Title	New transition metal complexes of 1-phenyl-2-((quinolin-2-ylmethylene)amino)ethan-1-ol Schiff base: Spectroscopic, X-ray, DFT, Hirshfeld surface analysis, biological and molecular docking studies

Abstract

In this research, a new Schiff base was prepared from phenylethanolamine and quinoline-2-carboxaldehyde, and then transition metal complexes were formed with the element's manganese, cobalt, nickel, copper, zinc, and palladium. The reported new compounds were characterized using different analytical and spectroscopic techniques such as elemental analysis (CHN), infrared spectroscopy (FTIR), proton nuclear magnetic resonance (^{1}HNMR), mass spectrometry, molar conductivity, magnetic measurements, electron paramagnetic resonance, (EPR), and thermal analysis (TGA, DTG). The structure of HL and its cobalt complex was also solved by single crystal X-ray diffraction technique. The results showed that the ligand acts as a tridentate in all compounds to give an octahedral geometry, except for the palladium compound, which is linked to the ligand through two atoms of nitrogen and oxygen, as well as two chlorine atoms, to give a square planar geometry. The general formula of the complexes is $[M(HL)_2]X_2$ where: (M= Mn, Co, Ni, Cu, Zn; X= ClO_4, CF_3SO_3 or NO_3), while the general formula of the palladium compound is $[Pd(HL)Cl_2]$.

The biological activity was studied against different types of positive and negative bacteria and fungi. The binding of these complexes to DNA was also investigated using UV-Vis spectrophotometry, viscosity measurements, and agarose gel electrophoresis, which proved the interaction of the complexes with DNA via intercalative binding mode.

Molecular geometries of HL and the reported complexes were investigated using the DFT-B3LYP level of theory. The quantum global reactivity descriptors were also calculated. Hirshfeld surface analysis of the ligand and cobalt complexes was investigated. Interesting structural features with unique hydrogen bonding formation were observed. Biological screening and molecular docking studies of the ligand and complexes were reported to explore their potential application as therapeutic drugs. The biological studies and molecular docking were correlated to each other and with the quantum reactivity descriptors. In general, computational modeling and a study of biological activity have proven that these compounds have significant biological activity against various types of bacteria, which in turn can be used as therapeutic agents, especially the cobalt compound, which outperformed Ampicillin as an antibacterial and Nystatin as an antifungal drug.