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Synthesis, Characterization, Theoretical Crystal Structures and Antitubercular Activity Study of (E)-N'-(2,4-Dihydroxybenzylidene) Nicotinohydrazide and Some of Its Metal Complexes

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Abstract : Nicotinic acid hydrazide and 2,4-dihydoxylbenzaldehyde were condensed at 20°C to form an acylhydrazone (H3L) with ONO coordination pattern. The structure of the acylhydrazone was elucidated by using CHN analyzer, ESI mass spectrometry, IR, 1H NMR, 13C NMR and 2D NMR such as COSY and HSQC. Thereafter, five novel metal complexes [Mn(II), Fe(II), Pt(II) Zn(II) and Pd(II)] of the hydrazone ligand were synthesized and their structural characterization were achieved by several physicochemical methods, namely elemental analysis, electronic spectra, infrared, EPR, molar conductivity and powder X-ray diffraction studies. Structural geometries of some of the compounds were supported by using Hyper Chem-8 program for the molecular mechanics and semi-empirical calculations. The stability energy (E) and electron potentials (eV) for the frontier molecules were calculated by using PM3 method. An octahedral geometry was suggested for both Pd(II) and Zn(II) complexes while both Mn(II) and Fe(II) complexes conformed with tetrahedral pyramidal. However, Pt(II) complex agreed with tetrahedral geometry. In vitro antitubercular activity study of the ligand and the metal complexes were evaluated against Mycobacterium tuberculosis, H37Rv, by using micro-diluted method. The results obtained revealed that (PtL1) (MIC = 0.56 µg/mL), (ZnL1) (MIC = 0.61 µg/mL), (MnL1) (MIC = 0.71 µg/mL) and (FeL1) (MIC = 0.82 µg/mL), exhibited a significant activity when compared with first line drugs such as isoniazid (INH) (MIC = 0.9 µg/mL). H3L1 exhibited lesser antitubercular activity with MIC value of 1.02 µg/mL. However, the metal complexes displayed higher cytoxicity but were found to be non-significant different (P ˂ 0.05) to isoniazid drug.

Keywords : hydrazones, electron spin resonance, thermogravimetric, powder X-ray diffraction, antitubercular agents
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