

COPPER(I) CHLORIDE π -COMPLEXES WITH ALLYLSULFANYL DERIVATIVES OF 4-AMINO-5-PHENYL-4*H*-1,2,4-TRIAZOLEFedko A. M.¹, Yanchak A. I.¹, Slyvka Yu. I.¹, Goreshnik E. A.², Mys'kiv M. G.¹¹Department of Inorganic Chemistry, Ivan Franko National University of Lviv,

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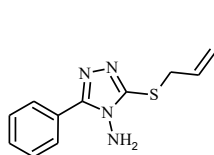
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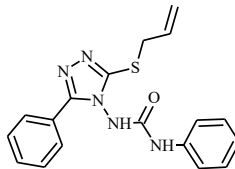
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1,2,4-Triazole derivatives have a wide range of applications in pharmaceutical chemistry and possess diverse pharmacological properties. These compounds also were found to be the excellent ligands for the crystal engineering of organometallic materials, possessing potential luminescent, catalytic, magnetic activity, etc.

In the present work, we present synthesis and crystal structures of two new CuCl π -complexes [Cu₂Cu^{II}(Triaz1)₂Cl₄] (**1**) and [Cu^I₄(Triaz2)₂Cl₄]·2H₂O·2C₃H₇OH (**2**) with 3-allylsulfanyl-4-amino-5-phenyl-4*H*-1,2,4-triazole (Triaz1) and N-phenyl-N'-{3-allylsulfanyl-4-amino-5-phenyl-4*H*-1,2,4-triazol-4-yl}urea (Triaz2).

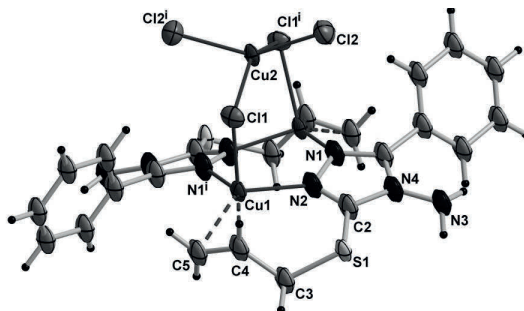


Triaz1



Triaz2

Crystals of complexes **1** and **2** were prepared by means of *ac* electrochemical synthesis from acetonitrile (for **1**) or *n*-propanol (for **2**) solutions of copper(II) chloride and corresponding Triaz. Complexes crystallize in the monoclinic system, **1**: Sp. gr. *C2/c*, $V = 3008.5(5) \text{ \AA}^3$, $Z = 4$; **2**: Sp. gr. *P2₁/c*, $V = 2600.3(3) \text{ \AA}^3$, $Z = 2$. The organometallic part in both complexes is represented by the {Cu₂(Triaz)₂}²⁺ dimers which are formed due to the chelating-bridging coordination behavior of the organic ligand. The Cu(I) cation adopts a close to a trigonal pyramidal coordination environment (2N, (C=C) + Cl). The basal plane of the coordination arrangement consists of the η^2 -allyl group and two N(*tr*) atoms. The axial site is occupied by a chlorine ion that is part of anionic inorganic fragments which are different in **1** and **2**. In structure **1** the anionic part is represented by {Cu^{II}Cl₄}²⁻ anion with a seesaw geometry, while in **2** – by closed to linear {Cu^ICl₂}⁻ fragment (Fig. 1).

Fig. 1. Fragment of crystal structure **2**. Symmetry code: (i) 1-x y, 1.5-z