The crystal structure of 2-(tetrazol-1-yl)pyridine complexes with Cu(II) and Co(II) chlorides

Y. V. Grigoriev, A. S. Lyakhov, L. S. Ivashkevich, S. V. Voitekhovich, A. I. Lesnikovich Research Institute for Physical Chemical Problems, Belarusian State University, Minsk, Belarus, e-mail: azole@bsu.by

As a part of our investigations concerned with the synthesis of tetrazole derivatives and their complexes with transition metals, 2-(tetrazol-1-yl)pyridine (L) was prepared by heterocyclization of 2-aminopyridine with triethyl orthoformate and sodium azide.

The interaction of L with $CuCl_2 \cdot 2H_2O$ (molar ratio 1 : 1) in ethanol at 70 °C results in two complexes: 1) CuL_2Cl_2 , deposited as a fine turquoise powder by cooling the reaction mixture to the room temperature; 2) $[CuLCl_2(H_2O)]_n$, crystallizing by slow evaporation of mother solution after separation of CuL_2Cl_2 to obtain crystals suitable for X-ray analysis. X-ray data of $[CuLCl_2(H_2O)]_n$ showed that it is monoclinic (S.G. $P2_1/n$). The compound presents 1*D* coordination polymer formed due to chlorine atoms (Cl1 and Cl2) acting as two bridges between neighboring copper atoms inside the chains. Both bridges, Cu–Cl1–Cu and Cu–Cl2–Cu, are asymmetrical, in which one bond Cu–Cl is of usual length and another bond is considerably elongated. The copper atoms have essentially elongated octahedral coordination, with the tetrazole ring N⁴, O atom of the water molecule together with two Cl atoms in the equatorial plane, and two Cl atoms in the axial sites.



CoL₂Cl₂(H₂O) complex was crystallized by slow evaporation at room temperature of ethanol solution containing L μ CoCl₂·6H₂O at molar ratio 2 : 1. According to single crystal X-ray analysis, it presents a molecular complex, crystallizing in the monoclinic space group $P2_1/c$. The cobalt atom forms a distorted octahedral coordination with O atom of the water molecule, two Cl and three N atoms of two ligands L. One ligand is bonded to the metal monodentately *via* the tetrazole ring N⁴ atom, whereas another one shows bidentate chelating binding through the terazole ring N² and the pyridine ring N atoms. It should be noted that the tetrazole N² atom, as a rule, is not coordinated by metal atoms in 1-substituted tetrazoles, and only solitary examples are known with this coordination.

Acknowledgment. This study is supported by Belarusian Republican Foundation for Fundamental Research, project X14P-038.