Inorganica Chimica Acta 387 (2012) 219–225

Contents lists available at SciVerse ScienceDirect

Inorganica Chimica Acta

journal homepage: www.elsevier.com/locate/ica

Organotin(IV) complexes of 2-hydroxyacetophenone-*N*(4)-cyclohexylthiosemicarbazone (H_2dact): Synthesis, spectral characterization, crystal structure and biological studies

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ARTICLE INFO

Article history:
Received 12 November 2011
Received in revised form 10 January 2012
Accepted 12 January 2012
Available online 24 January 2012

Keywords:
2-Hydroxyacetophenone-*N*(4)-cyclohexylthiosemicarbazone
Organotin(IV) complexes
Spectral analyses
Crystal structure
Cytotoxicity
Antibacterial activity

ABSTRACT

Four new organotin(IV) complexes of the type [MeSnCl(dact)] (**2**), [BuSnCl(dact)] (**3**), [PhSnCl(dact)] (**4**) and [Ph_2Sn(dact)] (**5**) were synthesized by the direct reaction of 2-hydroxyacetophenone-*N*(4)-cyclohexylthiosemicarbazone [H_2dact, (**1**)] and organotin(IV) chloride(s) in absolute methanol. The ligand [H_2dact, (**1**)] and its organotin(IV) complexes (**2–5**) have been characterized by CHN analyses, molar conductivity, UV–Vis, FT-IR, ^{1}H, ^{13}C and ^{119}Sn NMR spectral studies. The molecular structure of complex (**5**) has also been determined by single-crystal X-ray diffraction. The crystal structure of complex (**5**) showed that the ligand is doubly deprotonated at the oxygen and sulfur atoms and is coordinated to the tin(IV) atom through thiolate-S, azomethine-N and phenoxide-O atoms. X-ray diffraction studies indicated that complex (**5**) is a monomer and the central tin(IV) atom is five coordinated in a distorted trigonal bipyramidal geometry. The cytotoxicity of the ligand (**1**) as well as its organotin(IV) complexes (**2–5**) was studied against *Artemia salina*. The *in vitro* antibacterial activities of these compounds were also evaluated. The screening results have shown that the organotin(IV) complexes (**2–5**) have better antibacterial activity than the free ligand. Furthermore, it has been shown that diphenyltin(IV) derivative (**5**) exhibits significantly better activity than the monoorganotin(IV) derivatives (**2–4**).

1. Introduction

Thiosemicarbazones form an interesting class of compounds with a wide range of pharmacological applications [1,2]. Thiosemicarbazone usually act as chelating ligand with certain metal ions, bonding through the sulfur and hydrazine nitrogen atoms [3]. The heterocyclic thiosemicarbazones are of high interest because of their great versatility as ligands. This is due to the presence of several potential donor atoms, their flexibility and ability to coordinate either neutral or deprotonated forms. Seena and Kurup have synthesized and characterized dioxomolybdenum(IV) complexes with 2-hydroxyacetophenone-*N*(4)-cyclohexyl and *N*(4)-phenyl thiosemicarbazone which suggested that the Mo(IV) complex is penta-coordinated [4]. Rebolledo et al. have reported that Pd(II) complexes of 2-benzoylpyridine-*N*(4)-methyl/phenyl thiosemicarbazone ligands are active against the MCF-7, TK-10 and UACC-62 human tumor cell line [5]. For the past few years, studies of the coordination chemistry of thiosemicarbazone involved complexes with transition metal ions [6–9]. The synthesis and characterization of organotin(IV) complexes of Schiff base ligands have always attracted the attention of inorganic chemists and is well established in the literature [10–14]. Organotin(IV) complexes have been extensively studied due to their beneficial biological activities as well as their wide industrial and agricultural applications [15–21]. de Sousa et al. have reported organotin(IV) derivatives of 2-hydroxyacetophenone-*N*(4)-phenylthiosemicarbazone and found that the Sn(IV) atom adopts a strongly distorted trigonal bipyramidal configuration [22]. Although the organotin(IV) complexes exhibit important cytotoxic effects, but based on the literature review there is still very limited information available regarding the X-ray and biological studies of novel organotin(IV) complexes with substituted thiosemicarbazone ligands [23]. Previous works described the synthesis and structural studies of tin(IV)/organotin(IV) complexes with *N*(4)-substituted thiosemicarbazone ligand [24,25]. The particular interest of this work is a better understanding of the structural diversity of organotin(IV) complexes to delineate their biological properties. This paper reports the synthesis, spectral characterization and *in vitro* biological activity of organotin(IV) complexes (**2–5**). X-ray crystal structure of diphenyltin(IV) complex (**5**) is also described.

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doi:10.1016/j.ica.2012.01.020