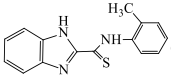
XRD STUDIES OF THE COMPLEX COMPOUND OF COPPER(II) WITH SUBSTITUTED HETEROCYCLIC THIOAMIDES

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The crystalline structure of compound (Fig. 1) is a salt of a complex cation and perchlorate anion (1:2 ratio). The complex cation consists of copper(II) cation, thioamide ligand  and isopropyl alcohol (1:2:1 ratio). The hydrogen atom of the hydroxyl group in isopropyl alcohol is objectively observed, which suggests that the copper atom is neutrally coordinated with the isopropyl alcohol molecule. The copper atom is the five-coordinated atom (coordination polyhedron – distorted square pyramid). The atoms of sulfur and nitrogen forming the basis of the pyramid do not lie in the same plane (the angle between the lines N(1)...S(1) and N(2)...S(2) is 26°), which is probably due to repulsion between sulfur atoms and atoms of bicyclic fragments (shortened intramolecular bonds S(1)...H(17) 2.88 Å (the sum of van der Waals radii 3.00 Å [1], S(2)...C(2) 3.33 Å (3.55 Å), S(2)...H(2) 2.75 Å (3.00 Å)). Bicyclic fragments of the ligands are flat with an accuracy of 0.01 Å. The five-member metal cycle Cu(1), S(1), C(8), C(7), N(1) is in the envelope conformation. The deviation of the S(1) atom from the mean square of other atoms is 0.1 Å. Metal cycle Cu(1), S(2), C(23), C(22), N(4) is flat with an accuracy of 0.01 Å. The thionic group S(1)=C(8) is somewhat turned relative to the bicyclic fragment (torsion angle S(1)–C(8)–C(7)–N(1) 8.9(6)°), whereas the thionic group S(2)=C(23) lies in the benzimidazole plane (torsion angle S(2)–C(23)–C(22)–N(4) 2.4(5)°). The atoms N(3) and N(6) have a trigonal-planar configuration, despite the shortened intramolecular bonds H(3N)…H(2N) 1.88 Å (2.32 Å), H(3N)…N(2) 2.43 Å (2.66 Å), H(6N)…H(5N) 1.78 Å (2.32 Å), H(6N)…N(5) 2.29 Å (2.32 Å).

Due to rotation around the bond Cl(1)–O(5) perchlorate anion $[ClO_4]^-$ in the copper(II) complex exists in two conformations with the contributions of 82 and 18%, respectively.

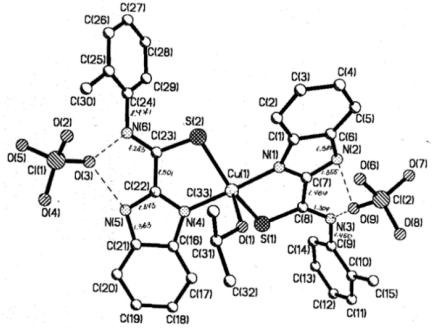


Fig. 1. Molecular structure of copper(II) complex

The most important bond lengths, Å: Cu(1)–S(1) 2.398(5), Cu(1)–N(1) 1.968(5), Cu(1)–S(2) 2.356(4), Cu(1)–N(4) 1.945(5), S(1)–C(8) 1.691(6), N(1)–C(7) 1.317(9), C(7)–C(8) 1.464(9), N(1)–C91) 1.388(4), N(2)–C(7) 1.355(8), N(3)–C(8) 1.305(8), S(2)–C(23) 1.687(7), N(40–C(22) 1.305(8), C(22)–C(23) 1.501(6) N(6)–C(23) 1.284(8), N(4)–C(16) 1.424(9), N(5)–C(22) 1,344(7). Valence angles, grad: N(1)–Cu(1)–S(1) 84.6(5), N(1)–Cu(1)–S(2) 93.5(5), N(4)–Cu(1)–S(2) 84.2(4), N(4)–Cu(1)–S(1) 96.9 (6), S(2)–Cu(1)–S(1) 145.8(7), N(4)–Cu(1)–N(1) 177.6(2), N(4)–Cu(1)–O(1) 91.0(2), N(1)–Cu(1)–O(1) 90.5(2), N(4)–Cu(1)–S(2) 84.2(4), O(1)–Cu(1)–S(2) 115.4(7)