The Molecular Structure of Dibromotrimethylsiloxyaluminium

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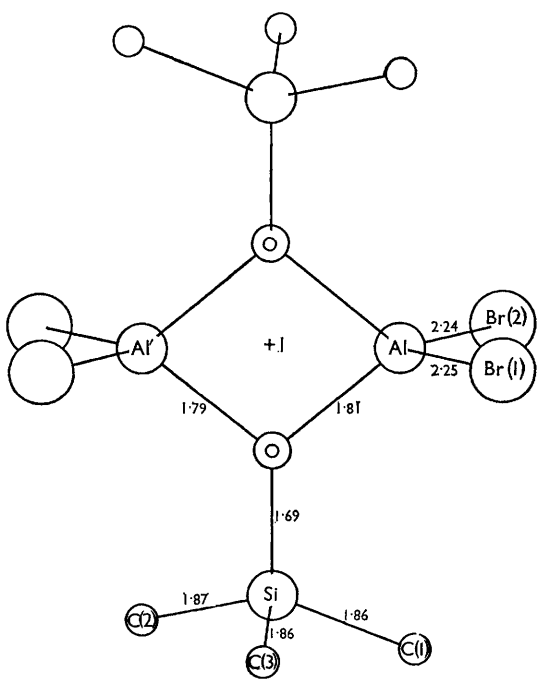
IN the course of investigations in this Institute on alumosiloxanes, the need was felt for more complete information about the structure of dihalogenotrimethylsiloxyaluminium. Accordingly an *X*-ray structural determination on dibromotrimethylsiloxyaluminium has been undertaken.

This compound, $Me_3SiOAlBr_2$, has colourless monoclinic crystals, with cell dimensions $a = 10{\cdot}206 \pm 0{\cdot}01$, $b = 9{\cdot}681 \pm 0{\cdot}005$, $c = 10{\cdot}402 \pm 0{\cdot}01$ Å; $\beta = 96° 33' \pm 5'$; $U = 1021$ Å^3. Assuming $Z = 4$, $D_c = 1{\cdot}796$ g.cm^{-3}; $F(000) = 524$. *Space group* $P2_1/n$ from systematic absences. Data from Weissenberg photographs, Cu-K_α radiation.

The *X*-ray intensities of 924 independent reflections were estimated visually. The positions of the bromine atoms were determined from a three-dimensional Patterson synthesis, and those of the other atoms from a series of F_o and F_o–F_c syntheses. After preliminary Fourier refinement, co-ordinates and anisotropic temperature-factors were refined by least squares. Values at the present stage ($R = 9{\cdot}4\%$) define the bond lengths (in Å) given in the Figure and the angles given in the Table.

The molecule is dimeric. Dimerization results in formation of a four-membered ring, in which each siloxy-group forms bonds with two aluminium atoms. By symmetry the ring must be planar. The silicon atoms lie approximately in this plane



TABLE

Bond Angles

Br(1)–Al–Br(2)	114°
Br(1)–Al–O	116°
Br(1)–Al–O′	111°
Br(2)–Al–O	113°
Br(2)–Al–O′	115°
O–Al–O′	85°
Al–O–Al′	95°
Si–O–Al	130°
Si–O–Al′	134°
O–Si–C(1)	106°
O–Si–C(2)	107°
O–Si–C(3)	106°
C(1)–Si–C(2)	118°
C(1)–Si–C(3)	107°
C(2)–Si–C(3)	111°

(0·15 Å from it). The Al–Br (σ = 0·01 Å), Si–O (σ = 0·02 Å), and Si–C (σ = 0·06 Å) bond lengths agree well with standard values.[1] The three bonds to the oxygen atom are coplanar with a maximum deviation of the oxygen atom of 0·05 Å. The Al–O bond length (1·80 Å, σ = 0·02 Å) is of interest as very few other values have been reported. Intermolecular contacts are between bromine atoms and methyl groups; none of these is less than 4·0 Å.

The results of the *X*-ray analysis confirm the model proposed by Schmidbaur and Schmidt[2] on the basis of physicochemical measurements.

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[1] L. E. Sutton *et al.*, "Tables of Interatomic Distances", *Chem. Soc. Special Publ.*, 1958, No. 11 and 1965, No. 18.
[2] H. Schmidbaur and M. Schmidt, *J. Amer. Chem. Soc.*, 1962, **84**, 1069.