The Crystal Structure of *cis*-Dichloro-*cis*-bis(dimethyl sulphoxide)-*trans*-dimethyltin(IV)

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cis-DICHLORO-*cis*-BIS(DIMETHYL SULPHOXIDE)-*trans*-DIMETHYLTIN(IV) appears from i.r.[1-3] and conductivity data to be an example of a six co-ordinate dimethyltin(IV) compound. Although a completely *trans*-co-ordination has been suggested,[3] the i.r. assignments (Sn–O and Sn–Cl stretching frequencies) are tenuous, and do not uniquely define the structure.

^1H n.m.r. spectra show a ^{119}Sn–Me coupling constant (*J* 86 c./sec., $CHCl_3$ solution)[1,3] substantially less than expected (*J* *ca.* 100 c/sec.) for a linear Me_2Sn skeleton.[4] This suggests about 40% *s* character in the tin bonding orbitals to carbon, and implies some distortion to the expected octahedral co-ordination.

However, the crystal structure shows *cis*-co-ordination of both the two chloro and two dimethyl sulphoxide (DMSO) ligands and a methyl–tin–methyl angle approaching linearity.

Crystal data: $C_6H_{18}Cl_2O_2S_2Sn$; $M = 375·9$; white, long prismatic crystals; orthorhombic, $a = 13·37 \pm 0·01$, $b = 15·57 \pm 0·01$, $c = 6·$ $0·01$ Å, $U = 1445$ Å^3, $D_m = 1·70$ (flotation), $Z = 4$, $D_c = 1·73$, $F(000) = 744$, space group $P2_12_12_1$ (D_2^4), Cu-K_α *X*-radiation, nickel-filtered, single-crystal oscillation, Weissenberg and precession photographs.

Rapid decomposition of the compound in air was prevented by sealing the crystals in Lindeman glass capillaries. Two crystals were used to record 950 non-zero reflections from ten levels (0*kl* to 9*kl*), on multiple film Weissenberg photographs. No corrections have been made for absorption, extinction, or anomalous dispersion.

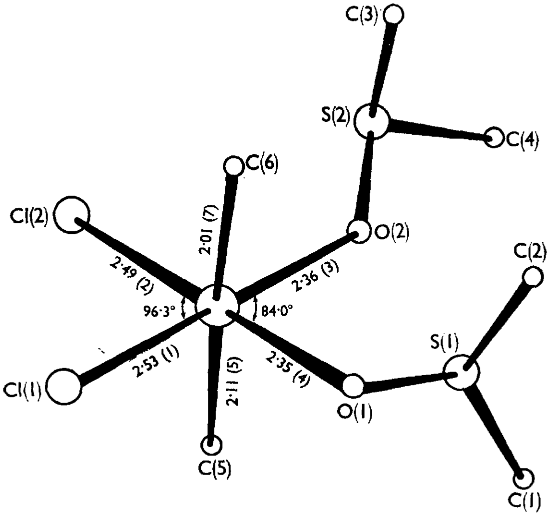

FIGURE. *Crystal structure of* cis-*dichloro*-cis-*bis(dimethylsulphoxide)*-trans-*dimethyltin* (IV). *All bond lengths quoted are provisional.*

Tin atomic co-ordinates were obtained from a three-dimensional Patterson synthesis. All other atoms, except hydrogen, were located in subsequent Fourier and difference Fourier syntheses. Five cycles of full-matrix least-squares refinement, using individual isotropic temperature factors, gave a conventional R value of 0·12.

The tin atom has a regular octahedral environment, with the DMSO groups co-ordinating through their oxygen atoms. For clarity of interpretation in the Figure, the *cis*-chlorine atoms and DMSO groups are shown in the basal plane, although the best least-squares plane contains Cl(1) O(2) C(5), and C(6), with the tin atom 0·1 Å out of the plane. The Sn–Cl and Sn–C bond lengths are comparable with those[5–8] reported, while the Sn–O bond length is significantly longer than another observation.[7] The configuration of the DMSO ligand is similar to a DMSO complex of Fe^{III} chloride.[9] The carbon–tin–carbon bond angle (172·4°) is larger than expected from ^1H n.m.r. evidence.

The large standard deviations in the bond lengths are mainly a result of the absence of cross-level data. Additional data will be collected about the remaining axes, and the completely refined structure will be published at a later date.

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