X-Ray Crystal and Molecular Structure of Trimethyltin Glycinate, a Polymeric, Trigonal Bipyramidal Tin Compound

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Summary Trimethyltin glycinate is shown by *X*-ray crystallography to be a linear polymer with amino-bridged trigonal bipyramidal units.

The reaction of trialkyltin hydroxide with amino-acids has been shown to yield a variety of structural types with the common stoicheiometry R_3SnAA (R = Me or cyclohexyl, AA = anion of the amino-acid). Trimethyltin glycinate appeared to be polymeric (room temperature ^{119m}Sn Mössbauer spectrum) and co-ordinated through the amino-nitrogen [$\nu(NH_2)$ 3311 cm^{-1}],[1] presumably ruling out the carboxylate-bridged structure common to trialkyl-tin acetates.[2]

Crystals of $Me_3Sn(O_2CCH_2NH_2)$ are tetragonal with $a = b = 7{\cdot}839$, $c = 14{\cdot}659$ Å, space group $P4_1$ or $P4_3$, $Z = 4$. The structural analysis was based on 645 independent reflections ($I_{obs}) > 3\sigma (I_{obs})$ (Cu-K_α), and R is currently 0·126. The essential stereochemistry is shown in the Figure; e.s.d.'s in the bond lengths average 0·03 (Sn–C, Sn–O, Sn–N) and 0·04 Å (C–C, C–O, C–N). The structure analysis confirms the presence of amino-nitrogen co-ordination and the predicted distorted trigonal bipyramidal geometry about the tin, the more electronegative substituents occupying the apical positions.[3] The Me_3Sn unit is distinctly non-planar (C_{3v} local symmetry with Sn atom displaced toward the carboxylate oxygen 0·12 Å from the mean plane of the methyl carbon atoms).

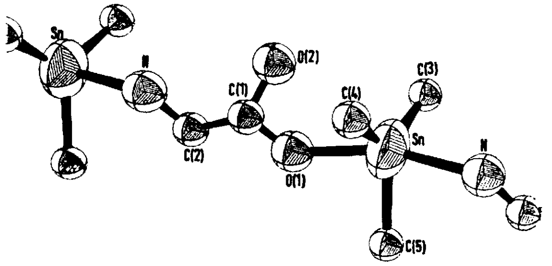

FIGURE. Stereochemistry of $Me_3Sn(O_2CCH_2NH_2)$ showing a portion of the one-dimensional chain. ∠ N–Sn–O(1) = 159·8°; mean Sn–C 2·14 Å; Sn–N 2·53 Å; Sn–O(1) = 2·27 Å.

The stereochemistry of the compound is determined by the geometrical requirements of the Me_3Sn unit. The five-membered chelate rings which are characteristic of amino-acid–metal complexes[4] are precluded in the linear arrangement of metal–ligand bonds required by fixing the oxygen and nitrogen atoms in the apical positions of the trigonal bipyramid at tin. The apical metal–ligand bonds formed by the co-ordination of the functional groups of two different ligand molecules result in infinite, one-dimensional chains. This type of bridging amino-acid co-ordination is only found in glycinatosilver(I) hemihydrate, where once again the preferred digonal co-ordination for Ag(I) determines the stereochemistry.[5]

Co-ordination occurs through a carboxylate oxygen and an amino nitrogen despite the generally believed greater affinity of tin for oxygen which would lead to the well established carboxylate bridged structure.[2,6] The observed stereochemistry presumably reflects the tendency of amino acids to utilize their functional groups as fully as possible in metal co-ordination.[4]

The tin carboxylate carbonyl [Sn–O(2)] contact distance is 3·22(3) Å indicating some weak interaction. The hydrogen atoms of the amino group are apparently used in hydrogen bonding, as illustrated by the intramolecular N–O(2) distance of 2·94(3) Å and an intermolecular contact distance of 2·67(3) Å with the adjacent symmetry related carboxylate carbonyl O(2).

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