

Magneto-structural, Stabilizing Interactions, Thermal, and Molecular Docking Studies of Cu(II) Complexes with Sorbic and 3-Phenylpropanoic Acids and N-donor Ligands

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Streszczenie

The first structurally characterized Cu(II) complex of sorbic acid (SA), compound **1** [Cu₂(μ-SA)₄(MET)₂], along with the Cu(II) complex of 3-phenylpropanoic acid (PPA), compound **2** [Cu₂(μ-PPA)₄(METB)₂], were synthesized and characterized. These complexes, supported by metronidazole (MET) and metronidazole benzoate (METB), were analyzed using FTIR, UV-vis spectroscopy, PXRD, thermal analysis, and single-crystal X-ray diffraction. Structural studies revealed dimeric arrangements with centrosymmetric *syn-syn* bidentate ligand coordination. Quantum Theory of Atoms in Molecules (QTAIM) and Natural Bond Orbital (NBO) analyses highlighted weak dispersion interactions, including CH...O, NO₂...HC, C-H...π, and π...π stacking, as well as tetrel-type stabilization. Molecular docking studies revealed that compound **2** exhibited the most favorable binding energy with *Candida albicans* receptors (4YDE and 3DRA), involving key interaction residues commonly found in active ligands. The magnetic properties of compounds **1** and **2** were thoroughly investigated, modeled, and analysed, yielding exchange coupling constants ($J = -320 \text{ cm}^{-1}$ for **1** and -330 cm^{-1} for **2**), demonstrating strong antiferromagnetic interactions within the dicopper(II) tetrakis(μ-carboxylato)-bridged blocks.

Słowa kluczowe

Sorbic acid, 3-phenylpropanoic acid, NBO, T-shaped π interactions, magnetic properties

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