 (19) | H34B—C34—H34C | 109.5 |

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| O1—Al1—Al2—O2 | −173.54 (10) | C2—C3—C8—C7 | −178.3 (2) |
| C16—Al1—Al2—O2 | 90.62 (12) | C4—C3—C8—C7 | 0.3 (3) |
| C17—Al1—Al2—O2 | −83.19 (12) | C7—C8—C9—C10 | 178.0 (2) |
| O2—Al1—Al2—O1 | 173.54 (10) | C3—C8—C9—C10 | −2.1 (3) |
| C16—Al1—Al2—O1 | −95.83 (12) | C8—C9—C10—C11 | −179.3 (2) |
| C17—Al1—Al2—O1 | 90.35 (12) | C8—C9—C10—C15 | 0.2 (3) |
| O1—Al1—Al2—C33 | −83.44 (12) | C9—C10—C11—C12 | 177.5 (2) |
| O2—Al1—Al2—C33 | 90.10 (12) | C15—C10—C11—C12 | −2.0 (3) |
| C16—Al1—Al2—C33 | −179.27 (12) | C10—C11—C12—C13 | 1.0 (4) |
| C17—Al1—Al2—C33 | 6.91 (14) | C11—C12—C13—C14 | 0.4 (4) |
| O1—Al1—Al2—C34 | 90.53 (11) | C12—C13—C14—C15 | −0.8 (3) |
| O2—Al1—Al2—C34 | −95.92 (12) | C3—C2—C15—C10 | −2.2 (3) |
| C16—Al1—Al2—C34 | −5.30 (13) | C1—C2—C15—C10 | 177.45 (16) |
| C17—Al1—Al2—C34 | −179.11 (12) | C3—C2—C15—C14 | 177.77 (17) |
| O2—Al1—O1—C1 | −176.03 (18) | C1—C2—C15—C14 | −2.6 (3) |
| C16—Al1—O1—C1 | −68.15 (19) | C9—C10—C15—C2 | 2.0 (3) |
| C17—Al1—O1—C1 | 75.81 (19) | C11—C10—C15—C2 | −178.52 (18) |
| Al2—Al1—O1—C1 | −171.8 (2) | C9—C10—C15—C14 | −177.99 (17) |
| O2—Al1—O1—Al2 | −4.20 (6) | C11—C10—C15—C14 | 1.5 (3) |
| C16—Al1—O1—Al2 | 103.68 (10) | C13—C14—C15—C2 | 179.87 (19) |
| C17—Al1—O1—Al2 | −112.36 (10) | C13—C14—C15—C10 | −0.2 (3) |
| O2—Al2—O1—C1 | 176.59 (17) | Al2—O2—C18—C19 | −26.6 (3) |
| C33—Al2—O1—C1 | −69.73 (19) | Al1—O2—C18—C19 | 161.38 (14) |
| C34—Al2—O1—C1 | 65.57 (18) | O2—C18—C19—C20 | 105.0 (2) |
| Al1—Al2—O1—C1 | 172.35 (19) | O2—C18—C19—C32 | −76.5 (2) |
| O2—Al2—O1—Al1 | 4.24 (6) | C32—C19—C20—C25 | −0.9 (3) |
| C33—Al2—O1—Al1 | 117.92 (11) | C18—C19—C20—C25 | 177.62 (16) |

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| C34—Al2—O1—Al1 | −106.78 (10) | C32—C19—C20—C21 | −179.83 (17) |
| O1—Al2—O2—C18 | −177.66 (19) | C18—C19—C20—C21 | −1.3 (3) |
| C33—Al2—O2—C18 | 72.7 (2) | C19—C20—C21—C22 | 176.45 (18) |
| C34—Al2—O2—C18 | −70.3 (2) | C25—C20—C21—C22 | −2.5 (3) |
| Al1—Al2—O2—C18 | −173.5 (2) | C20—C21—C22—C23 | 1.1 (3) |
| O1—Al2—O2—Al1 | −4.20 (6) | C21—C22—C23—C24 | 1.0 (3) |
| C33—Al2—O2—Al1 | −113.83 (11) | C22—C23—C24—C25 | −1.6 (3) |
| C34—Al2—O2—Al1 | 103.19 (10) | C23—C24—C25—C26 | −179.6 (2) |
| O1—Al1—O2—C18 | 178.43 (17) | C23—C24—C25—C20 | 0.0 (3) |
| C16—Al1—O2—C18 | 66.97 (19) | C19—C20—C25—C26 | 2.6 (3) |
| C17—Al1—O2—C18 | −68.82 (18) | C21—C20—C25—C26 | −178.35 (16) |
| Al2—Al1—O2—C18 | 174.21 (19) | C19—C20—C25—C24 | −177.04 (16) |
| O1—Al1—O2—Al2 | 4.22 (6) | C21—C20—C25—C24 | 2.0 (3) |
| C16—Al1—O2—Al2 | −107.24 (11) | C24—C25—C26—C27 | 177.8 (2) |
| C17—Al1—O2—Al2 | 116.97 (10) | C20—C25—C26—C27 | −1.9 (3) |
| Al1—O1—C1—C2 | −27.9 (3) | C25—C26—C27—C32 | −0.6 (3) |
| Al2—O1—C1—C2 | 162.27 (14) | C25—C26—C27—C28 | −179.2 (2) |
| O1—C1—C2—C15 | 100.4 (2) | C26—C27—C28—C29 | 176.7 (3) |
| O1—C1—C2—C3 | −79.9 (2) | C32—C27—C28—C29 | −2.0 (4) |
| C15—C2—C3—C8 | 0.3 (3) | C27—C28—C29—C30 | 1.1 (6) |
| C1—C2—C3—C8 | −179.36 (18) | C28—C29—C30—C31 | 0.5 (6) |
| C15—C2—C3—C4 | −178.3 (2) | C29—C30—C31—C32 | −1.2 (5) |
| C1—C2—C3—C4 | 2.1 (3) | C30—C31—C32—C27 | 0.3 (4) |
| C2—C3—C4—C5 | 178.5 (3) | C30—C31—C32—C19 | −179.4 (3) |
| C8—C3—C4—C5 | 0.0 (4) | C26—C27—C32—C31 | −177.4 (2) |
| C3—C4—C5—C6 | 0.8 (6) | C28—C27—C32—C31 | 1.3 (3) |
| C4—C5—C6—C7 | −1.9 (7) | C26—C27—C32—C19 | 2.3 (3) |
| C5—C6—C7—C8 | 2.3 (6) | C28—C27—C32—C19 | −179.02 (19) |
| C6—C7—C8—C9 | 178.5 (3) | C20—C19—C32—C31 | 178.1 (2) |
| C6—C7—C8—C3 | −1.4 (5) | C18—C19—C32—C31 | −0.4 (3) |
| C2—C3—C8—C9 | 1.8 (3) | C20—C19—C32—C27 | −1.6 (3) |
| C4—C3—C8—C9 | −179.6 (2) | C18—C19—C32—C27 | 179.90 (18) |