Structural Studies on some Benzimidazole Containing Compounds and Their Palladium and Platinum Complexes

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Abstract

This work has been carried out to investigate the structures of some newly prepared benzimidazole derivatives using elemental analysis, FT-IR, 1H NMR, electron impact mass spectrometry (MS), single crystal X-ray diffraction, X-ray powder diffraction, and electronic absorption measurements in different solvents and in solutions of different pH. The Pd(II) and Pt(II) solid complexes with different anions X; X = Cl, Br, I, SCN and NO3; have been synthesized as potential anticancer compounds and their structures were elucidated using elemental analysis, FT-IR, 1H NMR, MS, UV/vis., molar conductance, thermal analysis (TG and DTA) and X-ray powder diffraction. The activation thermodynamic parameters were calculated using non-isothermal methods. The molecular geometries, vibrational frequencies, and 1H NMR of the benzimidazoles L1-9 and their complexes have been calculated by using density functional method. Molecular orbital description HOMO and LUMO were done for the studied complexes. Natural bond orbital analysis (NBO) method was performed to provide details about the type of hybridization and the nature of bonding in the studied complexes. The synthesized ligands, in comparison to their metal complexes were screened for their antibacterial activity and cytotoxicity.

***Keywords*:** Benzimidazole; DFT; NBO; Cytotoxicity; Platinum complexes.