

**Homoleptic tin(IV) compounds containing tridentate ONS dithiocarbazate Schiff bases:
Synthesis, X-ray crystallography, DFT and cytotoxicity studies**

ABSTRACT

Six new tin(IV) compounds derived from tridentate dinegatively charged ONS dithiocarbazate Schiff bases derived from 2-hydroxy-3-methoxybenzaldehyde (H2L1, H2L2 and H2L3) and 2,3-dihydroxybenzaldehyde (H2L4, H2L5 and H2L6) (where H2Ln = di-acids of Schiff base) are reported. The compounds were characterised by elemental analysis, FT-IR and multinuclear NMR (¹H, ¹³C and ¹¹⁹Sn) spectroscopy. The crystal structures of tin(IV) [S-4-methylbenzyl-β-N-(2-hydroxy-3-methoxybenzylmethylene)dithiocarbazate] (2) and tin(IV) [S-benzyl-β-N-(2-hydroxy-3-methoxy benzylmethylene)dithiocarbazate] (3) were determined by X-ray single crystal diffraction analysis. X-ray crystallography showed the molecular geometries in homoleptic 2 and 3 to be quite similar in which the dinegative tridentate ligand coordinated the tin atoms via thiolate-S, phenoxide-O and imine-N atoms. The coordination geometries are based on an octahedron with like-atoms mutually trans. The experimental findings were validated by density functional theory (DFT) calculations at the B3LYP/LanL2DZ/6-311G(d,p) level of theory. All the tin(IV) compounds, except the insoluble compound 2 were screened for their in vitro cytotoxicity against a panel ten of cancer cell lines and one normal breast cell line (MCF-10 A) by MTT assay. Interestingly, the cytotoxicity of five tin(IV) compounds against HT29, MCF7 and MIA was higher than the reference drug, cisplatin.

Keyword: Tin complex; X-ray crystallography; Cytotoxicity