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Research paper

Synthesis, characterization and density functional theory of copper(II) complex and cobalt(II) coordination polymer for detection of nitroaromatic explosives

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ABSTRACT

In recent years there has been a significant interest to design luminescent materials to detect explosives with a great degree of selectivity, sensitivity, and fast response time. Two new luminescent compounds, [Cu(Biphen)(Meim)(H_2O)] 1 and [Co(BDC)(Meim)$_2$]$_n$ 2 (where HBiphen = biphenyl-4-carboxylic acid, H_2BDC = 1,4-benzenedicarboxylic acid and Meim = 1-methylimidazole) were synthesized under solvothermal and reflux conditions. The compounds were characterized by elemental analysis, FT-IR, thermogravimetric analysis, and electronic spectroscopy. Single Crystal X-ray Diffraction (SC-XRD) was used to determine their crystal structures. 1 crystallizes in the monoclinic space group *I*2/*a*, and the geometry around the metal center is square pyramidal connected by two (μ-N)$_2$ of Meim and two (μ-O)$_2$ of Biphen and a coordinated water molecule. 2 exhibits tetrahedral geometry connected by two (μ-N)$_2$ of Meim and two (μ-O)$_2$ halves of BDC in the triclinic space group *P*-1. Photophysical properties of the solid-state complexes were analyzed using fluorescence spectroscopy. 1 displayed high emissions at 430 nm (λ_{ex} = 264 nm) and 2 at 384 nm (λ_{ex} = 265 nm) which could be assigned to ligand to metal charge transfer (LMCT) due to the ligand's extended π-conjugation. Compounds 1 and 2 display selective nitroaromatic quenching response over other organic molecules having detection limits ranging between 1.66 ppm and 13.07 ppm, respectively. Density Functional Theory (DFT) revealed that potential interactions leading to the formation of adducts result from the transfer of electrons by hydrogen bonding and π-π stacking. Compound 2 was found to have greater ability to quench nitro analytes.