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Hexa-μ_2-isopropoxido-$\kappa^{12}O$:O-hexa-isopropoxidotetraaluminium(III)

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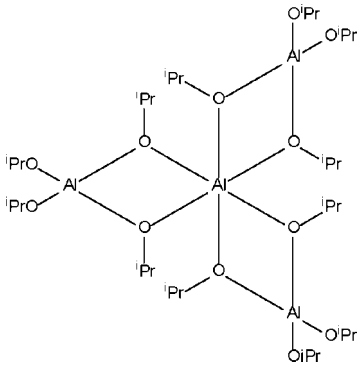
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.098; data-to-parameter ratio = 27.3.

In the tetranuclear title compound, $[Al_4(C_3H_7O)_{12}]$, one Al atom is six-coordinate, with an octahedral coordination geometry, whereas the other three are four-coordinate with tetrahedral geometries. Two of the three symmetry-independent Al atoms lie on special positions of site symmetry 2.

Related literature

The crystal structure of the title compound was first described in the enantiomorphic space group $P4_12_12$ [Amma (1963); see Folting *et al.* (1991), Turova *et al.* (1979) and Turova *et al.* (1978) for later reports]. For a comment on the occurrence of compounds crystallizing in pairs of enantiomorphic space groups, see Ng (2007).



Experimental

Crystal data

$[Al_4(C_3H_7O)_{12}]$
M_r = 816.95
Tetragonal, $P4_32_12$
a = 12.331 (2) Å
c = 31.641 (6) Å
V = 4811.1 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 293 (2) K
0.50 × 0.50 × 0.45 mm

Data collection

Stoe IPDS-II imaging-plate diffractometer
Absorption correction: analytical (*X-SHAPE*; Stoe & Cie, 2003)
T_{min} = 0.937, T_{max} = 0.955
15084 measured reflections
6434 independent reflections
5960 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.098
S = 1.05
6434 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 2626 Friedel pairs
Flack parameter: 0.0 (1)

Data collection: *X-RED32* (Stoe & Cie, 2001); cell refinement: *X-AREA* (Stoe & Cie, 2005); data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2066).

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supplementary materials

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Hexa-μ_2-isopropoxido-$\kappa^{12}O$:O-hexaisopropoxidotetraaluminium(III)

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Comment

Some achiral metal-organic compounds crystallize in one of the eleven pairs of enantiomorphic space groups; however, examples of the same compound belonging to one of each pair are rare. There is a short comment on such examples (Ng, 2007).

Experimental

The aluminium isopropoxide was an unexpected product from reaction of trimethyl aluminium (0.72 g, 0.01 mmol; 5 ml of 2*M* solution in toluene) and 1-methoxy-2-propanol (0.1 mol, 7.2 g, 10 ml). The solid obtained after removing the excess 1-methoxy-2-propanol under reduced pressure was recrystallized from mixture of hexane and dichloromethane (1:1).

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.96 – 0.98 Å), and were included in refinement in the riding model approximation, with U(H) set to 1.2 to 1.5 times U_{eq}(C).

Figures

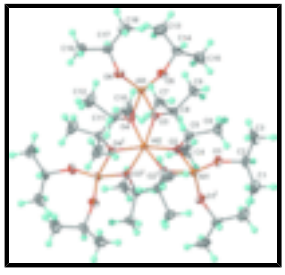


Fig. 1. **Figure 1**. Thermal ellipsoid plot of $[(C_3H_7O)_3Al]_4$. Displacement ellipsoids are drawn at the 50% probablity level, and H atoms are drawn as spheres of arbitrary radii. Symmetry codes are given in Table 1.

Hexa-μ$_2$-isopropoxido-κ^{12}O:O- hexaisopropoxidotetraaluminium(III)

Crystal data

$[Al_4(C_3H_7O)_{12}]$	$Z = 4$
$M_r = 816.95$	$F_{000} = 1792$
Tetragonal, $P4_32_12$	$D_x = 1.128$ Mg m^{-3}
Hall symbol: P 4nw 2abw	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.331$ (2) Å	Cell parameters from 5826 reflections
$b = 12.331$ (2) Å	$\theta = 1.8$–29.2°

c = 31.641 (6) Å	μ = 0.15 mm^{-1}
α = 90º	T = 293 (2) K
β = 90º	Irregular block, colorless
γ = 90º	0.50 × 0.50 × 0.45 mm
V = 4811.1 (14) Å^3	

Data collection

Stoe IPDS-II imaging-plate diffractometer	6434 independent reflections
Radiation source: medium-focus sealed tube	5960 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 29.2º
Rotation method scans	θ_{min} = 1.8º
Absorption correction: Analytical (X-SHAPE; Stoe & Cie, 2003)	h = −16→16
T_{min} = 0.937, T_{max} = 0.955	k = −5→16
15084 measured reflections	l = −35→43

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 1.3524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.098	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
6434 reflections	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
236 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (Flack, 1983), 2626 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.0 (1)

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

	x	y	z	U_{iso}*/U_{eq}
Al1	0.20008 (4)	1.20008 (4)	0.0000	0.02227 (13)
Al2	0.03496 (4)	1.03496 (4)	0.0000	0.01840 (12)
Al3	0.02619 (4)	0.88003 (4)	0.067181 (14)	0.02167 (10)
O1	0.33153 (10)	1.16747 (11)	0.01112 (4)	0.0313 (3)
O2	0.09447 (9)	1.15025 (9)	0.03410 (3)	0.0212 (2)
O3	0.12112 (9)	0.92722 (9)	0.02795 (3)	0.0206 (2)
O4	−0.06114 (9)	0.97909 (9)	0.04264 (3)	0.0213 (2)
O5	0.04236 (11)	0.91991 (11)	0.11805 (4)	0.0333 (3)
O6	0.00240 (11)	0.74607 (10)	0.05657 (4)	0.0314 (3)
C1	0.48650 (17)	1.27513 (19)	−0.00848 (7)	0.0456 (5)
H1A	0.4402	1.3279	−0.0216	0.068*

H1B	0.5086	1.2225	−0.0291	0.068*
H1C	0.5494	1.3106	0.0029	0.068*
C2	0.42514 (14)	1.21869 (15)	0.02697 (6)	0.0319 (4)
H2	0.4033	1.2731	0.0479	0.038*
C3	0.49532 (18)	1.1342 (2)	0.04860 (8)	0.0488 (5)
H3A	0.4546	1.0999	0.0707	0.073*
H3B	0.5583	1.1685	0.0604	0.073*
H3C	0.5175	1.0806	0.0283	0.073*
C4	0.00339 (18)	1.28344 (18)	0.07859 (6)	0.0395 (4)
H4A	−0.0648	1.2659	0.0656	0.059*
H4B	0.0369	1.3420	0.0635	0.059*
H4C	−0.0085	1.3048	0.1074	0.059*
C5	0.07732 (14)	1.18432 (14)	0.07744 (5)	0.0254 (3)
H5	0.0430	1.1251	0.0932	0.031*
C6	0.18536 (16)	1.21142 (16)	0.09791 (6)	0.0346 (4)
H6A	0.2316	1.1488	0.0972	0.052*
H6B	0.1736	1.2328	0.1267	0.052*
H6C	0.2192	1.2698	0.0828	0.052*
C7	0.25561 (15)	0.79397 (15)	0.00599 (6)	0.0322 (4)
H7A	0.2264	0.7945	−0.0221	0.048*
H7B	0.2204	0.7385	0.0223	0.048*
H7C	0.3321	0.7796	0.0048	0.048*
C8	0.23637 (13)	0.90413 (14)	0.02667 (5)	0.0248 (3)
H8	0.2729	0.9603	0.0100	0.030*
C9	0.28248 (15)	0.90408 (17)	0.07120 (6)	0.0341 (4)
H9A	0.2702	0.9736	0.0840	0.051*
H9B	0.3590	0.8898	0.0701	0.051*
H9C	0.2474	0.8488	0.0876	0.051*
C10	−0.19215 (17)	1.0540 (2)	0.09220 (7)	0.0432 (5)
H10A	−0.1545	1.1221	0.0911	0.065*
H10B	−0.1642	1.0113	0.1151	0.065*
H10C	−0.2681	1.0668	0.0965	0.065*
C11	−0.17585 (13)	0.99427 (14)	0.05127 (5)	0.0259 (3)
H11	−0.2068	1.0382	0.0284	0.031*
C12	−0.23402 (17)	0.88716 (19)	0.05205 (7)	0.0443 (5)
H12A	−0.2225	0.8501	0.0257	0.066*
H12B	−0.3102	0.8992	0.0561	0.066*
H12C	−0.2064	0.8437	0.0748	0.066*
C13	0.0016 (2)	0.8282 (2)	0.18290 (7)	0.0537 (6)
H13A	−0.0136	0.7621	0.1680	0.081*
H13B	−0.0641	0.8690	0.1862	0.081*
H13C	0.0309	0.8114	0.2102	0.081*
C14	0.08284 (16)	0.89431 (16)	0.15819 (5)	0.0315 (4)
H14	0.1498	0.8523	0.1550	0.038*
C15	0.1084 (2)	0.99959 (18)	0.18109 (6)	0.0459 (5)
H15A	0.1598	1.0407	0.1649	0.069*
H15B	0.1386	0.9836	0.2084	0.069*
H15C	0.0430	1.0409	0.1845	0.069*
C16	−0.0992 (2)	0.58198 (18)	0.05267 (8)	0.0489 (5)

H16A	−0.1571	0.6202	0.0389	0.073*
H16B	−0.1287	0.5242	0.0694	0.073*
H16C	−0.0510	0.5525	0.0318	0.073*
C17	−0.03744 (16)	0.65919 (14)	0.08080 (6)	0.0314 (4)
H17	−0.0874	0.6881	0.1021	0.038*
C18	0.05522 (19)	0.60221 (18)	0.10331 (7)	0.0442 (5)
H18A	0.0930	0.6532	0.1209	0.066*
H18B	0.1044	0.5727	0.0828	0.066*
H18C	0.0268	0.5447	0.1205	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.02132 (19)	0.02132 (19)	0.0242 (3)	−0.0026 (2)	−0.00022 (18)	0.00022 (18)
Al2	0.01869 (17)	0.01869 (17)	0.0178 (3)	0.0004 (2)	−0.00008 (16)	0.00008 (16)
Al3	0.0245 (2)	0.0214 (2)	0.01904 (19)	0.00060 (17)	0.00050 (17)	0.00200 (16)
O1	0.0229 (6)	0.0323 (6)	0.0386 (7)	−0.0037 (5)	−0.0041 (5)	−0.0029 (5)
O2	0.0237 (5)	0.0206 (5)	0.0193 (5)	−0.0019 (4)	0.0000 (4)	−0.0022 (4)
O3	0.0198 (5)	0.0209 (5)	0.0213 (5)	0.0022 (4)	−0.0011 (4)	0.0016 (4)
O4	0.0204 (5)	0.0225 (5)	0.0209 (5)	0.0007 (4)	0.0025 (4)	0.0013 (4)
O5	0.0397 (7)	0.0402 (7)	0.0201 (5)	0.0037 (6)	−0.0025 (5)	0.0009 (5)
O6	0.0410 (7)	0.0237 (6)	0.0295 (6)	−0.0027 (5)	0.0033 (5)	0.0044 (5)
C1	0.0304 (10)	0.0500 (12)	0.0562 (12)	−0.0068 (8)	0.0108 (9)	−0.0115 (10)
C2	0.0215 (8)	0.0356 (9)	0.0384 (9)	−0.0017 (7)	−0.0023 (7)	−0.0119 (7)
C3	0.0353 (11)	0.0579 (14)	0.0533 (12)	0.0062 (10)	−0.0174 (9)	−0.0117 (11)
C4	0.0455 (11)	0.0412 (10)	0.0319 (9)	0.0118 (9)	0.0003 (8)	−0.0096 (8)
C5	0.0306 (8)	0.0250 (8)	0.0208 (6)	−0.0008 (6)	0.0015 (6)	−0.0030 (6)
C6	0.0366 (10)	0.0387 (10)	0.0285 (8)	−0.0056 (8)	−0.0045 (7)	−0.0086 (7)
C7	0.0305 (9)	0.0298 (9)	0.0364 (9)	0.0072 (7)	0.0019 (7)	−0.0021 (7)
C8	0.0206 (7)	0.0262 (8)	0.0275 (7)	0.0027 (6)	−0.0006 (6)	0.0025 (6)
C9	0.0282 (9)	0.0410 (10)	0.0330 (8)	0.0067 (7)	−0.0070 (7)	−0.0021 (7)
C10	0.0310 (10)	0.0516 (13)	0.0471 (11)	−0.0002 (8)	0.0100 (8)	−0.0193 (9)
C11	0.0194 (7)	0.0303 (8)	0.0279 (7)	0.0029 (6)	0.0030 (6)	0.0045 (6)
C12	0.0323 (10)	0.0462 (12)	0.0545 (12)	−0.0112 (9)	0.0162 (9)	−0.0144 (10)
C13	0.0759 (17)	0.0562 (14)	0.0289 (9)	−0.0167 (12)	0.0121 (10)	0.0010 (9)
C14	0.0403 (10)	0.0345 (9)	0.0197 (7)	0.0013 (7)	−0.0013 (7)	0.0020 (6)
C15	0.0611 (14)	0.0456 (11)	0.0311 (8)	−0.0035 (10)	−0.0083 (9)	−0.0058 (8)
C16	0.0571 (14)	0.0316 (10)	0.0581 (13)	−0.0116 (10)	−0.0023 (11)	0.0011 (10)
C17	0.0388 (10)	0.0233 (8)	0.0319 (8)	−0.0007 (7)	0.0063 (7)	0.0046 (6)
C18	0.0532 (13)	0.0340 (10)	0.0454 (11)	0.0064 (9)	0.0025 (10)	0.0110 (9)

Geometric parameters (Å, °)

Al1—O1^{i}	1.7066 (13)	C6—H6B	0.9600
Al1—O1	1.7066 (13)	C6—H6C	0.9600
Al1—O2	1.7994 (12)	C7—C8	1.526 (2)
Al1—O2^{i}	1.7994 (12)	C7—H7A	0.9600
Al1—Al2	2.8794 (9)	C7—H7B	0.9600

Al2—O3^{i}	1.9172 (11)	C7—H7C	0.9600
Al2—O3	1.9172 (11)	C8—C9	1.519 (2)
Al2—O4	1.9234 (11)	C8—H8	0.9800
Al2—O4^{i}	1.9234 (11)	C9—H9A	0.9600
Al2—O2	1.9297 (12)	C9—H9B	0.9600
Al2—O2^{i}	1.9297 (12)	C9—H9C	0.9600
Al2—Al3^{i}	2.8601 (7)	C10—C11	1.503 (2)
Al2—Al3	2.8601 (6)	C10—H10A	0.9600
Al3—O5	1.6946 (13)	C10—H10B	0.9600
Al3—O6	1.7110 (14)	C10—H10C	0.9600
Al3—O4	1.8039 (12)	C11—C12	1.503 (3)
Al3—O3	1.8027 (12)	C11—H11	0.9800
O1—C2	1.408 (2)	C12—H12A	0.9600
O2—C5	1.4496 (18)	C12—H12B	0.9600
O3—C8	1.4499 (19)	C12—H12C	0.9600
O4—C11	1.4527 (19)	C13—C14	1.509 (3)
O5—C14	1.4007 (19)	C13—H13A	0.9600
O6—C17	1.406 (2)	C13—H13B	0.9600
C1—C2	1.522 (3)	C13—H13C	0.9600
C1—H1A	0.9600	C14—C15	1.520 (3)
C1—H1B	0.9600	C14—H14	0.9800
C1—H1C	0.9600	C15—H15A	0.9600
C2—C3	1.518 (3)	C15—H15B	0.9600
C2—H2	0.9800	C15—H15C	0.9600
C3—H3A	0.9600	C16—C17	1.509 (3)
C3—H3B	0.9600	C16—H16A	0.9600
C3—H3C	0.9600	C16—H16B	0.9600
C4—C5	1.525 (3)	C16—H16C	0.9600
C4—H4A	0.9600	C17—C18	1.519 (3)
C4—H4B	0.9600	C17—H17	0.9800
C4—H4C	0.9600	C18—H18A	0.9600
C5—C6	1.519 (2)	C18—H18B	0.9600
C5—H5	0.9800	C18—H18C	0.9600
C6—H6A	0.9600		
O1^{i}—Al1—O1	119.34 (9)	H4A—C4—H4B	109.5
O1^{i}—Al1—O2	106.11 (6)	C5—C4—H4C	109.5
O1—Al1—O2	118.89 (6)	H4A—C4—H4C	109.5
O1^{i}—Al1—O2^{i}	118.89 (6)	H4B—C4—H4C	109.5
O1—Al1—O2^{i}	106.11 (6)	O2—C5—C6	109.83 (14)
O2—Al1—O2^{i}	82.26 (7)	O2—C5—C4	110.00 (14)
O1^{i}—Al1—Al2	120.33 (5)	C6—C5—C4	109.74 (15)
O1—Al1—Al2	120.33 (5)	O2—C5—H5	109.1
O2—Al1—Al2	41.13 (4)	C6—C5—H5	109.1
O2^{i}—Al1—Al2	41.13 (4)	C4—C5—H5	109.1
O3^{i}—Al2—O3	168.73 (8)	C5—C6—H6A	109.5
O3^{i}—Al2—O4	95.46 (5)	C5—C6—H6B	109.5

O3—Al2—O4	76.68 (5)	H6A—C6—H6B	109.5
O3^{i}—Al2—O4^{i}	76.68 (5)	C5—C6—H6C	109.5
O3—Al2—O4^{i}	95.46 (5)	H6A—C6—H6C	109.5
O4—Al2—O4^{i}	92.91 (7)	H6B—C6—H6C	109.5
O3^{i}—Al2—O2	96.50 (5)	C8—C7—H7A	109.5
O3—Al2—O2	92.40 (5)	C8—C7—H7B	109.5
O4—Al2—O2	96.08 (5)	H7A—C7—H7B	109.5
O4^{i}—Al2—O2	169.22 (5)	C8—C7—H7C	109.5
O3^{i}—Al2—O2^{i}	92.40 (5)	H7A—C7—H7C	109.5
O3—Al2—O2^{i}	96.50 (5)	H7B—C7—H7C	109.5
O4—Al2—O2^{i}	169.22 (5)	O3—C8—C9	109.93 (13)
O4^{i}—Al2—O2^{i}	96.08 (5)	O3—C8—C7	109.82 (14)
O2—Al2—O2^{i}	75.67 (7)	C9—C8—C7	109.82 (14)
O3^{i}—Al2—Al3^{i}	38.30 (3)	O3—C8—H8	109.1
O3—Al2—Al3^{i}	133.38 (4)	C9—C8—H8	109.1
O4—Al2—Al3^{i}	95.53 (4)	C7—C8—H8	109.1
O4^{i}—Al2—Al3^{i}	38.38 (3)	C8—C9—H9A	109.5
O2—Al2—Al3^{i}	134.23 (4)	C8—C9—H9B	109.5
O2^{i}—Al2—Al3^{i}	95.21 (4)	H9A—C9—H9B	109.5
O3^{i}—Al2—Al3	133.38 (4)	C8—C9—H9C	109.5
O3—Al2—Al3	38.30 (3)	H9A—C9—H9C	109.5
O4—Al2—Al3	38.38 (3)	H9B—C9—H9C	109.5
O4^{i}—Al2—Al3	95.53 (4)	C11—C10—H10A	109.5
O2—Al2—Al3	95.21 (3)	C11—C10—H10B	109.5
O2^{i}—Al2—Al3	134.23 (4)	H10A—C10—H10B	109.5
Al3^{i}—Al2—Al3	120.12 (3)	C11—C10—H10C	109.5
O3^{i}—Al2—Al1	95.63 (4)	H10A—C10—H10C	109.5
O3—Al2—Al1	95.63 (4)	H10B—C10—H10C	109.5
O4—Al2—Al1	133.55 (4)	O4—C11—C10	110.79 (14)
O4^{i}—Al2—Al1	133.55 (4)	O4—C11—C12	110.76 (14)
O2—Al2—Al1	37.83 (3)	C10—C11—C12	110.65 (16)
O2^{i}—Al2—Al1	37.83 (3)	O4—C11—H11	108.2
Al3^{i}—Al2—Al1	119.938 (16)	C10—C11—H11	108.2
Al3—Al2—Al1	119.938 (15)	C12—C11—H11	108.2
O5—Al3—O6	119.13 (7)	C11—C12—H12A	109.5
O5—Al3—O4	106.41 (6)	C11—C12—H12B	109.5
O6—Al3—O4	117.83 (6)	H12A—C12—H12B	109.5
O5—Al3—O3	118.94 (7)	C11—C12—H12C	109.5
O6—Al3—O3	106.72 (6)	H12A—C12—H12C	109.5
O4—Al3—O3	82.69 (5)	H12B—C12—H12C	109.5
O5—Al3—Al2	120.50 (5)	C14—C13—H13A	109.5
O6—Al3—Al2	120.36 (5)	C14—C13—H13B	109.5
O4—Al3—Al2	41.45 (4)	H13A—C13—H13B	109.5
O3—Al3—Al2	41.24 (4)	C14—C13—H13C	109.5

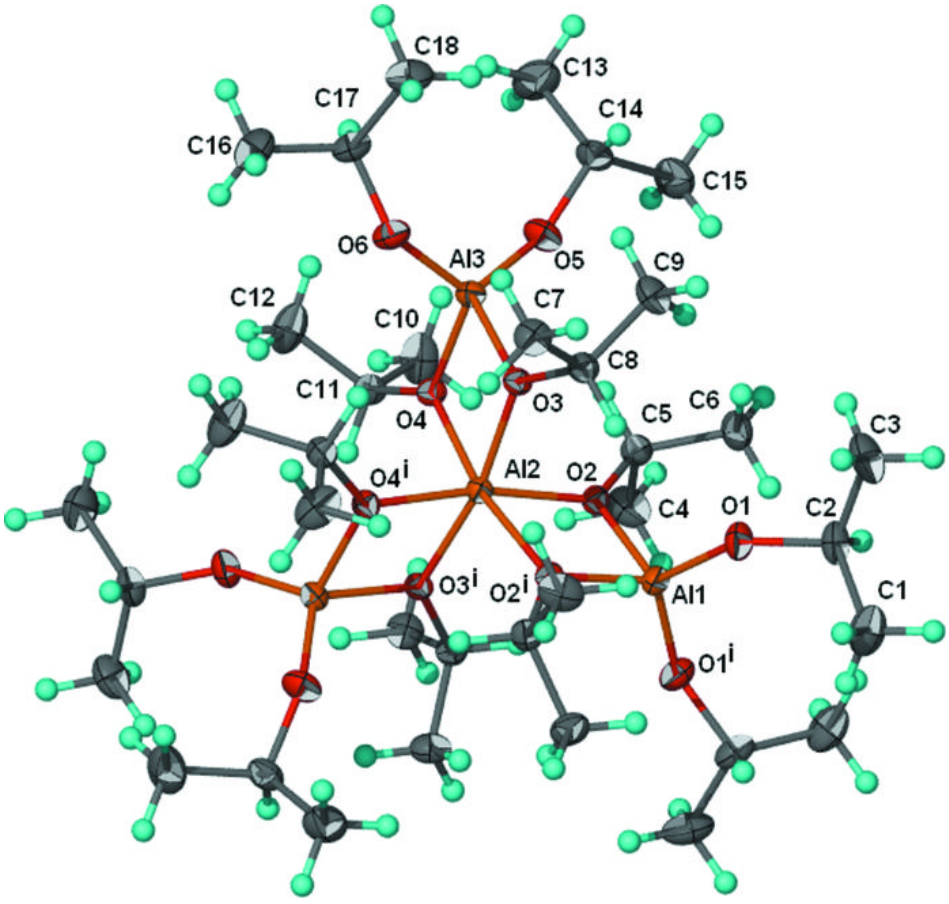
C2—O1—Al1	138.27 (12)	H13A—C13—H13C	109.5
C5—O2—Al1	125.02 (10)	H13B—C13—H13C	109.5
C5—O2—Al2	133.39 (10)	O5—C14—C13	110.79 (17)
Al1—O2—Al2	101.03 (5)	O5—C14—C15	108.29 (16)
C8—O3—Al3	126.32 (10)	C13—C14—C15	110.60 (17)
C8—O3—Al2	131.78 (10)	O5—C14—H14	109.0
Al3—O3—Al2	100.46 (6)	C13—C14—H14	109.0
C11—O4—Al3	125.99 (10)	C15—C14—H14	109.0
C11—O4—Al2	133.27 (9)	C14—C15—H15A	109.5
Al3—O4—Al2	100.18 (5)	C14—C15—H15B	109.5
C14—O5—Al3	146.90 (13)	H15A—C15—H15B	109.5
C17—O6—Al3	133.51 (12)	C14—C15—H15C	109.5
C2—C1—H1A	109.5	H15A—C15—H15C	109.5
C2—C1—H1B	109.5	H15B—C15—H15C	109.5
H1A—C1—H1B	109.5	C17—C16—H16A	109.5
C2—C1—H1C	109.5	C17—C16—H16B	109.5
H1A—C1—H1C	109.5	H16A—C16—H16B	109.5
H1B—C1—H1C	109.5	C17—C16—H16C	109.5
O1—C2—C3	108.66 (16)	H16A—C16—H16C	109.5
O1—C2—C1	110.51 (16)	H16B—C16—H16C	109.5
C3—C2—C1	111.28 (17)	O6—C17—C16	109.60 (16)
O1—C2—H2	108.8	O6—C17—C18	110.21 (16)
C3—C2—H2	108.8	C16—C17—C18	111.36 (17)
C1—C2—H2	108.8	O6—C17—H17	108.5
C2—C3—H3A	109.5	C16—C17—H17	108.5
C2—C3—H3B	109.5	C18—C17—H17	108.5
H3A—C3—H3B	109.5	C17—C18—H18A	109.5
C2—C3—H3C	109.5	C17—C18—H18B	109.5
H3A—C3—H3C	109.5	H18A—C18—H18B	109.5
H3B—C3—H3C	109.5	C17—C18—H18C	109.5
C5—C4—H4A	109.5	H18A—C18—H18C	109.5
C5—C4—H4B	109.5	H18B—C18—H18C	109.5
$O1^{i}$—Al1—Al2—$O3^{i}$	13.79 (6)	Al1—Al2—O2—C5	−171.47 (17)
O1—Al1—Al2—$O3^{i}$	−166.21 (6)	$O3^{i}$—Al2—O2—Al1	−90.82 (6)
O2—Al1—Al2—$O3^{i}$	93.36 (6)	O3—Al2—O2—Al1	96.10 (5)
$O2^{i}$—Al1—Al2—$O3^{i}$	−86.64 (6)	O4—Al2—O2—Al1	172.95 (5)
$O1^{i}$—Al1—Al2—O3	−166.21 (6)	$O4^{i}$—Al2—O2—Al1	−40.7 (3)
O1—Al1—Al2—O3	13.79 (6)	$O2^{i}$—Al2—O2—Al1	0.0
O2—Al1—Al2—O3	−86.64 (6)	$Al3^{i}$—Al2—O2—Al1	−83.23 (6)
$O2^{i}$—Al1—Al2—O3	93.36 (6)	Al3—Al2—O2—Al1	134.39 (4)
$O1^{i}$—Al1—Al2—O4	−89.25 (7)	O5—Al3—O3—C8	63.16 (14)
O1—Al1—Al2—O4	90.75 (7)	O6—Al3—O3—C8	−75.17 (13)
O2—Al1—Al2—O4	−9.69 (7)	O4—Al3—O3—C8	167.90 (12)
$O2^{i}$—Al1—Al2—O4	170.31 (7)	Al2—Al3—O3—C8	167.58 (15)
$O1^{i}$—Al1—Al2—$O4^{i}$	90.75 (7)	O5—Al3—O3—Al2	−104.43 (7)
O1—Al1—Al2—$O4^{i}$	−89.25 (7)	O6—Al3—O3—Al2	117.25 (6)

O2—Al1—Al2—O4^{i}	170.31 (7)	O4—Al3—O3—Al2	0.32 (5)
O2^{i}—Al1—Al2—O4^{i}	−9.69 (7)	O3^{i}—Al2—O3—C8	146.61 (13)
O1^{i}—Al1—Al2—O2	−79.57 (7)	O4—Al2—O3—C8	−166.87 (13)
O1—Al1—Al2—O2	100.43 (7)	O4^{i}—Al2—O3—C8	101.43 (13)
O2^{i}—Al1—Al2—O2	180.0	O2—Al2—O3—C8	−71.19 (13)
O1^{i}—Al1—Al2—O2^{i}	100.43 (7)	O2^{i}—Al2—O3—C8	4.65 (13)
O1—Al1—Al2—O2^{i}	−79.57 (7)	Al3^{i}—Al2—O3—C8	108.15 (13)
O2—Al1—Al2—O2^{i}	180.0	Al3—Al2—O3—C8	−166.57 (16)
O1^{i}—Al1—Al2—Al3^{i}	45.23 (5)	Al1—Al2—O3—C8	−33.39 (13)
O1—Al1—Al2—Al3^{i}	−134.77 (5)	O3^{i}—Al2—O3—Al3	−46.8 (2)
O2—Al1—Al2—Al3^{i}	124.80 (6)	O4—Al2—O3—Al3	−0.30 (5)
O2^{i}—Al1—Al2—Al3^{i}	−55.20 (6)	O4^{i}—Al2—O3—Al3	−92.01 (6)
O1^{i}—Al1—Al2—Al3	−134.77 (5)	O2—Al2—O3—Al3	95.38 (6)
O1—Al1—Al2—Al3	45.23 (5)	O2^{i}—Al2—O3—Al3	171.22 (5)
O2—Al1—Al2—Al3	−55.20 (6)	Al3^{i}—Al2—O3—Al3	−85.28 (6)
O2^{i}—Al1—Al2—Al3	124.80 (6)	Al1—Al2—O3—Al3	133.17 (4)
O3^{i}—Al2—Al3—O5	−90.94 (8)	O5—Al3—O4—C11	−69.86 (13)
O3—Al2—Al3—O5	100.37 (8)	O6—Al3—O4—C11	66.96 (13)
O4—Al2—Al3—O5	−80.11 (8)	O3—Al3—O4—C11	172.05 (12)
O4^{i}—Al2—Al3—O5	−167.81 (7)	Al2—Al3—O4—C11	172.37 (15)
O2—Al2—Al3—O5	13.10 (7)	O5—Al3—O4—Al2	117.77 (7)
O2^{i}—Al2—Al3—O5	88.15 (8)	O6—Al3—O4—Al2	−105.41 (7)
Al3^{i}—Al2—Al3—O5	−136.51 (6)	O3—Al3—O4—Al2	−0.32 (5)
Al1—Al2—Al3—O5	43.49 (6)	O3^{i}—Al2—O4—C11	0.60 (14)
O3^{i}—Al2—Al3—O6	88.04 (8)	O3—Al2—O4—C11	−171.21 (14)
O3—Al2—Al3—O6	−80.66 (8)	O4^{i}—Al2—O4—C11	−76.28 (13)
O4—Al2—Al3—O6	98.86 (8)	O2—Al2—O4—C11	97.76 (14)
O4^{i}—Al2—Al3—O6	11.16 (7)	O2^{i}—Al2—O4—C11	137.2 (2)
O2—Al2—Al3—O6	−167.92 (7)	Al3^{i}—Al2—O4—C11	−37.88 (13)
O2^{i}—Al2—Al3—O6	−92.88 (8)	Al3—Al2—O4—C11	−171.51 (16)
Al3^{i}—Al2—Al3—O6	42.46 (6)	Al1—Al2—O4—C11	103.72 (13)
Al1—Al2—Al3—O6	−137.54 (6)	O3^{i}—Al2—O4—Al3	172.12 (5)
O3^{i}—Al2—Al3—O4	−10.83 (7)	O3—Al2—O4—Al3	0.30 (5)
O3—Al2—Al3—O4	−179.52 (8)	O4^{i}—Al2—O4—Al3	95.23 (6)
O4^{i}—Al2—Al3—O4	−87.70 (8)	O2—Al2—O4—Al3	−90.73 (5)
O2—Al2—Al3—O4	93.21 (6)	O2^{i}—Al2—O4—Al3	−51.3 (3)
O2^{i}—Al2—Al3—O4	168.26 (8)	Al3^{i}—Al2—O4—Al3	133.63 (4)
Al3^{i}—Al2—Al3—O4	−56.40 (5)	Al1—Al2—O4—Al3	−84.77 (6)
Al1—Al2—Al3—O4	123.60 (5)	O6—Al3—O5—C14	35.9 (3)
O3^{i}—Al2—Al3—O3	168.70 (7)	O4—Al3—O5—C14	172.1 (2)
O4—Al2—Al3—O3	179.52 (8)	O3—Al3—O5—C14	−97.3 (2)
O4^{i}—Al2—Al3—O3	91.82 (6)	Al2—Al3—O5—C14	−145.1 (2)

O2—Al2—Al3—O3	−87.26 (7)	O5—Al3—O6—C17	21.18 (19)
O2^{i}—Al2—Al3—O3	−12.22 (7)	O4—Al3—O6—C17	−110.12 (16)
Al3^{i}—Al2—Al3—O3	123.12 (6)	O3—Al3—O6—C17	159.41 (16)
Al1—Al2—Al3—O3	−56.88 (6)	Al2—Al3—O6—C17	−157.81 (15)
O1^{i}—Al1—O1—C2	25.16 (16)	Al1—O1—C2—C3	152.14 (16)
O2—Al1—O1—C2	−107.20 (18)	Al1—O1—C2—C1	−85.5 (2)
O2^{i}—Al1—O1—C2	162.84 (17)	Al1—O2—C5—C6	−32.61 (18)
Al2—Al1—O1—C2	−154.84 (16)	Al2—O2—C5—C6	137.16 (13)
O1^{i}—Al1—O2—C5	−69.64 (13)	Al1—O2—C5—C4	88.28 (16)
O1—Al1—O2—C5	68.26 (13)	Al2—O2—C5—C4	−101.95 (17)
O2^{i}—Al1—O2—C5	172.44 (15)	Al3—O3—C8—C9	−37.91 (19)
Al2—Al1—O2—C5	172.44 (15)	Al2—O3—C8—C9	125.61 (13)
O1^{i}—Al1—O2—Al2	117.92 (6)	Al3—O3—C8—C7	83.03 (15)
O1—Al1—O2—Al2	−104.18 (7)	Al2—O3—C8—C7	−113.45 (14)
O2^{i}—Al1—O2—Al2	0.0	Al3—O4—C11—C10	77.18 (18)
O3^{i}—Al2—O2—C5	97.71 (14)	Al2—O4—C11—C10	−113.17 (16)
O3—Al2—O2—C5	−75.37 (14)	Al3—O4—C11—C12	−46.01 (19)
O4—Al2—O2—C5	1.48 (14)	Al2—O4—C11—C12	123.65 (15)
O4^{i}—Al2—O2—C5	147.8 (2)	Al3—O5—C14—C13	−85.5 (3)
O2^{i}—Al2—O2—C5	−171.47 (17)	Al3—O5—C14—C15	153.1 (2)
Al3^{i}—Al2—O2—C5	105.30 (13)	Al3—O6—C17—C16	148.14 (16)
Al3—Al2—O2—C5	−37.08 (14)	Al3—O6—C17—C18	−89.0 (2)

Symmetry codes: (i) *y*−1, *x*+1, −*z*.

Fig. 1


C18
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O4i
Al2
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O3i
O2i
Al1
C1
O1i