

GAS-PHASE INTERACTIONS OF ORGANOTINS WITH GLYCINE

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Due to the wide industrial applications considerable amounts of the organotins have entered various ecosystems^[1]. Depending on the nature and the number of the organic groups bound to the Sn cation, some organotins show specific effects to different organisms even at very low concentrations^[2]. While organotins compounds have emerged as potentially biologically active compounds^[3]. During the last few years it is noticeable that organotins compounds occupy an important place in cancer chemotherapy reports^[4]. Considerable efforts have been directed to study the interaction of organotins with amino acids and peptides. To the best of our knowledge the interaction of amino acids with organotins or peptides by mass spectrometry has not been explored so far.

In this respect, the gas phase interaction of organotins with glycine was studied by means of mass spectrometry.

Interaction between di-organotins and glycine gives rise exclusively to a singly charged complexes of general formula $[(R)_2Sn(AA)-H]^+$ associated with formal deprotonation of glycine. MS/MS experiments show the loss of H₂O, CO and H₂O+CO. On the other hand losses of 57, 58 and 73 Daltons are specific of organotins and correspond to the formation of $[(R)_2SnOH]^+$, $[(R)_2SnNH_2]^+$ and $[(R)_2SnH]^+$ ions, respectively. A systematic study of the spectra obtained with labeled glycine concludes that the hydride in $[(R)_2SnH]^+$ is specifically a C(α) hydrogen. As regards tri-organotins only Trimethyltin showed interaction in gas phase. The abundant ion corresponds to $[(CH_3)_3Sn(AA)]^+$ which is dissociate by elimination of the intact ligand leading to carbocation $[(CH_3)_3Sn]^+$. In order to rationalize our experimental findings, we performed DFT calculations for the various systems. The most stable $[(R)_2Sn(Gly)-H]^+$ forms involve a bidentate interaction with the carboxylate group, while for triorganotins, the most stable coordination mode corresponds to monodentate interaction with zwitterionic amino acids. Finally the potential energy surfaces associated with the main fragmentation processes have also been explored.

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