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THE CRYSTAL STRUCTURE AND ANTITUMOR ACTIVITY OF 1,6-DINITRATO-BIS[2-(5-METHYLSULFANYL)-4-(PROP-2-EN-1-YL)-4--(1,2,4-TRIAZOL-3-YL)PYRIDINE]COPPER

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The aim of this work is the determination of structural features and biological properties of the coordination compound obtained by the reaction between copper(II) nitrate and 2-formylpyridine 4-allyl-S-methylisothiosemicarbazone.

The experiment showed that mentioned above substances react in ethanolic solutions regardless of the combined molar ratios forming fine-crystalline dark green coordination compound with composition $C_{22}H_{24}N_{10}O_6S_2Cu$ (**I**). The X-ray diffraction analysis of obtained monocrystals of the complex **I** showed that there is not any molecule of initial isothiosemicarbazone. The coordination compound **I** is a square-bipyramidal copper(II) complex which contains two ligands of 2-(5-methylsulfanyl)-4-(prop-2-en-1-yl)-4-(1,2,4-triazol-3-yl)pyridine (L). This ligand has formed in the reaction mixture as a result of oxidative cyclization of 2-formylpyridine 4-allyl-S-methylisothiosemicarbazone. These molecules L are in the inner sphere of the coordination compound in the equatorial plane. They behave like bidentate ligands coordinating to the central atom of copper by pyridinic and azomethinic nitrogen atoms forming five-membered metallacycles. Such case of template cyclization of thiosemicarbazone ligand has been previously described in the literature source [1]. The apical positions are occupied by two monodentate nitrate ions.

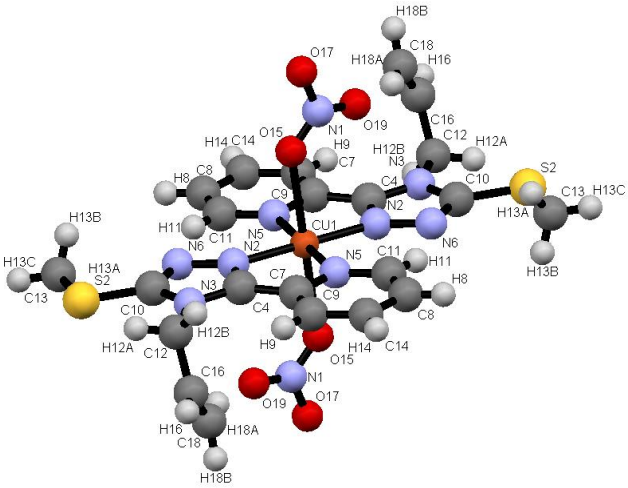

Fig. 1. The crystal structure of **I**

It is known that coordination compounds with such ligands in many cases manifest biological activity. Therefore, it was studied antitumor activity of this coordination compound. It was determined that thee synthesized complex selectively inhibits the growth and proliferation of human promyelocytic leukemia HL-60 cells at the concentration 10^{-5}mol/L for 98%. At the concentration 10^{-6} mol/L and 10^{-7} mol/L it inhibits 6 and 3% of these cells, respectively.

This work showed that the study of new biometal coordination compounds with ligands obtained from heterocyclic aldehyde, ketones and thiosemicarbazones has prospects.

References:

1. V.V. Bon, S.I. Orysyk, V.I. Pekhnyo. Russian Journal of Coordination Chemistry, 2011, Vol. 37, No. 2, pp. 149–152.

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