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Complexes of Organometallic Compounds. XLIV. Synthesis and Mössbauer Spectroscopic Studies of Glylcylglycinato-O,N,N(2–)diorganotin (IV) Complexes

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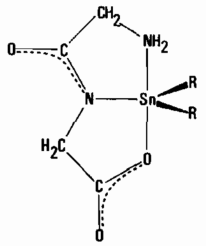
The present communication concerns our recent results on the interaction of R_2Sn^{IV} moieties (R = Me, Bu^n, Oct^n) with the dianion of glycylglycine, the simplest dipeptide, which may behave as a ONN tridentate ligand.[1] The investigation is an extension of our previous work on organometal–tridentate ligand complexes;[2] it is also the first part of a research project on the coordination of tin by ligands bearing functional groups present in biological molecules. The planned project is justified by the widespread and increasing practical uses of organotin compounds,[3] their consequent diffusion into the environment and their toxicity, which, albeit low,[4] cannot be ignored. The present status of the knowledge in the field is limited to few derivatives of triorganotin(IV) with aminoacids and dipeptides,[5,6] where bases presumably behave as bridging bismonodentate.[6]

The title compounds have been synthesized by 1:1 reaction of Me_2SnCl_2 with $^{(-)}OOCCH_2N^{(-)}COCH_2NH_2$ (from glycylglycine and sodium metoxide 1:2), and of R_2SnO (R = Bu^n, Oct^n) with the dipeptide, in methanol. The related analytical data are in the Table. The Mössbauer spectra were determined with the Laben–Elscint equipment described elsewhere,[7] operating at constant acceleration with a sawtooth waveform; the parameters reported in the Table have been determined.

It clearly appears that the obtained R_2Sn(Gly-Gly) solid crystalline compounds have 1:1 R_2Sn^{IV}:Gly-Gly stoichiometric composition (see Table). Their probable configuration in the solid state is here qualitatively inferred from Mössbauer data: isomer shifts, δ, are consistent with those of R_2Sntrid (where trid^{2-} are "planar" ligands with ONO and SNO donor atoms), while quadrupole splittings, ΔE, are in the range observed for complexes Me_2SnONO.[2b] Earlier spectroscopic work leads to assume a trigonal bipyramidal type configuration for R_2Sntrid, where C atoms of the organotin moiety and ligand N are lying in equatorial position, and OO or OS ligand atoms are axial; ONO, ONS atoms would be located in a plane.[2] These hypotheses have been essentially confirmed by the crystal and molecular structures of three of these compounds, although actual configurations are consistenly distorted from the ideal trigonal bipyramid.[8] The configuration (I) may then be tentatively advanced for Alk_2Sn(Gly-Gly) [which would then be glycylglycinato-O,N,N(2–)dialkyltin(IV)], mainly on the basis of the above mentioned similarity between ΔE values, taking also into account the symmetry of the coordinated ligand.[1]



(I)

TABLE. Analytical Data [% found (calcd.)], and Mössbauer Parameters (at liquid N_2 temperature).

Compound[a]	M.p. (°C)	C	H	N	O	Sn	δ[b]	ΔE[c]	Γav[d]
Me_2Sn(Gly-Gly)	273 (dec.)	25.82) (25.84)	4.55 (4.34)	10.03 (10.04)	17.31 (17.21)	42.45 (42.56)	1.26	3.29	1.14
Bu^n_2Sn(Gly-Gly)	196–197	39.51 (39.70)	6.80 (6.66)	7.62 (7.72)	13.35 (13.22)	32.85 (32.69)	1.35	3.19	1.09
Oct^n_2Sn(Gly-Gly)	135–137	50.59 (50.55)	8.42 (8.48)	6.05 (5.89)	10.21 (10.10)	24.90 (24.97)	1.37	3.43	0.97

[a] Gly-Gly = glycylglycinato(2–). [b] Isomer shift with respect to $BaSnO_3$–$BaSnO_3$ RT spectra. [c] Nuclear quadrupole splitting. [d] Full width at half height of the resonant peaks, average.

On the other hand, polymeric structures with bridging glycylglycinato(2–) cannot be excluded at the present status of the research. Further work is in progress, including theoretical treatment of ΔE parameters and also on the crystal and molecular structure of a representative compound.

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