

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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Source: Renewable Energy

Volume: 50 **Issue:** 17 **Pages:** 8158-8167 **DOI:** 10.1021/ic200635g **Published:** Sep 5 2011

Document Type: Article

Language: English

Abstract: The organotin(IV) compounds [Me₂Sn(L)(2)] (1), [Et₂Sn(L)(2)] (2), [(Bu₂Sn)-Bu-n(L)(2)] (3), [(n)Oct₂Sn(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; Coordination Compounds; Anticancer Complexes; Cancer-Chemotherapy; Ruthenium Complexes; Crystal-Structures; Cell-Growth; NMR-Spectra

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Funding:

Funding Agency	Grant Number
Foundation for Science and Technology (FCT), Portugal	PEst-OE/QUI/UI0100/2011 SFRH/BPD/44773/2008
Ministry of Science and Technology of China	2009ZX09103-104

Publisher: Amer Chemical SOC

Publisher Address: 1155 16TH ST, NW, Washington, DC 20036 USA

ISSN: 0020-1669

Citation: SHANG, Xianmei; MENG, Xianggao; ALEGRIA, Elisabete C. B. A.; LI, Qingshan; GUEDES DA SILVA, M. Fátima C.; KUZNETSOV, Maxim L.; POMBEIRO, Armando J. L. - Syntheses, Molecular Structures, Electrochemical Behavior, Theoretical Study, and Antitumor Activities of Organotin(IV) Complexes

Containing 1-(4-Chlorophenyl)-1-cyclopentanecarboxylato Ligands. Renewable Energy. ISSN 0020-1669.
Vol. 50, n.º 17 (2011) p. 8158-8167.