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1D and 2D porosity in monomeric copper(II) complexes with 1-piperidineacetic acid and 1-piperidineacetamide

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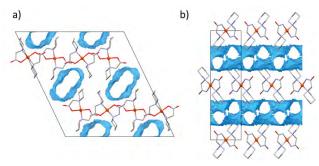
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1-piperidineacetic acid (HPAA) and 1-piperidineacetamide (HPAAM) can be treated as N-alkylated glycine and N-alkylated glycinamide. N-alkylated amino acids and their derivatives can find application as synthetic building blocks and play an important role in studies related to the structural properties and biological activity [1], [2]. Copper(II) complexes with amino acids and their derivatives were shown to be very interesting compounds for various fields of research, such as bioinorganic chemistry, medicinal chemistry and crystal engineering. Due to versatile noncovalent interactions, these complexes have the ability to form porous structures, coordination polymers, or other different architectures in the solid state [3]. Interestingly, only a few bis(N,N-dialkylamino acidato)copper and bis(N,N-dialkylamino acetamidato)copper complexes have been structurally characterized until now.

In this research we have synthesized and structurally characterized one ligand, HPAAM (1), two copper(II) complexes $[Cu(PAA)_2(H_2O)] \cdot 3H_2O$ (2) and $[Cu(PAAM)_2] \cdot 3H_2O$ (3), and a sodium salt [Na(PAA)(μ -H₂O)₄(H₂O)]·H₂O (4). Although the only difference between the ligands is the presence of either the carboxylic or the amide group, the influence on the supramolecular architectures of the copper(II) complexes is significant. In 2 a square-pyramidal complex is formed with two O,N-donating PAA ligands in the basal plane and a water molecule occupying the apical position. The molecules are connected into a 2D network through hydrogen bonds. 1D infinite channels of water molecules are formed (Fig. 1a). On the other hand, 1-piperidineacetamide forms a square-planar copper(II) complex hydrogen bonded into a 3D network with 2D infinite channels of water molecules (Fig. 1b). Both copper complexes exhibit trans-coordination, which is not as common in this type of complexes as the *cis*- coordination, probably due to bulky hydrophobic ligands. 1-piperidineacetic acid crystallized from an aqueous solution as a sodium salt forming a 2D coordination polymer 4 with sodium ions.

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Figure 1. a) 1D channels of water molecules in structure of 2; b) 2D channels of water molecules in structure of 3. Hydrogen atoms are omitted for clarity.



References:

[1] Gilon, C. et al. (2003). Houben-Weyl Methods of Organic Chemistry: Synthesis of Peptides and peptidomimetics, Vol. E 22c, edited by M. Goodman et al., pp. 215–271. Thieme: Stuttgart, Germany

[2] Belliotti, T. R. et al. (2005). J. Med. Chem. 48, 2294–2307.[3] Vušak, D. et al. (2017). Cryst. Growth Des. 17, 6049–6061.

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