

Copper(II) Complexes of 1,3-Dimethyl-(5-(8'-quinolinylazo)-6-aminouracil: Structures, Magnetism and Biological activity

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Streszczenie

Two Cu(II)-complexes were synthesized using 1,3-dimethyl-5-(8'-quinolinylazo)-6-aminouracil (**H₂L**) ligand in combination with thiocyanide (SCN⁻) and azide (N₃⁻) pseudohalides as co-ligands. The thiocyanide (SCN⁻) co-ligand guided to form monomeric aquo-isothiocyanato-Cu(II) complex, [Cu^{II}(HL)(NCS)(H₂O)] (**1**) of H₂L. Under similar reaction condition, the azide (N₃⁻) co-ligand led to form polymeric azido-Cu(II) complex, [Cu^{II}(L')(N₃)]_n, (**2**) of HL', where HL' was an *in situ* generated new ligand, 1,3-dimethyl-(5-(8'-quinolinylazo)-6-hydroxouracil (HL') from H₂L. Both are tridentate ligands with different uracil-donor sites (H₂L: N_qN_aN_u, HL': N_qN_aO_u). The complexes are monoclinic with space groups C2/c (Z = 8) and P2₁/n (Z = 4) for **1** and **2**, respectively. They possess slightly distorted square-pyramidal coordination around Cu^{II} ions with elongation at the axial sites (Cu1-O3 (water) bond is 2.2698(13)Å for **1** and Cu1-O_{μ-uracil} bond is 2.5525(13)Å for **2**). The polymeric nature of **2** is availed through one of the exocyclic-C = O groups of HL', making Cu...Cu spacing to 7.9973(3)Å. 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 **1** is devoid of any significant interaction between the mononuclear units. Magnetic properties show weak ferromagnetic exchange coupling within the chain (*J* = 0.61 cm⁻¹) in **2**. The TD-DFT study reveals that ILCT, LMCT and d-d types of electronic transitions are involved in both the complexes. The evaluated biological efficacy of the compounds against plant pathogens it is revealed that the complex **1** has an antibacterial and complex **2** has antifungal properties.

Słowa kluczowe

Quinolinyl-azo-uracil, Copper(II)-complex, Structures, Ferromagnetism, Plant pathogens

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