

Butyltin(IV) citrates and tartrates: structural characterization and their interaction with nucleotides.

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Streszczenie

Butyltin complexes with biologically important hydroxyacids, citric $\text{HOOCCH}_2\text{C}(\text{OH})(\text{COOH})\text{CH}_2\text{COOH}$ ($\text{C}_6\text{H}_8\text{O}_7$) acid and (2*R*,3*R*)-(+)-tartaric $\text{HOOCCH}(\text{OH})\text{CH}(\text{OH})\text{COOH}$ ($\text{C}_4\text{H}_6\text{O}_6$) acid: $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_6\text{H}_6\text{O}_7)]$ (**1**), $[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_6\text{H}_7\text{O}_7)]$ (**2**), $(\text{phenH})_2[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_6\text{H}_5\text{O}_7)]$ (**3**), $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_4\text{H}_4\text{O}_6)]$ (**4**), $[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_4\text{H}_5\text{O}_6)]$ (**5**), $(\text{phenH})[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_4\text{H}_4\text{O}_6)]$ (**6**) and $[\{\text{Sn}(\text{C}_4\text{H}_9)_3\}_2(\text{C}_4\text{H}_4\text{O}_6)]$ (**7**) have been synthesized and characterized by ESI-MS, IR and ^1H , ^{13}C and ^{119}Sn NMR spectra. Their structures and properties in solid state and solutions were proposed on the basis of the spectroscopic data and density functional theory (DFT) calculations at B3LYP/3-21G** level. Complexes in solutions in polar solvents are five-coordinate as evidenced by ^{13}C and ^{119}Sn NMR spectra. Geometries of the five-coordinate complexes were optimized with B3LYP/3-21G** calculations. The ^{13}C , ^{31}P and ^{119}Sn NMR spectra prove that complexes effectively interact with AMP, ATP and DAMP nucleotides forming Sn-OP bonds and N...H-O (nucleotide-carboxylate ligand) hydrogen bonds. In the case of dibutyltin complexes (**1** and **4**) nucleotides may also be coordinated as a chelating ligands via phosphate group and N7 atom of adenine residue.

Słowa kluczowe

Dibutyltin, Tributyltin, Citrate, Tartrate, Nucleotide, DFT

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