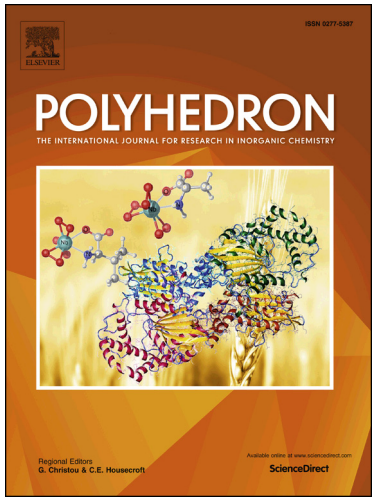

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Coordination environment of new Co(II), Ni(II) and Cu(II) complexes with 4-bromophenoxyacetic acid: Structural, spectroscopic and theoretical studies

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Abstract:

We report the synthesis of new Co(II), Ni(II) and Cu(II) complexes with 4-bromophenoxyacetic acid. We characterize these compounds structurally using various laboratory (XRF, IR, UV-VIS) and synchrotron (EXAFS, XANES) spectroscopic methods, magnetic measurements and DFT calculations. We found that in the powder form of complexes Co(II) and Ni(II) cations are coordinated by two monodentate carboxylate ligands and the first coordination sphere is completed by water molecules that form an octahedron. The coordination polyhedron of Cu(II) exhibits a distorted tetragonal-pyramidal geometry with two ligands coordinating in bidentate and monodentate fashion via carboxylate O atoms and two water molecules.

The X-ray single crystal structure analysis performed for Cu(II) complex after its recrystallization from *N,N*–dimethylformamide (DMF) solution revealed the formation of dinuclear complex. In crystals, the carboxylate O atoms occupy the bases of two tetragonal pyramids formed around two Cu(II) ions with the DMF molecules in the apical positions.