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Coordination behaviour and DFT studies of Copper(II) complexes of a novel chromone derived tetradentate Schiff base

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New Schiff base chelates of Copper(II) derived from the Schiff base ligand ethylenediaminobi(chromone-3-carbaldehyde) (FCED), *viz.*, [Cu(FCED)Cl]Cl (**1**), [Cu(FCED)Br]Br (**2**), $[Cu(FCED)(NO_3)](NO_3)$ (**3**) and $[Cu(FCED)](ClO_4)_2$ (**4**) have been synthesized and characterized. Microanalytical data, molar conductance and magnetic susceptibility values have been obtained and IR, UV-Visible, EPR spectral studies, TG/DTA, and DFT studies have been carried out to suggest the tentative structures of the complexes. The ligand acts as a neutral tetradentate ONNO donor ligand and the bonding sites are Nitrogen atoms of azomethine groups and Oxygen atoms of carbonyl groups. A square pyramidal geometry is suggested for complexes **1**, **2** and **3** and a square planar geometry is suggested for **4**. The crystal data indicate that the complex **3** crystallizes in monoclinic P21/n space group with a distorted square pyramidal structure and the π-π stacking interactions results in polymeric chains in unit cell of the complex.

Keywords: Copper(II) complexes, Schiff base, Spectra, Magnetic susceptibility, Single crystal structures, π-π Stacking interactions, DFT studies