The Crystal Structure of $(Me_3Sn)_2N_2C$

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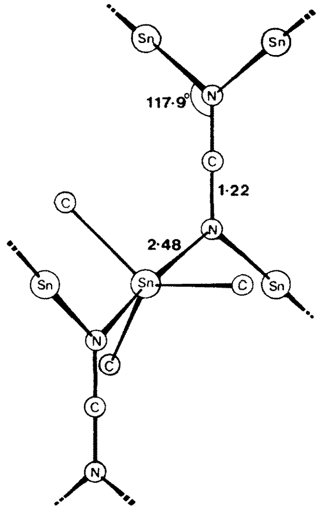
Summary The crystal structure of $(Me_3Sn)_2N_2C$ consists of an infinite helical network of planar trimethyltin groups linked by linear NCN units.

CRYSTALS of methyltin halides and pseudohalides contain molecular units strongly linked by asymmetric halogen and pseudohalogen bridges; for example the crystal structure[1] of trimethyltin isothiocyanate consists of zig-zag $-S \cdots Sn-N=C=S \cdots Sn-$ chains, bent only at sulphur, with nearly planar trimethyltin groups, whereas in the cyanide[2] planar Me_3Sn groups are linked by disordered CN units to form linear chains. In order to study a trimethyltin pseudohalide in which no free donor atoms would be available for this type of interaction, we have prepared and characterised $(Me_3Sn)_2N_2C$. By analogy with $(H_3SiN)_2C$, we had expected that this would possess a carbodi-imide rather than a cyanamide structure.[3]

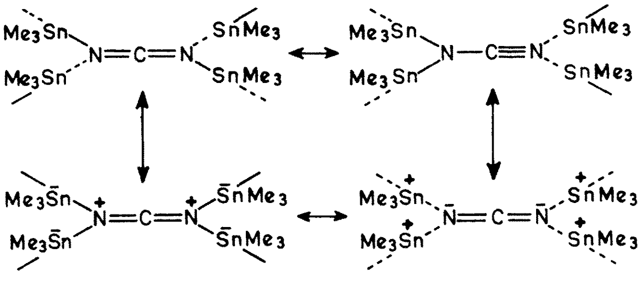
The compound was prepared by the reaction of trimethyltin chloride with silver cyanamide in refluxing benzene; needle-shaped crystals were grown by slow evaporation of a toluene solution under reduced pressure. The formula $C_7H_{18}N_2Sn_2$ was confirmed by elemental analysis and by the presence of a strong molecular ion in the mass spectrum.



FIGURE

The crystals are hexagonal, $P6_222$; $a = b =$ 8·74 (1), $c =$ 14·28 (2) Å; $Z =$ 3 for $D_c =$ 1·94, consistent with approximate density determinations by flotation. Intensities were estimated visually from equi-inclination Weissenberg photographs taken with Cu-K_α radiation. Statistical tests[4] strongly indicated that the structure was non-centrosymmetric. The structure was solved by Patterson and Fourier methods, and refined by full-matrix least-squares with anisotropic temperature factors for the tin atoms, and isotropic temperature factors for the carbon and nitrogen atoms, to a conventional 'R index' of 0·058 for 233 unique observed reflections. Friedel's law has so far been assumed in averaging equivalent reflections.

There is a diad axis along one Sn–C bond, so the trimethyltin group is exactly planar, with a mean Sn–C bond length of 2·14 (3) Å. The Sn–N bonds [2·48 (1) Å] are all crystallographically equivalent. The distortions from an accurately trigonal bipyramidal $N-SnC_3-N$ conformation are probably a packing effect: the NSnN angle is173·0(2)°. The Sn_2NCNSn_2 moieties have exact D_2 (222) symmetry with a dihedral angle of 64° between the two Sn_2NC planes. The trimethyltin groups are linked by NCN units to form helices about screw triad axes parallel to the Z (needle) axis; the NCN units are also parallel to the Z axis, and are each part of two helices of the same hand. The Sn–N bond is about 0·35 Å longer than in the alkyltin isothiocyanates,[1,5,6] but similar to the Sn–(C,N) distance in the disordered trimethyltin cyanide.[2] The structure can be considered to be intermediate between carbodi-imide, cyanamide, and ionic structures:



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