

Pseudohalide coligands guided structural motifs, magnetism and BSA-interactions of copper(II) complexes derived from 1,3-dimethyl-6-aminouracil

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Streszczenie

Two novel copper(II) complexes with mononuclear (**1**) and 1D polynuclear (**2**) structural motifs were synthesized using the novel planar tridentate ligand 1,3-dimethyl-5-(thiazolyl-azo)-6-aminouracil, H_2L (triclinic, $P\bar{1}$ space group and $Z = 2$) and pseudohalide coligands, namely azido and thiocyanato ligands. **1** is a monomeric-azo-azido complex with the monoclinic crystal system and $P2_1/n$ space group, whereas **2** is a 1D polynuclear coordination polymer of Cu(II)-azo- μ -SCN (μ -SCN is bonded in the end-to-end (anti mode) manner) with the orthorhombic crystal system and $Pbca$ space group. The crystallographic study, magneto-structural study and EPR spectra revealed distinctly that both complexes possess a slightly distorted square-pyramidal geometry about the Cu(II) ion. The observed and/or theoretical TDDFT bands show the nature of multiple intraligand, ligand-to-metal, metal-to-ligand charge transfer and d-d transitions. Direct current (dc) variable-temperature magnetic susceptibility measurements on polycrystalline samples of **1** and **2** were carried out in the temperature range 1.8–300 K. The copper(II) ions remain non-interacting at 300 K ($\chi_m T$: $0.417 \text{ cm}^3 \text{ mol}^{-1} \text{ K}$ for **1** and $0.361 \text{ cm}^3 \text{ mol}^{-1} \text{ K}$ for **2**). The Weiss constant for **1** is -2.3 K and for **2** it is 0.96 K , indicating that weak antiferromagnetic and weak ferromagnetic interactions exist in **1** and **2**, respectively. As expected, complex **1** exhibits an intermolecular type of interaction ($\chi' = -1.37(1) \text{ cm}^{-1}$), whereas **2** exhibits an intramolecular magnetic interaction ($J = 1.17(2) \text{ cm}^{-1}$) between the Cu(II) ions. The cause of the weak ferromagnetic coupling in **2** may be due to the orthogonality of the magnetic orbitals ($d_{x^2-y^2}$) involved in the equatorial-axial singly bridging SCN moiety. All the compounds show excellent binding interactions (K_A) with BSA, with the order complex **1** ($1.993 \times 10^4 \text{ M}^{-1}$) > complex **2** ($6.072 \times 10^3 \text{ M}^{-1}$) > free ligand ($2.619 \times 10^3 \text{ M}^{-1}$).

Słowa kluczowe

Thiazolyl-azo-6-aminouracil, Copper(II) complexes, X-ray structures, Magnetic coupling, BSA interactions

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