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Key indicators

Single-crystal X-ray study
 $T = 100\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.02\text{ \AA}$
 Disorder in main residue
 R factor = 0.058
 wR factor = 0.110
 Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

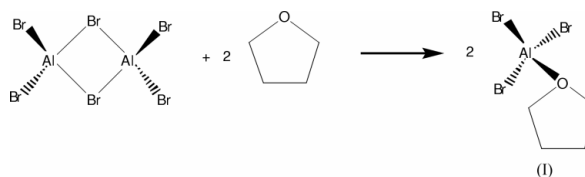
Tribromo(tetrahydrofuran)aluminium(III)

In the title compound, $[\text{AlBr}_3(\text{C}_4\text{H}_8\text{O})]$, (I), the Al atom, the O atom and one of the Br atoms are located on a crystallographic mirror plane; as a result, there is one half molecule in the asymmetric unit. Tetrahydrofuran shows a disorder due to puckering of the five-membered ring. (I) is isomorphous with $[\text{AlCl}_3(\text{C}_4\text{H}_8\text{O})]$ and $[\text{GaCl}_3(\text{C}_4\text{H}_8\text{O})]$.

Received 9 April 2003
 Accepted 15 April 2003
 Online 30 April 2003

Comment

Recently, we reported the X-ray crystal structure analysis of $[\text{GaCl}_3(\text{C}_4\text{H}_8\text{O})]$ ($\text{C}_4\text{H}_8\text{O} = \text{THF}$; Scholz *et al.*, 2002). Halides of group 13 elements have found widespread use as starting materials in inorganic chemistry. The synthesis of group 13 element clusters depends, on the one hand, on the oxidation state of elements in the halides, and, on the other hand, on the solvent used. AlBr_3 features a cyclic, dimeric arrangement in non-donor solvents like alkenes or benzene. In contrast, monomeric adducts of AlBr_3 are formed in the presence of Lewis bases. We were interested in the syntheses of aluminium cluster compounds with bulky substituents, such as the supersilyl (tri-*tert*-butylsilyl) group. Therefore, we have prepared a solution of $\text{AlBr}_3(\text{THF})$ in pentane. Colourless crystals of the title compound, (I), were grown from this solution at ambient temperature.



The molecule of (I) is located on a crystallographic mirror plane, passing through atoms Al1, O1 and Br1 (Fig. 1 and

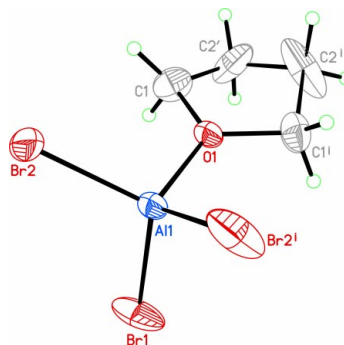


Figure 1

A perspective view of the title compound, (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Only one of the two disordered conformations of tetrahydrofuran is shown. [Symmetry code: (i) $x, \frac{1}{2} - y, z$.]

Table 1). All other atoms occupy general positions. As a result, there is one half molecule in the asymmetric unit. The crystal structure of (I) is isomorphous with those of $[\text{AlCl}_3(\text{C}_4\text{H}_8\text{O})]$ (Engelhardt *et al.*, 1996) and $[\text{GaCl}_3(\text{C}_4\text{H}_8\text{O})]$ (Scholz *et al.*, 2002).

Experimental

Colourless crystals of the title compound, (I), were obtained from a solution of 0.168 g (0.63 mmol) AlBr_3 and 0.5 ml tetrahydrofuran in 5 ml pentane at ambient temperature.

Crystal data

$[\text{AlBr}_3(\text{C}_4\text{H}_8\text{O})]$	$D_x = 2.313 \text{ Mg m}^{-3}$
$M_r = 338.81$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/m$	Cell parameters from 4175 reflections
$a = 6.3475 (11) \text{ \AA}$	$\theta = 2.1\text{--}25.2^\circ$
$b = 10.779 (2) \text{ \AA}$	$\mu = 12.46 \text{ mm}^{-1}$
$c = 7.4326 (12) \text{ \AA}$	$T = 100 (2) \text{ K}$
$\beta = 106.971 (13)^\circ$	Plate, colourless
$V = 486.39 (15) \text{ \AA}^3$	$0.12 \times 0.08 \times 0.05 \text{ mm}$
$Z = 2$	

Data collection

Stoe IPDS-II two-circle diffractometer	918 independent reflections
ω scans	714 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (MULABS; Spek, 1990; Blessing, 1995)	$R_{\text{int}} = 0.082$
$T_{\text{min}} = 0.302$, $T_{\text{max}} = 0.546$	$\theta_{\text{max}} = 25.1^\circ$
4060 measured reflections	$h = -7 \rightarrow 7$
	$k = -12 \rightarrow 12$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0137P)^2 + 5.177P]$
$R[F^2 > 2\sigma(F^2)] = 0.058$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.11$	$\Delta\rho_{\text{max}} = 1.07 \text{ e \AA}^{-3}$
918 reflections	$\Delta\rho_{\text{min}} = -1.82 \text{ e \AA}^{-3}$
55 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Al1—O1	1.823 (8)	Al1—Br2	2.264 (2)
Al1—Br1	2.262 (4)		
O1—Al1—Br1	107.3 (3)	Br1—Al1—Br2	111.72 (10)
O1—Al1—Br2	106.24 (17)	Br2'—Al1—Br2	113.13 (18)

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

All H atoms were refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$], using a riding model with $\text{C—H} = 0.99 \text{ \AA}$. Atom C2 is disordered, and it was, therefore, refined employing a split model. It was assumed that the probabilities of the two conformations, $\text{C1—C2—C2}^i\text{—C1}^i$ and $\text{C1—C2}'\text{—C2}^i\text{—C1}^i$ are each 50% [symmetry code: (i) $x, \frac{1}{2} - y, z$]. Furthermore, the two C1—C2 and $\text{C1—C2}'$ distances as well as the C2—C2^i and $\text{C2}'\text{—C2}^i$ distances were restrained to be the same length. However, the anisotropic displacement parameter of C2 has a max/min ratio of 18.8. The maximum and minimum electron-density peaks are located 0.46 and 1.03 \AA from Br2, respectively.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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