

New heteroleptic L-argininato copper(II) complex with bromide and N, N' - heterocyclic ligands - synthesis, supramolecular, spectroscopic, magnetic and theoretical investigations

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Streszczenie

A new heteroleptic $[\text{CuBr}(\text{L-Arg})(\text{bpy})]\text{Br}\cdot 2\text{H}_2\text{O}$ (**1**) ($\text{L-Arg} = \text{L-Arginine}$, $\text{bpy} = 2,2'$ -bipyridine) complex has been synthesized and its molecular and supramolecular structure aspects have been discussed based on the X-ray single crystal structure and Hirshfeld analyses. In addition, the properties of complex **1** have been elucidated using different spectroscopic methods (FT-IR / FIR, Raman, NIR-Vis-UV, Q- / X- band EPR) and magnetic measurements. In this complex, the bromide anion occupies the apex of a slightly distorted square pyramid ($\tau = 0.12$). The $[\text{CuBr}(\text{L-Arg})(\text{bpy})]^+$ complex units exhibit a ribbon-like organization, with Cu(II) metal centers located at the corners of triangles where the shortest Cu...Cu distance is 5.579 Å. The aromatic moieties of bpy are aligned nearly parallel leading to $\pi\cdots\pi$ interactions. Both, non-bonded and coordinated, Br^- ions act as hydrogen-bond acceptors for guanidinium groups. Hirshfeld analysis indicated the importance of the $\text{Br}\cdots\text{H}$ (17.9 – 18.4 %), $\text{O}\cdots\text{H}$ (14.9–15.2 %), and $\text{H}\cdots\text{H}$ (42.3–43.1 %) interactions in the molecular packing of the studied complex. Atoms in molecules (AIM) calculations indicated mainly the closed shell character for the Cu–N, Cu–O and Cu–Br coordination interactions. The G value calculated using the Q-band EPR spectra parameters $g_{\parallel} = 2.235$ and $g_{\perp} = 2.05$ is 4.7, what indicating negligible coupling and that local tetragonal axes are aligned parallel. A negative value of Weiss temperature $\theta_{\text{CW}} = -0.32$ K indicates the presence of weak antiferromagnetic coupling between the neighboring Cu(II) ions mediated through hydrogen bonds and π - π stacking of aromatic moieties of bpy. The value of $g_{\text{av}} = 2.113$ obtained from Q-band EPR spectra is consistent with that corresponding to the Curie constant ($C = 0.4138$ emu K mol^{-1}), *i.e.* $g = 2.101$, and that obtained from the best fitting to the Brillouin function: $g = 2.139$.

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