

Structural, magnetic and quantum-chemical study of dinuclear copper(II) thiophenecarboxylate and furancarboxylate complexes.

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The synthesis, spectral and magnetic properties, crystal and electronic structures of five dimeric copper(II) carboxylates, $[\text{Cu}_2(2\text{-tpc})_4(\text{H}_2\text{O})_2]$ (**1**), $[\text{Cu}_2(2\text{-tpc})_4(\text{DMSO})_2]$ (**2**) (where 2-tpc is 2-thiophenecarboxylate and DMSO is dimethylsulfoxide), $[\text{Cu}_2(5\text{-Me-2-tpc})_4(\text{DMSO})_2]\cdot 2\text{caffeine}$ (**3**), $[\text{Cu}_2(5\text{-Me-2-tpc})_4(\text{H}_2\text{O})_2]\cdot 0.488[(5\text{-Me-2-tpcH}\cdot\text{H}_2\text{O})_2]\cdot 0.012[\text{Cu}(5\text{-Me-2-tpc})_2(\text{H}_2\text{O})_2]$ (**4**) (where 5-Me-2-tpcH and 5-Me-2-tpc are 5-methyl-2-thiophenecarboxylic acid and its deprotonated anion, respectively) and $[\text{Cu}_2(2\text{-fuc})_4(\text{H}_2\text{O})_2]\cdot 2.5\text{H}_2\text{O}$ (**5**) (where 2-fuc is 2-furancarboxylate), are reported. All five complexes adopt dimeric paddle-wheel cage structures as revealed by X-ray analyses. Moreover, the crystal structure of **4** contains, apart from dimeric paddle-wheel molecules, also other molecules that exist as a result of substitutional disorders. EPR spectra and magnetic measurements for **1**, **4** and **5** confirmed an antiferromagnetic intramolecular interaction between the Cu(II) ions with $-2J$ coupling constants of 319, 334 and 327 cm^{-1} , respectively. Density functional calculations (B3LYP hybrid functional) have been carried out on the experimental geometries in order to study the magnetic properties of the respective complexes. The computed values of $2J$ are overestimated by ca $110\text{--}180\text{ cm}^{-1}$. Our calculations show that the coexistence of various conformers can be the source of different exchange coupling constants, despite their similar electronic structure parameters.

Słowa kluczowe

Cu(II) complexes, Paddle wheel structures, Carboxylates, Magnetism, Density functional theory

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