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Nature of metal-ligand bond in some metal complexes of a number of tetradentate(N_2O_2) asymmetric Schiff base ligands

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Schiff-base ligands and their coordination compounds have attracted the researchers' attention and taken an important area in chemistry as compounds having azomethine linkage (C═N) [1]. This interest is still growing due to their attractive properties, simple synthesis, stability, low toxicity, good biocompatibility [2] and diverse fields of applications in industry, medicine, analytic and catalysis [3]. To the best of our knowledge the nature of bond in metal complexes of salen type ligands have never been studied. Herein, we want to report a theoretical study on the strength and nature of metal−ligand bond in tetradentate (N_2O_2) asymmetric Schiff base ligands (Salpyr). The goemetry of all complexes were optimzed at BP86-D3/TZ2P level of theory using ADF program. Then, the nature of bond in the mentioned complexes was studied with an Energy Decomposion Analysis of metal−ligand bond.

Keywords: Theoretical Study, Schiff base complexes, Interaction and stabilization energies, Nature of bond

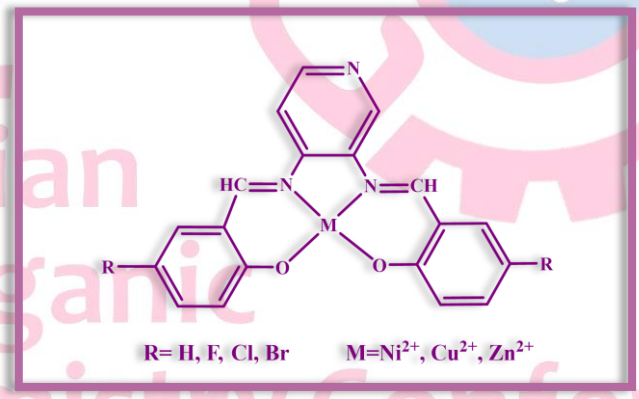


Figure 1. Chemical structure of metal complexes studied here

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