

Antiferromagnetic cyclic tetrameric copper(II) complex and 8-azaxanthine derived from 1,3-dimethyl-5-(5'-methyl-3'-isoxazolyl-azo)-6-aminouracil: structures, non-covalent interactions and magnetism

Autorzy

Nishan Das
Nishithendu Bikash Nandi
Julia Kłak
Lesław Sieroń
Alexander S. Novikov
Waldemar Maniukiewicz
Tarun Kumar Misra

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The synthesis of uracil derivatives and their conversion to a number of potential compounds have drawn attention of researchers aiming to develop innovative materials. Therefore, a novel azo ligand, 1,3-dimethyl-5-(5'-methyl-3'-isoxazolyl-azo)-6-aminouracil (H_2L , **1**), was synthesized from 1,3-dimethyl-6-aminouracil and 3-amino-5-methyl-isoxazole. Compound **1** was converted to an 8-azaxanthine derivative, 1,3-dimethyl-8-(5'-methyl-3'-isoxazolyl)azaxanthine (**2**), *via* its reaction with $Cu(NO_3)_2 \cdot 6H_2O$ in DMF solution. Alternatively, when **1** reacted with $Cu(CH_3COO)_2 \cdot H_2O$ in the presence of NaN_3 in methanol, an antiferromagnetic Cu(II) complex (**3**) was formed, where Cu(II) is found to be coordinated with the *in situ*-generated novel ligand 1,3-dimethyl-5-(but-2-one-3-ene-4-amino-azo)-6-aminouracil (L^1) and azide ions. The structures of these compounds (**1–3**) were characterized using single crystal X-ray analysis. Complex **3** is a tetrameric assembly of Cu(II) with a nearly parallelogram shape. Its Cu(II) centers are interconnected through doubly end-on azide ($\mu_{1,1}$ -azide) bridges and doubly end-to-end azo ($\mu_{1,2}$ -azo) bridges. The theoretical study shows the presence of non-covalent interactions, including H-bonding and stacking interactions. Magnetic studies of **3**, a nearly parallelogram tetranuclear Cu(II) unit with side lengths of 3.7839(6) Å and 4.7727(8) Å, revealed that it possesses strong antiferromagnetic interactions, as evidenced by its exchange coupling constant $J_1 = -250$ (1) cm^{-1} through end-on azide bridging between the Cu(II) ions (Cu–N–Cu, 116°). Thus, the present study not only introduces a strong antiferromagnetic material, but also establishes a notable correlation between its structure and magnetic properties.

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