


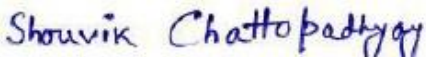
## Abstract

**“Studies on some mono-, di- and tri-nuclear complexes of transition and non transition metals with N,O donor Schiff bases and their reduced analogues”**

**Submitted by:** Smt. Ipsita Mondal, **[Index No.: 1/22/Chem./27]**

Several manganese(III), zinc(II) and cadmium(II) complexes with have been synthesized using different Schiff base and reduced Schiff base ligands. The complexes were characterized by elemental analysis, spectral study and single crystal X-ray diffraction analysis. The energetic features of Br $\cdots$ B interactions, hydrogen bonding and  $\pi\cdots\pi$  stacking interactions in some complexes have been calculated using DFT calculations and further corroborated with NCI plot index computational tools. Bader's Quantum Theory of Atoms-in-Molecules (QTAIM) was used to obtain insight into the physical nature of weak non-covalent interactions in both complexes. Additionally, the Reduced Density Gradient (NCI-RDG) methods nicely established the presence of such non-covalent intermolecular interactions. In terms of applications, some complexes showed good catalase mimicking activity (catalytic decomposition of hydrogen peroxide into oxygen and water). Some zinc complexes showed strong fluorescence, which may be quenched in presence of different nitroaromatic substances. The complexes were used for the detection of nitroaromatic explosives via turn-off fluorescence response.

  
16.02.2024  
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16.02.2024  
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