INTERNATIONAL SYMPOSIUM ON CRYSTALLOGRAPHY
100 YEARS OF HISTORY FORTALEZA 2014

Blucher Physics Proceedings
Janeiro de 2015, Número 3, Volume 1

OXORHENIUM(V) COMPLEXES WITH A S-BENZYLDITHIOCARBAZATE LIGAND: SYNTHESIS AND CHARACTERIZATION

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In this study was performed the synthesis and characterization of two new oxorhenium(V) complexes with the 5-hydroxy-3-methyl-5-phenyl-pyrazoline-1-(S-benzyldithiocarbazate) ligand (H_2bdtc): ReOBr(bdtc)(triphenylphosphine) (**1**) and ReO(bdtc)(cysteamine) (**2**). In the characterization of the structures were employed different techniques like elemental analysis, spectroscopic methods (ESI-MS, IR, ^{1}H and ^{31}P NMR), and by X-ray diffraction. In addition, a detailed quantum chemical study will support in understanding the different electronic properties of the both compound, which will clarify the experimental data available for these molecules. The **1** purple prism monocrystals was crystallized with a monoclinic system and a $P2_1/n$ space group. The complex **2** is a different case, where it was observed red prism monocrystals with a $P2_1/c$ space group after the crystallization. Comparing both structures, the main information we can take is the different coordination arrangements that $bdtc^{2-}$ can assume, where is detected a planar one for **1** and a facial one for the complex **2**. Moreover, understanding the second order perturbation energy (E_2) allows the determination of the strength between donor and acceptor NBO, while the Quantum Theory of Atoms in Molecules will be employed in the understanding of intermolecular interactions predicted between the ligands.