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New Organotin (IV) Derivatives of 1-Phenyl-1H-Tetrazole-5-Thiol, a Five-Membered Nitrogen Heterocycle

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NEW ORGANOTIN (IV) DERIVATIVES OF 1-PHENYL-1H-TETRAZOLE-5-THIOL, A FIVE-MEMBERED NITROGEN HETEROCYCLE

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Abstract The structural characterization of two organotin (IV) derivatives of the five-membered heterocycle 1-phenyl-1H-tetrazole-5-thiol is discussed.

INTRODUCTION

The compound 1-phenyl-1H-tetrazole-5-thiol is a 5-membered nitrogen heterocycle containing a thiocarbonyl group in exocyclic position. The ring has several potential donor sites which may lead to various coordination modes in metal derivatives.

Although the first Main Group organometallic derivatives of the heterocycle were regarded to have the ring bound to the metal through the non-substituted nitrogen atom adjacent to the thioketo group, recently the X-ray characterization¹⁻² of some organotin (IV) derivatives showed more complex coordination patterns that involve sulfur and nitrogen as well.

In this work we report the synthesis and structural characterization, in solution and in solid state of two triorganotin (IV) derivatives of 1-phenyl-1H-tetrazole-5-thiol, namely $\text{Bz}_3\text{SnSCN}_4\text{Ph}$ and $\text{Me}_3\text{SnSCN}_4\text{Ph}$.

RESULTS AND DISCUSSION

The compounds $\text{R}_3\text{SnSCN}_4\text{Ph}$, $\text{R} = \text{Bz}, \text{Me}$, were obtained from the ammonium salt of the ligand reacting with the corresponding triorganotin (IV) chlorides.

Multinuclear (^1H , ^{13}C and ^{119}Sn) NMR data² suggest a monomeric tetrahedral structure in solution for both compounds, where the tetrazolethiolate anion is bound to the triorganotin group through sulfur, without evidence for further Sn-N interactions.

Both compounds were characterized in the solid state by single crystal X-ray diffraction.

The compound $\text{Bz}_3\text{SnSCN}_4\text{Ph}^2$ is a polymer with C_3SnSN_2 cores and built through *intermolecular* dative $\text{N} \rightarrow \text{Sn}$ bonds, the geometry around the metal being best described as a distorted capped trigonal bipyramid. In this compound the thiotetrazolate ring can be considered as a *bimetallic triconnective* bridge, while in the di-n-butyl derivative^{1,2} the ligand is found to act as a *monometallic biconnective* group, thus giving an idea of how complex the coordination of this heterocycle to metal atoms can be.

In the compound $\text{Me}_3\text{SnSCN}_4\text{Ph}^3$, the main coordination site of the ring towards the metal is the sulfur atom, though *intermolecular* $\text{Sn} \cdots \text{N}$ bonds result in the buildup of an unusual trimeric structure which defines a 15-membered $\text{Sn}_3\text{S}_3\text{C}_3\text{N}_6$ macrocycle, or alternatively, if the weak *intramolecular* $\text{Sn} \cdots \text{N}$ interactions (3.285 Å) are taken into account, a novel, 9-membered, tin-nitrogen inorganic ring of composition Sn_3N_6 arises (Figure 1).

