

Butyltin(IV) 2-sulfobenzoates: synthesis, structural characterization and their cytostatic and antibacterial activities.

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Abstract

Three butyltin complexes with 2-sulfobenzoic acid $[\text{Sn}(\text{C}(4)\text{H}(9))_2\{\text{O}(3)\text{SC}(6)\text{H}(4)\text{COO}-2\}(\text{H}(2)\text{O})]\cdot(\text{C}(2)\text{H}(5)\text{OH})$ (1), $[\text{Sn}(\text{C}(4)\text{H}(9))_3\{\text{O}(3)\text{SC}(6)\text{H}(4)\text{COOH}-2\}]$ (2) and $[\text{Sn}(2)(\text{C}(4)\text{H}(9))_6\{\mu-\text{O}(3)\text{SC}(6)\text{H}(4)\text{COO}-2\}]$ (3) have been synthesized and characterized by IR and $(1)\text{H}$, $(13)\text{C}$ and $(119)\text{Sn}$ NMR spectra. They show interesting properties in solid state and solutions because there are many modes of coordination of the Sbz ligand. The structure of complex 1 has been determined by X-ray crystallography. It is a chain compound with 2-sulfonatobenzoate coordinated to Sn atoms as a bridging and chelate ligand via O atoms of COO and SO(3) groups. In solutions the chains dissociate giving mainly mononuclear complexes. The NMR spectra and calculation at the DFT B3LYP/3-21G** level indicate that in solutions of compounds 1, 2 and 3 in polar solvents, many complexes showing dynamic properties are formed. Density functional theory (DFT) calculations showed that many five- and six-coordinate isomers and conformers can exist in equilibrium. All compounds effectively interact with AMP and ATP. The NMR spectra showed that nucleotides are coordinated to Sn atoms via PO(4) groups. The complexes are very active cytostatic agents against tumor strains. They are more effective than cisplatin. It is interesting that activity of 3 against non-tumor cell NHDF is lower than against tumor cells. Antibacterial activity of 1 and 2 has been investigated. Compound 2 is a very effective agent against Gram-positive bacteria. Antibacterial activity of 1 is lower than that of 2. Activity of 1 both against Gram-positive and Gram-negative bacteria is similar.

Słowa kluczowe

butyltin 2-sulfobenzoates, dibutyltin, tributyltin, cytostatic activity, antibacterial activity

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