



Dinuclear Copper(II) Complex with Hemiaminal N,O-Donor Ligand

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Streszczenie

Novel copper(II) coordination compounds with hemiaminal N,O-donor ligands were obtained and synthesized in a one-pot reaction from three appropriate substrates (aldehyde, amine, and copper(II) chloride) in methanol. A dinuclear complex with a $[\text{Cu}_2\text{Cl}_2(\text{hemiaminal})_2(\text{amine})_2]$ coordination mode was obtained. The complex consists of two five-coordinated central Cu(II) cations with square pyramidal geometry and C_i molecular symmetry. The hemiaminal oxygen atom forms a bridge between the two metallic centers, and that coordination bond is a factor stabilizing these hemiaminal moieties, generally regarded as unstable intermediates. We analyzed the energetic and physicochemical properties of the $[\text{Cu}_2\text{Cl}_2(\text{hemiaminal})_2(\text{amine})_2]$ complex using density functional theory (DFT). First of all, we predicted the geometrical parameters, molecular electrostatic potential, HOMO and LUMO energies, and reactivity indices to indicate the free radical scavenging capacity. Based on the topological analysis of charge densities, we also characterized the properties of hydrogen bonds. Moreover, the antimicrobial properties of the complex were investigated, and it exhibited the highest activity against Gram-positive bacteria and *Candida albicans*.

Słowa kluczowe

hemiaminal, stable intermediate, coordination compound, copper complex, biological activity, DFT calculation, topological analysis

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