

Crystal structure and quantum-chemical calculations of a trimethylaluminium–THF adduct

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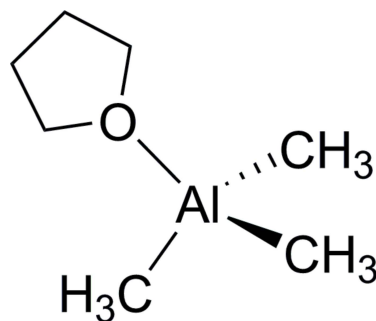
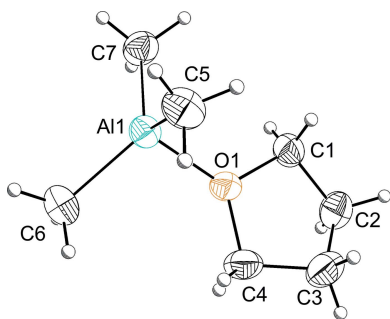
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Keywords: crystal structure; aluminium; trimethylaluminium; thf; adduct; monomer; angle.**CCDC reference:** 1588683**Supporting information:** this article has supporting information at journals.iucr.org/e

The title compound, trimethyl(tetrahydrofuran- κO)aluminium(III), $[\text{Al}(\text{CH}_3)_3(\text{C}_4\text{H}_8\text{O})]$, is an addition product of trimethylaluminium and tetrahydrofuran (THF). Instead of a dimeric structure, which is very common for these types of compounds, a monomeric molecular structure is observed. The C–Al–C angles in the molecule are very different from the C–Al–C angles found in dimeric molecular structures, leading to a different symmetry around the Al^{III} atom. The reasons for these differences are discussed.

1. Chemical context

Similar to diborane, trimethylaluminium is present as a dimer at room temperature. Analogously, two monomers are connected by two three-center–two-electron bonds bridging both molecules. The monomer of trimethylaluminium can be observed at high temperatures and low pressure with a trigonal-planar symmetry in the gas phase (Almenningen *et al.*, 1971). The most important use of trimethylaluminium is in the production of methylaluminoxane, which is used to activate the Ziegler–Natta catalysts for olefin polymerization (Andresen *et al.*, 1976). Another known and important application is in the synthesis of Tebbe's reagent, which is used for methylenation reactions in organic synthesis (Herrmann, 1982). The monomeric structure of trimethylaluminium in THF could lead to a higher reactivity of this compound in these applications. Different THF adducts of trimethylaluminium are known (Kong *et al.*, 1995; Vidyaratne *et al.*, 2009; Tanner *et al.*, 1993), but on the one hand the trimethylaluminium–THF adduct is obtained as a co-crystallate and on the other it is part of a calcium sandwich complex. Many ether adducts of AlMe_3 are also known (see *e.g.* Robinson *et al.*, 1985, 1987; Zhao *et al.*, 1999; Leman *et al.*, 1993; Hsiao *et al.*, 2016; Zhang *et al.*, 1985; Atwood *et al.*, 1983). We decided to synthesize the THF adduct of trimethylaluminium specifically to analyse its properties.



2. Structural commentary

In the presence of THF, no dimeric trimethylaluminium, but instead a monomeric trimethylaluminium–thf adduct was formed. It was synthesized from a trimethylaluminium solution in *n*-heptane under inert conditions. Crystals of this compound are pyrophoric, sensitive to moisture, oxygen and high temperature. As a consequence, they were handled and prepared at low temperature under an argon atmosphere. The title compound (Fig. 1) shows a structure between trigonal-planar and tetrahedral symmetry, as indicated by the three C–Al–C angles [116.43 (9), 116.24 (9), 114.97 (9)°; Table 1]. As a result of the weak interaction between aluminium and oxygen, an elongated Al–O bond distance is observed [1.9131 (13) Å]. The Al–O bond distance is very similar to those in known aluminium–THF adducts [Lehmkuhl *et al.*, 1985 (CSD recode DENGIM; Groom *et al.*, 2016); Schnitter *et al.*, 1997 (refcode NIKJEW)] and other molecular structures where this compound could be obtained as a co-crystallate [Kong *et al.*, 1995 (YUGWEC); Vidyaratne *et al.*, 2009 (IHEYOK)]. Even longer Al–O bonds can be observed in the molecular structure of a dioxane–trimethylaluminium adduct [2.02 (2) Å; Atwood & Stucky, 1967 (TMALOX)] and in the molecular structure of trimethylaluminium with 18-crown-6 [2.005 (6) Å; Atwood *et al.*, 1982 (BOYVEQ)]. The dimeric aluminium structure (AFODUU) observed by Sharma *et al.* (2002) shows very short Al–O bonds for the terminal and bridging isopropoxy groups bound to the tetra-coordinated positions [1.799 (3)–1.685 (3) Å], indicating a strong interaction between aluminium and oxygen in these cases. These results support the weak interaction between aluminium and oxygen in the title compound, leading to a slight distortion of the trimethylaluminium and a structure between trigonal-planar and tetrahedral symmetry. In contrast to the monomeric structure, the dimeric molecular structure of trimethylaluminium features one large C–Al–C angle and two smaller C–Al–C angles [123.55 (1), 107.26 (1), 106.79 (1)°]. As a result of the lower electron density of the two bridging

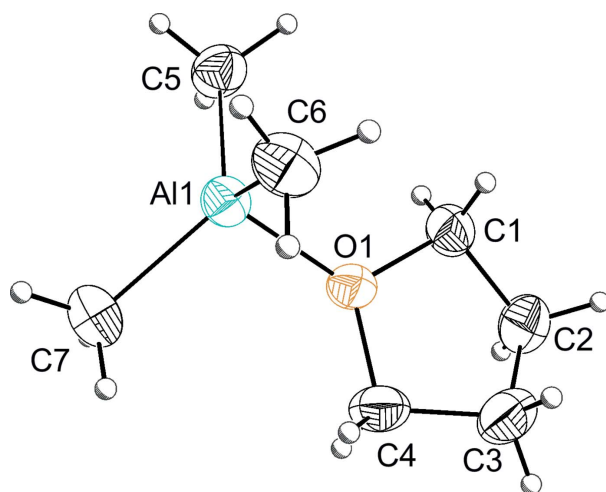


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

Table 1
Selected geometric parameters (Å, °).

O1–Al1	1.9131 (13)	C6–Al1	1.976 (2)
C5–Al1	1.9671 (19)	C7–Al1	1.965 (2)
C5–Al1–C6	116.43 (9)	C1–O1–Al1	122.45 (10)
C5–Al1–C7	116.24 (9)	C4–O1–Al1	124.00 (11)
C6–Al1–C7	114.97 (9)	C4–O1–C1	109.40 (13)

Al–C bonds, less space is required in the coordination sphere of the aluminium atom. In comparison with an ideal tetrahedral coordination sphere, there is a smaller angle for the bridging bonds and a larger angle for the terminal bonds (Stammler *et al.*, 2015). These results are supported by further dimeric molecular structures of trimethylaluminium. Nikiforov *et al.* (2008) reported a titanium complex (BOFNOA) with a trimethylaluminium unit with one large C–Al–C angle and two smaller C–Al–C angles [119.32 (13), 103.34 (13), 103.39 (12)° and 115.86 (13), 106.78 (13), 100.29 (12)°]. Occhipinti *et al.* (2011) reported the synthesis and stability of homoleptic metal(III) tetramethylaluminates, which feature one large C–Al–C angle for the terminal bonds and two smaller C–Al–C angles for the bridging bonds. For the crystal structure of Tm(AlMe₄)₃, a large C–Al–C angle for the terminal bonds [118.55 (7) or 119.5 (2)°] and two smaller angles [104.84 (7), 108.64 (7)° or 105.43 (6), 108.86 (7)°] were observed.

3. Quantum-chemical calculations

Quantum-chemical calculations with the minnesota functional M062X, basis set 6–311+G(2df,p) and the solvent model (PCM) were applied to verify the C–Al and C–O bond lengths as well as the C–Al–C angles. Apparently, a simple gas-phase calculation is not sufficient to describe the crystal precisely, and leads to different results than found in the monomeric molecular structure of this compound. Therefore we decided to use the solvent model (PCM). Götz *et al.* (2010) have recently evaluated the ability of an embedded-cluster model with polarizable continuum solvents (PCM) to reproduce the crystal environmental effects. Those models were used to reproduce the crystal environmental effects on QTAIM parameters inside the tetrameric unit of solid MeLi (Götz *et al.*, 2013).

The NBO analysis of the Al–C bond indicates an occupancy of 82% for carbon and an occupancy of 18% for aluminium. The carbon part of the bond consists of 34% *s*-character and 66% *p*-character, whereas the aluminium part of the bond consists of 29% *s*-character, 70% *p*-character and 1% *d*-character. These results are in good agreement with the observed C–Al–C angles [116.43 (9), 116.24 (9), 114.97 (9)°]. The greater electronegativity of carbon provides more *p*-character in the Al–C bond, resulting in smaller angles than 120°. The NBO analysis for the Al–O bond indicates an occupancy of 94% for oxygen and an occupancy of 6% for aluminium. The oxygen part of the bond consists of 41% *s*-character and 59% *p*-character whereas the aluminium

Table 2
NBO analysis.

Al—O	Al	O	Al—C	Al	C
Occupancy	5.70%	94.30%		18.22%	81.78%
<i>s</i>	14.29%	41.14%		28.82%	33.59%
<i>p</i>	83.68%	58.84%		70.24%	66.39%
<i>d</i>	1.95%	0.01%		0.91%	0.01%

part of the bond consists of 14% *s*-character and 84% *p*-character and 2% *d*-character. The details of the NBO analysis are summarized in Table 2.

4. Database survey

The basic building unit, trimethylaluminium, has been known for a long time and has been completely characterized (Lewis & Rundle, 1953; Vranka & Amma 1967). Studies using single crystal X-ray analysis have been made, determining the exact structure, and were found in a search of the Cambridge Structural Database (Groom *et al.*, 2016). A dimeric structure with bridging methyl groups can be obtained, which is formed by two monomers that share a center of symmetry. An interior Al—C—Al angle of about 74° and an exterior C—Al—C angle of about 124° were observed. Furthermore the Al—C distances have significant differences. The Al—C bridging distance is 2.14 Å, whereas the Al—C terminal distance is about 2.00 Å. Trimethylaluminium–THF adducts have been reported already. On the one hand this compound was observed as a co-crystallate of a self-activating ethylene trimerization catalyst (IHEYOK; Vidyaratne *et al.*, 2009) and on the other hand as a co-crystallate of an unusual transition-metal cluster (YUGWEC; Kong *et al.*, 1995). The co-crystallate has not been further analysed.

5. Synthesis and crystallization

Trimethylaluminium is predominately a dimer in hydrocarbon solution. The structure was obtained treating 200 mg (1.38 mmol, 1.0 eq.) of a 2 M solution of trimethylaluminium in *n*-heptane with 0.08 ml (1.38 mmol, 1.0 eq.) THF under inert conditions. The sample was stored under an argon atmosphere at 193 K for two weeks and crystallized as colourless blocks. The yield was not determined. The crystals are pyrophoric and were prepared with the help of 'X-Temp 2' (Heine & Stalke, 1992; Stalke, 1998). Further methods of analysis or characterization were not possible because of the high reactivity of this compound.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.98 Å, $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl hydrogen atoms and C—H = 0.99 Å, $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene hydrogen atoms.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Al(CH ₃) ₃ (C ₄ H ₈ O)]
<i>M_r</i>	144.18
Crystal system, space group	Monoclinic, <i>P</i> ₂ / <i>c</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.7034 (6), 9.1228 (7), 13.6833 (11)
β (°)	98.845 (8)
<i>V</i> (Å ³)	950.18 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.15
Crystal size (mm)	0.4 × 0.4 × 0.2
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Sapphire3
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2010)
<i>T</i> _{min} – <i>T</i> _{max}	0.767, 0.971
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	16552, 2071, 1664
<i>R</i> _{int}	0.085
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.054, 0.152, 1.09
No. of reflections	2071
No. of parameters	85
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.89, -0.33

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010), *SIR2004* (Burla *et al.*, 2007), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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References

- Almenningen, A., Halvorsen, S. & Haaland, A. (1971). *Acta Chem. Scand.* **25**, 1937–1945.
- Andresen, A., Cordes, H.-G., Herwig, J., Kaminsky, W., Merck, A., Mottweiler, R., Pein, J., Sinn, H. & Vollmer, H.-J. (1976). *Angew. Chem. Int. Ed. Engl.* **15**, 630–632.
- Atwood, J. L., Hrcncir, D. C., Shakir, R., Dalton, M. S., Priester, R. D. & Rogers, R. D. (1982). *Organometallics*, **1**, 1021–1025.
- Atwood, J. L., Priester, R. D., Rogers, R. D. & Canada, L. G. (1983). *J. Inclusion Phenom.* **1**, 61–69.
- Atwood, J. L. & Stucky, G. D. (1967). *J. Am. Chem. Soc.* **89**, 5362–5366.
- Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G., Siliqi, D. & Spagna, R. (2007). *J. Appl. Cryst.* **40**, 609–613.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Götz, K., Gessner, V. H., Unkelbach, C., Kaupp, M. & Strohm, C. (2013). *Z. Anorg. Allg. Chem.* **639**, 2077–2085.
- Götz, K., Meier, F., Gatti, C., Burow, A., Sierka, M., Sauer, J. & Kaupp, M. (2010). *J. Comput. Chem.* **31**, 2568–2576.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst. B* **72**, 171–179.
- Heine, A. & Stalke, D. (1992). *Angew. Chem. Int. Ed. Engl.* **31**, 854–855.
- Herrmann, W. A. (1982). *Adv. Organomet. Chem.* **20**, 195–197.
- Hsiao, H.-C., Datta, A., Chen, Y.-F., Chang, W., Lee, T.-Y., Lin, C.-H. & Huang, J.-H. (2016). *J. Organomet. Chem.* **804**, 35–41.

- Kong, G., Harakas, G. N. & Whittlesey, B. R. (1995). *J. Am. Chem. Soc.* **117**, 3502–3509.
- Lehmkuhl, H., Mehler, K., Shakoor, A., Krüger, C., Tsay, Y.-H., Benn, R., Ruffiniska, A. & Schroth, A. (1985). *Chem. Ber.* **118**, 4248–4258.
- Leman, J. T., Landry, C. C. & Barron, A. R. (1993). *Main Group Met. Chem.* **16**, 193–199.
- Lewis, P. H. & Rundle, R. E. (1953). *J. Chem. Phys.* **21**, 986–992.
- Nikiforov, G. B., Roesky, H. W., Heisen, B. C. & Oswald, R. B. (2008). *Organometallics*, **27**, 2544–2548.
- Occhipinti, G., Meermann, C., Dietrich, H. M., Litlabø, R., Auras, F., Törnroos, K. W., Maichle-Mössner, C., Jensen, V. R. & Anwender, R. (2011). *J. Am. Chem. Soc.* **133**, 6323–6337.
- Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction, Yarnton, England.
- Robinson, G. H., Bott, S. G., Elgamal, H., Hunter, W. E. & Atwood, J. L. (1985). *J. Inclusion Phenom.* **3**, 65–69.
- Robinson, G. H., Hunter, W. E., Bott, S. G. & Atwood, J. L. (1987). *J. Organomet. Chem.* **326**, 9–16.
- Schnitter, C., Roesky, H. W., Albers, T., Schmidt, H.-G., Röpken, C., Parisini, E. & Sheldrick, G. M. (1997). *Chem. Eur. J.* **3**, 1783–1792.
- Sharma, N., Sharma, R. K., Bohra, R., Drake, J. E., Hursthouse, M. B. & Light, M. E. (2002). *J. Chem. Soc. Dalton Trans.* 1631–1634.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Stalke, D. (1998). *Chem. Soc. Rev.* **27**, 171–178.
- Stammler, H.-G., Blomeyer, S., Berger, R. J. F. & Mitzel, N. W. (2015). *Angew. Chem. Int. Ed.* **54**, 13816–13820.
- Tanner, P. S., Williams, R. A. & Hanusa, T. P. (1993). *Inorg. Chem.* **32**, 2234–2235.
- Vidyaratne, I., Nikiforov, G. B., Gorelsky, S. I., Gambarotta, S., Duchateau, R. & Korobkov, I. (2009). *Angew. Chem. Int. Ed.* **48**, 6552–6556.
- Vranka, R. G. & Amma, E. L. (1967). *J. Am. Chem. Soc.* **89**, 3121–3126.
- Zhang, H., Means, C. M., Means, N. C. & Atwood, J. L. (1985). *J. Crystallogr. Spectrosc. Res.* **15**, 445–452.
- Zhao, Q., Sun, H.-S. & You, X.-Z. (1999). *J. Organomet. Chem.* **572**, 59–64.

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Trimethyl(tetrahydrofuran- κ O)aluminium(III)

Crystal data

[Al(CH₃)₃(C₄H₈O)]
 $M_r = 144.18$
 Monoclinic, $P2_1/c$
 $a = 7.7034$ (6) Å
 $b = 9.1228$ (7) Å
 $c = 13.6833$ (11) Å
 $\beta = 98.845$ (8)°
 $V = 950.18$ (13) Å³
 $Z = 4$

$F(000) = 320$
 $D_x = 1.008$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 8661 reflections
 $\theta = 2.2$ – 29.4 °
 $\mu = 0.15$ mm⁻¹
 $T = 150$ K
 Block, colourless
 $0.4 \times 0.4 \times 0.2$ mm

Data collection

Oxford Diffraction Xcalibur Sapphire3
 diffractometer
 Radiation source: Enhance (Mo) X-ray Source
 Graphite monochromator
 Detector resolution: 16.0560 pixels mm⁻¹
 ω scans
 Absorption correction: multi-scan
 (CrysAlis PRO; Oxford Diffraction, 2010)
 $T_{\min} = 0.767$, $T_{\max} = 0.971$

16552 measured reflections
 2071 independent reflections
 1664 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.085$
 $\theta_{\max} = 27.0$ °, $\theta_{\min} = 2.7$ °
 $h = -9 \rightarrow 9$
 $k = -11 \rightarrow 11$
 $l = -17 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.152$
 $S = 1.09$
 2071 reflections
 85 parameters
 0 restraints

Primary atom site location: structure-invariant
 direct methods
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.101P)^2 + 0.0468P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.89 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$$

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.23608 (15)	0.37473 (13)	0.62125 (9)	0.0358 (3)
C1	0.4234 (2)	0.3761 (2)	0.61379 (15)	0.0403 (4)
H1A	0.4953	0.3839	0.6801	0.048*
H1B	0.4521	0.4592	0.5726	0.048*
C2	0.4549 (3)	0.2322 (2)	0.56601 (16)	0.0500 (5)
H2A	0.5778	0.1990	0.5853	0.060*
H2B	0.4284	0.2389	0.4930	0.060*
C3	0.3280 (3)	0.1316 (2)	0.60652 (16)	0.0507 (5)
H3A	0.3019	0.0440	0.5642	0.061*
H3B	0.3748	0.1000	0.6747	0.061*
C4	0.1680 (3)	0.2259 (2)	0.60476 (16)	0.0445 (5)
H4B	0.0906	0.2184	0.5401	0.053*
H4A	0.1006	0.1966	0.6576	0.053*
C5	0.2460 (3)	0.7005 (2)	0.65333 (15)	0.0439 (5)
H5A	0.3731	0.6915	0.6742	0.066*
H5B	0.2022	0.7858	0.6856	0.066*
H5C	0.2212	0.7130	0.5814	0.066*
C6	0.1905 (3)	0.4582 (2)	0.83000 (15)	0.0461 (5)
H6A	0.1225	0.3705	0.8410	0.069*
H6B	0.1635	0.5367	0.8742	0.069*
H6C	0.3162	0.4354	0.8438	0.069*
C7	-0.1208 (3)	0.5008 (2)	0.63514 (15)	0.0436 (5)
H7A	-0.1357	0.5156	0.5634	0.065*
H7B	-0.1902	0.5737	0.6648	0.065*
H7C	-0.1608	0.4021	0.6493	0.065*
All	0.12856 (7)	0.52245 (6)	0.69114 (4)	0.0335 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0322 (7)	0.0311 (6)	0.0447 (7)	-0.0050 (5)	0.0082 (5)	-0.0018 (5)
C1	0.0311 (9)	0.0408 (10)	0.0500 (11)	-0.0005 (7)	0.0088 (7)	0.0007 (8)
C2	0.0481 (11)	0.0471 (12)	0.0560 (13)	0.0081 (9)	0.0119 (9)	-0.0046 (9)
C3	0.0624 (14)	0.0336 (10)	0.0554 (13)	0.0024 (9)	0.0067 (10)	0.0011 (8)
C4	0.0451 (10)	0.0351 (10)	0.0535 (12)	-0.0111 (8)	0.0087 (8)	-0.0039 (8)
C5	0.0456 (11)	0.0368 (10)	0.0508 (12)	-0.0022 (8)	0.0117 (8)	0.0014 (8)
C6	0.0474 (11)	0.0526 (12)	0.0368 (10)	-0.0045 (9)	0.0021 (8)	0.0038 (8)
C7	0.0342 (10)	0.0541 (12)	0.0419 (11)	0.0013 (8)	0.0037 (8)	0.0035 (8)

All	0.0318 (3)	0.0352 (3)	0.0336 (3)	-0.0007 (2)	0.0048 (2)	0.00140 (19)
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Geometric parameters (Å, °)

O1—C1	1.462 (2)	C3—C4	1.500 (3)
O1—C4	1.460 (2)	C5—A11	1.9671 (19)
O1—A11	1.9131 (13)	C6—A11	1.976 (2)
C1—C2	1.503 (3)	C7—A11	1.965 (2)
C2—C3	1.508 (3)		
O1—C1—C2	104.49 (15)	C5—A11—C6	116.43 (9)
C1—C2—C3	102.38 (16)	C5—A11—C7	116.24 (9)
C4—C3—C2	102.87 (16)	C6—A11—C7	114.97 (9)
O1—C4—C3	104.82 (15)	C1—O1—A11	122.45 (10)
O1—A11—C5	101.44 (7)	C4—O1—A11	124.00 (11)
O1—A11—C6	102.27 (8)	C4—O1—C1	109.40 (13)
O1—A11—C7	101.92 (8)		

Selected geometric parameters (Å, °).

O1—A11	1.9131 (13)
C5—A11	1.9671 (19)
C6—A11	1.976 (2)
C7—A11	1.965 (2)
C5—A11—C6	116.43 (9)
C7—A11—C5	116.24 (9)
C7—A11—C6	114.97 (9)
C1—O1—A11	122.45 (10)
C4—O1—A11	124.00 (11)
C4—O1—C1	109.40 (13)
