Crystal and Molecular Structure of Triphenyltin *N*-Benzoyl-*N*-phenylhydroxamate

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Summary $Ph_3Sn \cdot O \cdot NPh \cdot CO \cdot Ph$ possesses a trigonal bipyramidal arrangement of groups about tin, to which the carbonyl oxygen is intramolecularly co-ordinated.

ALTHOUGH monomeric in benzene solution, triphenyltin *N*-benzoyl-*N*-phenylhydroxamate (I), exhibits several strong peaks in the mass spectrum of the solid which are attributable to the presence of dimeric species involving SnOSnO rings.[1] We have carried out a single crystal *X*-ray study of this compound to investigate this possibility.

Colourless crystals of (I) are monoclinic, space group $P2_1/C$, $a = 12 \cdot 28$, $b = 17 \cdot 62$, $c = 15 \cdot 41$ Å, $\beta = 128 \cdot 37°$. The intensities of 3549 independent non-zero reflections were recorded on a four-circle diffractometer using Cu-K_α radiation. The structure was derived from the three-dimensional Patterson function, and has been refined to R 0·049 by block-diagonal matrix least-squares with anisotropic temperature factors for all atoms.

The structure, (Figure), consists of a trigonal bipyramidal arrangement of groups around tin. The three phenyl groups are not equivalent; two occupy similar equatorial positions, whilst the third occupies an axial position with a not unexpectedly longer tin–carbon bond distance. The hydroxamic acid residue, covalently bound at an equatorial site, forms an almost planar five-membered Sn·O·N·C:O ring by the intramolecular co-ordination of the carbonyl oxygen to tin at the remaining axial site. The metal–ligand bond distances compare favourably with those determined previously for similar model compounds, as do those for the organic residue, save for the N–O distance (1·38 Å) which is significantly lower than in *O*-carbamoyl hydroxylamine[2] (1·46 Å) and hydroxylamine hydrochloride[3] (1·47 Å). The shortest intermolecular tin–oxygen distances are in excess of 6·5 Å. Therefore the compound is clearly monomeric in the crystalline state, and as such is the first example of a compound possessing the *cis*-R_3SnX_2 trigonal bipyramidal configuration reported. We are unable to offer any explanation for the observation in the mass spectrum of fragments containing two tin atoms. Conclusions concerning intermolecular association in the solid state .drawn from mass spectral data must therefore be regarded with caution.

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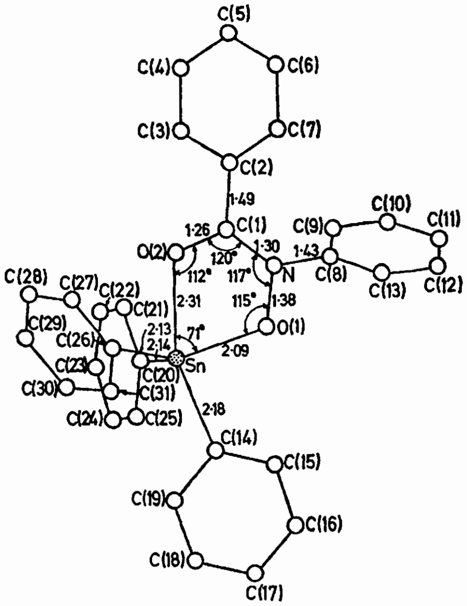

FIGURE

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