Molecular Structure of Trimethylaluminium–Trimethylamine by Electron Diffraction

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Summary The molecular structure of the complex trimethylaluminium–trimethylamine has been determined by electron diffraction; the structures of acceptor and donor are found to be different from those of the isolated molecules.

WE have determined the molecular structure of trimethylaluminium–trimethylamine, using gas-phase electron diffraction, by recording the electron scattering pattern from the vapour with a source temperature of 65 °C (corresponding to a vapour pressure of *ca.* 15 mm[1]) and a nozzle temperature of 80°. The molecule has C_{3v} symmetry with staggered methyl groups. The main molecular parameters are listed in the Table (estimated standard deviations in parentheses) along with the corresponding structure parameters of monomeric trimethylaluminium[2] and trimethylamine[3] also obtained by gas-phase electron diffraction.

Formation of the complex leads to significant increase of the Al–C and N–C bond lengths as well as to deformation of the planar acceptor molecule. The Al–N bond is substantially longer than the Al–N bond found in Cl_3AlNMe_3 by *X*-ray diffraction from the crystal, 1·96(1) Å.[4]

Substitution of the methyl groups by the more electronegative chlorine atoms helps to remove negative charge from the aluminium atom making possible a stronger dative Al–N bond. It is of interest that the N–C bonds in Cl_3AlNMe_3 appear to be longer than in Me_3AlNMe_3; the three bond distances are 1·48(2), 1·55(2) and 1·58(2) Å.[4]

TABLE

	Me_3AlNMe_3[a]	$AlMe_3$[b]
Al–C	1·987(5) Å	1·957(3) Å
$\angle C_3$–Al–C* ..	102·4(0·3)°	90°
		$N(Me)_3$[c]
N–C	1·474(3) Å	1·454(2) Å
$\angle C_3$–N–C*	109·3(0·4)°	108·3(0·2)°
Al–N	2·099(10) Å	

* C_3 is the three-fold axis of the molecule.
[a] This work; [b] ref. 2; [c] ref. 3.

There has been some discussion as to whether the B–N bond distance in Me_3BNMe_3 is substantially greater than in the trimethylamine complexes of borontrihalides.[5–7] The differences observed between the analogous aluminium derivatives seems to indicate that it is. We are presently studying the bonding in all these compounds by CNDO calculations.

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