



The influence of ancillary NCS^- ions on structural, spectroscopic, magnetic and biological properties of copper(II) l-argininato complex

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Artykuł

The anions are one of the factors that govern the self-organization of the crystal structure involving $[\text{Cu}(\text{I-Arg})]^{2+}$ cation complex. Therefore, the crystals of hexa-coordinated *l*-argininato copper(II) complex with coordinated isothiocyanato ions, *trans*- $[\text{Cu}(\text{I-Arg})_2(\text{NCS})_2] \cdot 2\text{H}_2\text{O}$ (**1**), were synthesized and studied by X-ray structural analysis, spectroscopic techniques (FT-IR, Raman, X- and Q-band EPR, NIR-Vis-UV), magnetic and thermal methods. The distortion of elongated octahedron ($T = 0.757$) shows the static character. The complex presents a monomeric nature but the $[\text{Cu}(\text{I-Arg})_2(\text{NCS})_2]$ units are bound via O-H...O, N-H...O and N-H...N hydrogen bonds forming two dimensional layers. One broad band with three well-marked maxima at $15,850\text{ cm}^{-1}$, $16,630\text{ cm}^{-1}$ and $17,500\text{ cm}^{-1}$ are generated by ${}^2\text{B}_{1g}(\text{d}_{x^2-y^2}) \rightarrow \text{A}_{1g}(\text{d}_{z^2})$, ${}^2\text{B}_{2g}(\text{d}_{xy})$ and ${}^2\text{E}_g(\text{d}_{xz} \approx \text{d}_{yz})$ transitions. The values of g tensor components $g_{\perp}=g_x=g_y$ 2.056 (77 K) / 2.057 (298 K) agree well with the $g_{\perp}$ found for other *trans*- N_2O_2 chromophore with two chelating *l*-Arg-ligands in copper(II) xy plane. The relation of g_z ($g_{\parallel}=2.245$) $\gg g_x=g_y$ ($g_{\perp}=2.056$) > 2.0023 is characteristic for $\text{d}_{x^2-y^2}$ orbital of unpaired electron ground state in the axial symmetry of copper(II) environment. The field induced slow magnetic relaxation is observed, despite the lack of the zero-field splitting of Cu(II) monomeric complex **1**. Due to the labile character and the preference for distorted coordination geometries leading to plasticity of copper(II) coordination sphere, the comprehensive spectroscopic studies of the complexes arising in aqueous solutions when complex **1** was in aqueous solutions, were conducted (NIR-Vis-UV, EPR). The antimicrobial activity of **1** was evaluated against the yeast, dermatophyte and bacteria. *Microsporum gypseum* was the most sensitive strain, with a 4-time lower MIC comparing to the reference drug - Fluconazole.

Słowa kluczowe

Copper(II), *l*-Arginine, Isothiocyanate ions, Crystal structure, Spectroscopy (FT-IR, Raman, EPR, NIR-Vis-UV), Thermal properties, Magnetism, Solution studies

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