Title: Syntheses, Molecular Structures, Electrochemical Behavior, Theoretical Study, and Antitumor Activities of Organotin(IV) Complexes Containing 1-(4-Chlorophenyl)-1-cyclopentanecarboxylato Ligands

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Abstract: The organotin(IV) compounds [Me2Sn(L)(2)] (1), [Et(2)sn(L)(2)] (2), [(Bu2Sn)-Bu-n(L)(2)] (3), [(n)Oct(2)Sn(L)(2)] (4), [Ph2Sn(L)(2)] (5), and [PhOSnL](6) (6) have been synthesized from the reactions of 1-(4-chlorophenyl)-1-cyclopentanecarboxylic acid (HL) with the corresponding diorganotin(IV) oxide or dichloride. They were characterized by IR and multinuclear NMR spectroscopies, elemental analysis, cyclic voltammetry, and, for 2, 3, 4 and 6, single crystal X-ray diffraction analysis. While 1-5 are mononuclear diorganotin (IV) compounds, the X-ray diffraction of 6 discloses a hexameric drumlike structure with a prismatic Sn6O6 core. All these complexes undergo irreversible reductions and were screened for their in vitro antitumor activities toward HL-60, BGC-823, Bel-7402, and KB human cancer cell lines. Within the mononuclear compounds, the most active ones (3, 5) are easiest to reduce (least cathodic reduction potentials), while the least active ones (1, 4) are the most difficult to reduce. Structural rearrangements (i.e., Sn-O bond cleavages and trans-to-cis isomerization) induced by reduction, which eventually can favor the bioactivity, are disclosed by theoretical/electrochemical studies.

KeyWords Plus: Redox Properties; Diorganotin(IV) Complexes; Organometallic Chemistry; Coordinatio-Compounds; Anticancer Complexes; Cancer-Chemotherapy; Ruthenium Complexes; Crystal-Structures; Cell-Growth; NMR-Spectra

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