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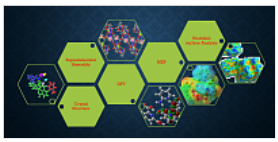
Co(II) coordination compound: structural and computational insights via crystal structure, DFT, MEP, NBO and Hirshfeld surface analyzes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A new coordination compound of Co(II) [Co(pydc) $_2$](pydcH $_2$)(Hapy)(H $_2$ O) $_5$ (**1**) (where, pydcH $_2$ = pyridine-2,6-dicarboxylic acid; Hapy = protonated 2-aminopyridine)was synthesized and characterized by single crystal X-ray diffraction (SC-XRD) analyses. Crystallographic analysis (CIF file CCDC no. 2236169) revealed that complex **1** has distorted octahedral geometry with pydc coordinated as a tridentate ligand to a metal ion. The electronic structure of the complex was determined using DFT calculations with pseudo potential of LANL2DZ basis function for Cobalt atom while B3LYP/GEN level using 6-31+G * basis set for other atoms. The optimized structure can reproduce the crystal structure with good accuracy at this computational level. Frontier molecular orbital analysis and molecular electrostatic potential (MEP) have been evaluated to understand the reactivity characteristics of the complex. Natural bond orbital (NBO) analysis illustrates the charge transfer between the donor and acceptor sites of the investigated complex. Further, the intermolecular contacts of the complex are analyzed through Hirshfeld surface analysis and finger print plots.

Keywords: *cobalt complex, crystal structure, DFT, Hirshfeld surface*