MS36-P13

Novel isostructural and isoeletronic nickel(II) and palladium(II) complexes: Crystallographic and spectroscopic evaluation

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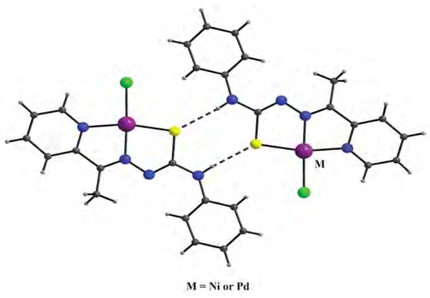
Metal complexes with biologically important ligands have received a great attention in the last decades. The thiosemicarbazones and their complexes it is a permanent fiel of research due the numerous pharmacological properties and applications, with anticancer, bactericidal and fungicidal activity.[1] The activity of the coordination compounds of transition metals is normally increased compared to the free thiosemicarbazones and depends largely on their structure and properties.[2] So the crystallographic elucidation of these compounds is important and fundamental to evaluate their possible applications. We describe the synthesis of two new complexes, [Ni(L)Cl] (1) and [Pd(L)Cl] (2), with the ligand 2-acetylpyridine N^4-phenylthiosemicarbazone (HL). The compounds have been characterized by elemental analysis and spectral (IR, UV-Vis, ^{1}H NMR, and ^{13}C NMR) measurements. Crystal and molecular structures of both complexes have been determined by single crystal X-ray analysis. It was found that the ligand coordinates with tridentate NNS donor atoms, in its deprotonatd tiona form. The chlorine ion is present in the coordination sphere for the both center atoms of the complexes, with Ni-Cl distance of 2.163(10) Å and Pd-Cl of 2.298(8) Å and displays the square-planar geometry with significantly distortion. The compounds are isoeletronic with d8 configuration and isostructural, also observed at spectroscopy analyses. Interestingly, the intermolecular hydrogen bonds have also been observed in both complexes and are responsible for the formation of a dimer-like structure in the crystal structure. For the purpose of complexation, all the techniques employed were compared with results obtained for the complex agent, and thus, to study with more clarity the influence of the metals in the structure, stability and property of these ligands. The biological potential applications of the compounds have been studied against cancer cells.



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Keywords: hydrogen bons, dimer, transition metals

MS36-P14

Structurally diverse of [Mn(salen)(NCS/NCSe)] complexes

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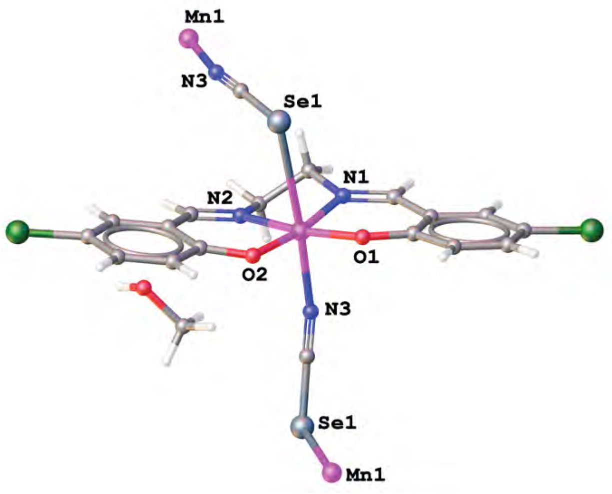
Manganese(III)-salen complexes are subject of three research studies: (i) the design of models of Mn-containing proteins and enzymes, (ii) the development of catalysts for oxidations of organic substrates, and (iii) study of magnetism of Mn(III) complexes. Manganese(III)-salen complexes are interesting synthetic systems that can act as mimetic of catecholase, peroxidase, catalase and superoxide dismutase [1-3].

In this study, a series of thiocyanate- and selenocyanate- manganese(III) complexes derived from Schiff based obtained by the condensation of salicylaldehyde, 5-bromo-salicylaldehyde, 5-chloro-salicylaldehyde, 3,5-dibromo-salicylaldehyde or 3,5-dichlorosalicylaldehyde and 1,2-diamineethane have been synthesized and characterized using single-crystal X-ray crystallography in the cases of [Mn(3,5-Br$_2$salen)(μ-NCS)]$_n$ (1), [Mn(3,5-Br$_2$salen)(μ-NCSe)]$_n$ (2), [Mn(3,5-Cl$_2$salen)(μ-NCS)]$_n$ (3), [[Mn(3,5-Cl$_2$salen)(μ-NCSe)]$_n$ (4), [Mn(5-Clsalen)(μ-NCSe)]$_n$.nMeOH (5), [Mn(5-Brsalen)(NCS)]$_2$ (6), [Mn(5-Clsalen)(NCS)]$_2$ (7) and [Mn(5-Brsalen)(NCSe)]$_2$ (8). The complexes 1–5 form 1D coordination polymers with thiocyanate or selenocyanate bridging ligands. The compounds 2, 4 and 5 are first examples of manganese(III) complexes with bridging selenocyanate ligands. The compounds 6–8 are dinuclear molecular complexes with terminal thiocyanate or selenocyanate ligands.



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Keywords: Coordination polymer, Mn(III)-salen, Crystal structure