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Theoretical Treatment,Synthesis and Characterization of Some New Schiff Base Transition Metal Complexes

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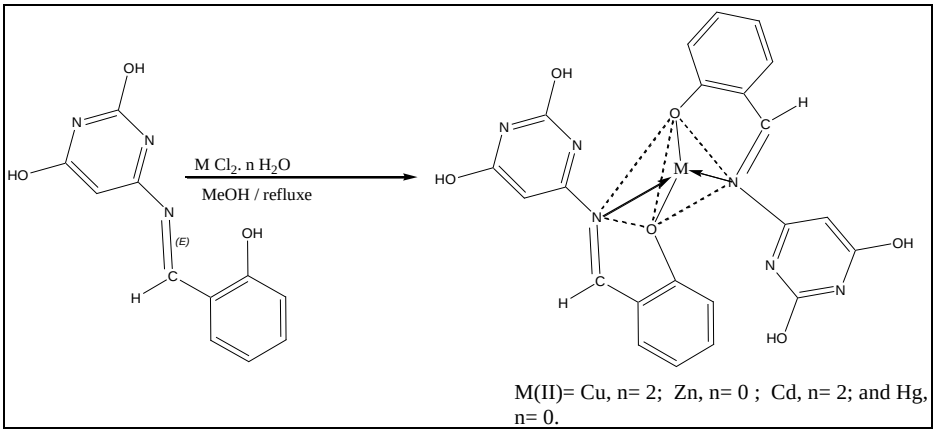
ABSTRACT

The complexes of Schiff base (6-[2-Hydroxy-benzylidene)-amino]-pyrimidine-2,4-diol) (L) with Cu(II), Zn(II), Cd(II) and Hg(II) were prepared. The Schiff base and complexes have been characterized by FT-IR,[1]H-NMR UV-Vis, Mass spectra, magnetic moment, elemental microanalyses (C.H.N.) and molar conductance. The work also includes a theoretical treatment of the formed complexes in the gas phase. This was done using the (hyperchem-8) program for the molecular mechanics and semi-empirical calculations. The electrostatic potential of the free ligands was calculated to investigate the reactive sites of the molecules. The heat of formation(ΔHf°) and binding energy(ΔEb) at 298K for the free ligands and its metal complexes were calculated by using PM3 method.

Graphical Abstract:



Preparation of the Complexes

Keywords: Theoretical treatment, Schiff base, complex, (PM3) method.