

SYNTHESIS AND CRYSTAL STRUCTURE CHARACTERIZATION OF NOVEL COPPER(I) π -COMPLEXES WITH N-ALLYL-1,2,3-TRIAZOLE

Fedko A. M., Slyvka Yu. I., Mys'kiv M. G.

Ivan Franko National University of Lviv, Kyryla i Mefodiya 6, 79005 Lviv, Ukraine
af98@i.ua

1,2,3-Triazoles, being an important type of heterocyclic compounds, have a wide range of application in different spheres, in particular, they known as photostabilizers of polymers, optical brightening agents, corrosion inhibitors, dyestuffs. Due to their biological activity they find application in medicine as antibacterial, antiviral and anticancer agents. Moreover, due to triazole structure features they can mimic different functional groups, justifying their wide employment as bioisosteres. It was also investigated that triazole-based complexes with Cu(I) display NLO properties. Its exploration may be useful in the study of cancer progression mechanism which is accompanied with the change of copper(I) level in damaged tissues. Since a number of copper(I) π -complexes with benzotriazole allyl derivatives has been already studied, we present in this work firstly obtained Cu(I) π -compounds with allyl derivatives of monocyclic 1,2,3-triazole.

[Cu(C₅H₇N₃)Br] (**1**),
[Cu(C₅H₇N₃)₂CH₃C₆H₄SO₃] (**2**) and
[Cu(C₅H₇N₃)CF₃COO] (**3**) are novel π -complexes, which are obtained by means of an alternating current electrochemical technique starting from non-water solution of CuBr₂, Cu(CH₃C₆H₄SO₃)₂·xH₂O, Cu(CF₃COO)₂·xH₂O with the mixture of 1- and 2-allyl-1,2,3-triazole-1,2,3. The crystal structures of **1–3** (Table) were determined by means of single crystal X-ray diffraction. In all of the structures the crystallographically independent copper(I) atom with trigonal pyramidal environment is present. Isomer-selective complexation has been observed: in compounds **1** and **2** 1-N-allyl-1,2,3-triazole plays bridging role, but, in the complex **3** (Fig.) tridentate 2-N-allyl-1,2,3-triazole fully realizes its coordination abilities performing chelate-bridging π,σ -function. The structures of complexes **1–3** possess polymeric chains. Presence of Br[–] anion in **2** leads to doubling of infinite chains. These chains, in turn, are associated into 3D structure by non-valent weak interactions.

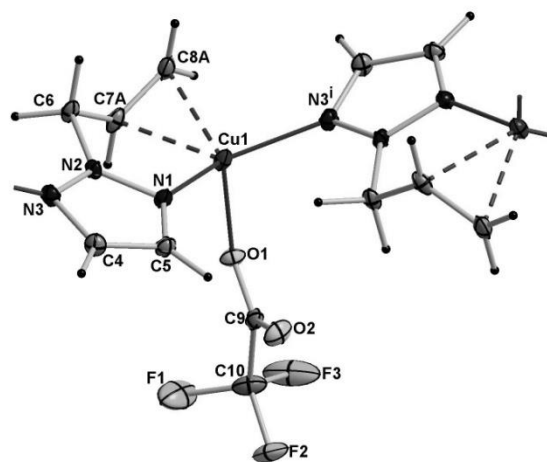


Fig. Fragment of crystal structure 3

Table. Selected crystal data for **1–3** π -compounds

No	Composition	Space group	V, Å ³	Z	Density g/cm ³	Coordination type
1	[Cu(L1)Br]	P-1	377,2(3)	2	2,224	σ, π
2	[Cu(L1) ₂ CH ₃ C ₆ H ₄ SO ₃]	P2 ₁ /c	1970,4(12)	4	1,527	σ, σ, π
3	[Cu(L2)CF ₃ COO]	P2 ₁ /n	964,8(6)	4	1,967	σ, π

It should be noted, that complex **2** is the first example of structurally characterized copper(I) *p*-toluenesulfonate π -complex.