Journal of Inorganic and General Chemistry
ZAAC
Zeitschrift für anorganische und allgemeine Chemie

DOI: 10.1002/zaac.202000425

ARTICLE

Synthesis, structural and DFT investigation of $Zn(nba)_2(meim)_2$ for adsorptive removal of eosin yellow dye from aqueous solution

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A novel Zn(II) mixed-ligand complex, $Zn(nba)_2(meim)_2$ (**1**), synthesized from $Zn(NO_3)_2.6H_2O$, nitrobenzoic acid (Hnba) and 1-methylimidazole (meim) is reported. The complex was characterized by elemental analysis, FT-IR, powder and single crystal X-ray crystallography and TGA/DSC. **1** exhibits a tetrahedral geometry for Zn(II), which is coordinated to two carboxylate oxygen atoms from two nba anions and two imidazole nitrogen atoms from two meim molecules. Thermal analysis shows the stability of **1** up to 260 °C. The adsorption of eosin yellow (EY) dye on **1** was investigated. The adsorption capacity of **1** for EY amounted to 65.32 mg/g, fitting best into Langmuir isotherm and pseudo second order kinetic models. From DFT studies, it was determined that adsorption is predominantly due to electrostatic, hydrogen bonding and π-π interactions.