

## Influence of nitrogen donor ligands on the coordination modes of copper(II) 2-nitrobenzoate complexes: structures, DFT calculations and magnetic properties.

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### Streszczenie

Three novel copper(II) 2-nitrobenzoate complexes,  $[\text{Cu}(\text{g-pic})_2(2\text{-nitrobenzoate})_2]$  **1**,  $[\text{Cu}(\text{b-pic})_2(2\text{-nitrobenzoate})_2(\text{H}_2\text{O})_2]$  **2** and  $[\text{Cu}_2(\text{H}_2\text{tea})_2(2\text{-nitrobenzoate})_2]2(\text{H}_2\text{O})$  **3** (where g-pic = 4-methylpyridine, b-pic = 3-methylpyridine and H<sub>2</sub>tea = mono deprotonated triethanolamine), were isolated by addition of g-pic, b-pic and H<sub>3</sub>tea to the hydrated copper(II) 2-nitrobenzoate,  $[\text{Cu}_2(2\text{-nitrobenzoate})_4(\text{H}_2\text{O})_2]2\text{H}_2\text{O}$ , suspended in a methanol : water (4 : 1) mixture. The newly synthesized complexes have been characterized by elemental analyses, thermogravimetric analysis (TGA), spectroscopic techniques (EPR, IR and UV/Visible), magnetic susceptibility measurements, single crystal X-ray structure determination and DFT study. All compounds crystallize in the monoclinic crystal system with the P2<sub>1</sub>/c space group. X-ray structure determination revealed the presence of monomers in both **1** and **2** and dimer in **3** with the deprotonated oxygen atom of the H<sub>2</sub>tea ligand bridging two Cu(II) atoms. Two co-crystallized water molecules are also present in **3**. The crystal lattice is stabilized by C–HO hydrogen bonding interactions in **1** and O–HO, C–HO hydrogen bonding interactions in **2** and **3**. The dimeric complex exhibits relatively strong ferromagnetic exchange with  $J = 100 \text{ cm}^{-1}$  (corresponding to  $H = JS_1S_2$ ). The zero-field splitting parameters (zfs) of the dimer triplet states D and E were derived from HF EPR spectra recorded at moderately low temperatures. The sign of D was determined from low-temperature HF EPR spectra.

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