The crystal structure of aqua(N-salicylidene-methylester-L-glutamato)Cu(II) monohydrate has been determined. The structure was refined by SHELXL-97 to R = 0.0344 for 5318 unique reflections taken at the temperature 183 K, 229 parameters being refined. The crystal structure consists of the molecular units [Cu(N-sal-5-met-L-glu)(H2O)] connected by three dimensional network of hydrogen bonds. The coordination polyhedron in the complex is approximately square-pyramidal with the pentacoordinated Cu(II) atom. The base of the pyramid is formed by the phenolic O3, carboxylic O5 and azometine N1 atoms of the Schiff-base anion and by O4 atom of the water molecule. The apex of the pyramid contains weakly bonded O6 atom of the carboxylic group of another molecule. The base of the pyramid bond distances are $1.9267(14)$, $1.9492(14)$, $1.9312(16)$ and $1.9715(14)$ Å, respectively. The apical bond length is $2.3929(15)$ Å. The chemical quantum mechanical calculations of the electron structure were done by Gaussian98 program package using B3LYP/SVP method and basis set. The calculation of Mulliken population analysis, and contributions of individual atomic orbitals to Cu-O and Cu-N bonds were done for doublet as the most stable multiplet state. Calculated bond populations indicated that while the bonds Cu1 to O3, N1 and O5 are almost equivalent ($0.211, 0.228, 0.201$), respectively, the Cu1-O4 bond is significantly weaker ($0.137$). Synthesis and structure determination of title compound was stimulated due to found antimicrobial activities of Cu(II) complexes containing Schiff - bases derived from salicylaldehyde and L-glutamic acid as well as its methyl and ethyl esters.

Keywords: Cu(II) COMPLEX SCHIFF BASE B3LYP

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**STRUCTURE AND BIOLOGICAL ACTIVITY OF Zn(II) COMPLEX WITH TRIS(BENZIMIDAZOL-2-YLMETHYL)AMINE(NTB) LIGAND**

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Since the structures of superoxide dismutase (SOD) exhibit that most of the coordinated atoms around metal ions are from imidazole groups of histidine, which are the primary ligands in distorted coordination geometry [1-2], an important step should be to design to synthetic models of SOD in which ligands should contain imidazole groups. In order to elucidate the properties of SOD model compounds, a new Zn (II) mononuclear complex with NTB was synthesized with stoichiometry of $\text{ZnNTB}_2(\text{NO}_3)_2\text{dipy}_2\text{dmf}_2\text{dipy}$ (dipy: 4,4-dipyridyl). The complex was characterized with element analysis, UV and IR spectra. The crystal structure was determined using X-ray diffraction method. A total of 7975 reflections were collected on a Bruker AXS Smart-1000 CCD diffractometer. 4844 observed reflections were used in the structure analysis and refinements with 514 variables. The structure was solved by direct and fourier synthesis method. The crystallographic parameters are as follows:

$\text{Zn} \cdot \text{H}_2 \text{O} \cdot \text{NTB} \cdot 2 \text{H}_2 \text{O}$.$\text{Cu} \cdot \text{O} \cdot \text{NTB} \cdot 2 \text{H}_2 \text{O}$

The reaction of copper(II) carboxylates with 4-aminoypyridine (4-apy) were investigated and their products structurally characterized by single crystal X-ray diffraction. Reaction of Cu(II) acetate resulted in two isomers of the composition $\text{Cu(acetate)}_2(4\text{-apy})_2$ with markedly different stability; the violet form - unstable in air and the blue - stable form. In both isomers the ligands are arranged around the copper atom in a trans mode. The 4-apy ligands lie almost in the plane in the violet form, while they are twisted with respect to each other in the blue form. Variations were observed also in the coordination of the acetate groups to the copper ion.

Monomeric complexes of the same stoichiometry were obtained also by the reaction of Cu(II) hexanoxate (hex) and heptanoxate (hep) with 4-apy. The violet Cu(hex)$_2$(4-apy)$_2$ and Cu(hex)$_2$(4-apy)$_2$, are isomortic and possess trans geometry of the ligands around the copper centre. Reaction of 4-apy with Cu(II) octanate lead to a formation of a novel, unprecedented basic centrosymmetric tetranuclear compound of composition $\text{Cu4(octa)}_2(\text{OH})_2(4\text{-apy})_2$, Molecule contains bidentate bridging and monoatomic bridging carboxylate groups, triply bridging hydroxyl groups and 4-aminoypyridine as a terminal ligand. In all five compounds 4-apy is coordinated through endocyclic nitrogen atom only.

Keywords: COPPER(II) COMPLEXES CARBOXYLATES AMINO PYRIDINE

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**THE X-RAY INVESTIGATION OF CO(III) DIOXIMATE COMPLEXES WITH BF$_4$ OR CF$_3$SO$_3$ ANIONS**

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An investigation of Co(III) dioximate complexes, has shown that the reaction conditions play a determining role on their composition, structure and biological properties. X-ray analysis of five new Co(III) dioximates, with tetrafluoroborate and triflate anions, $\text{[Co(DH)}_2(\text{NH}_3)_2\text{BF}_4$, $\text{[Co(MH)}_2(\text{Thio)}_2\text{BF}_4$, $\text{[Co(NioxH)}_2(\text{Py)}_2\text{BF}_4$, $\text{[Co(DH)}_2(\text{Thio)}_2\text{CF}_3$SO$_3$ and $\text{[Co(DH)}_2(\text{Py})_2\text{CF}_3$SO$_3$], indicates that the metal has a normal octahedral environment. The 4-N equatorial plane (eq), formed by two residues of (DH), (MH) and (NioxH) (DH: dimethylglyoxime, MH: methylglyoxime and NioxH: nioxyme), are coplanar within 1.2-1.6°. The mean Co-N$_{eq}$ distance is 1.886 Å. The apical positions of the polyhedron are occupied by the nitrogen and sulphur atoms of the NH$_3$, Thio or Py ligands. The mean Co-N(NH$_3$) , Co-S(Thio) and Co-N(Py) distances are 1.964, 2.281 and 1.963 Å, respectively. The DH ligands are linked by two O…H…O intramolecular hydrogen bonds, mean O…O distance of 2.52 Å. The nature of the equatorially coordinated ligand, or the different neutral ligands in the trans positions, does not change the configuration of the complex cation. Biological tests indicate that the tetrafluoroborate complexes have a much stronger influence on the enzymatic activity of the genera Aspergillus niger 33, as an amylase producer, compared to the triflate complex.

Keywords: COPPER(II) COMPLEXES, ANION, HYDROGEN BOND

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**CRYSTAL AND ELECTRONIC STRUCTURE OF AQUA-SALICYLIDENE-METHYLESTER-L-GLUTAMATO(Cu(II)) MONOHYDRATE**

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Reactions of copper(II) carboxylates with 4-aminoypyridine (4-apy) were investigated and their products structurally characterized by single crystal X-ray diffraction. Reaction of Cu(II) acetate resulted in two isomers of the composition $\text{Cu(acetate)}_2(4\text{-apy})_2$ with markedly different stability; the violet form - unstable in air and the blue - stable form. In both isomers the ligands are arranged around the copper atom in a trans mode. The 4-apy ligands lie almost in the plane in the violet form, while they are twisted with respect to each other in the blue form. Variations were observed also in the coordination of the acetate groups to the copper ion.

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Keywords: Cu(II) COMPLEX SCHIFF BASE B3LYP

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