**Mononuclear Cu(II) complexes with polypyridyl ligands, 2,4,6-tris(2-pyridyl)-1,3,5-triazine (tptz) and bis(2-pyridylcarbonyl)amido (bpca); Study of catalytic effect of Cu(II) in hydrolysis reaction of tptz**

Khatereh Abdi

k.abdi@ch.iut.ac.ir

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Department of Chemistry

Isfahan University of Technology, Isfahan 84156-83111, Iran

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**Supervisor: Hassan Hadadzadeh, hadad@cc.iut.ac.ir**

**Abstract**

In this thesis, two mononuclear polypyridyl complexes of Cu(II), [Cu(tptz)Cl2]·2H2O and [Cu(tptz)2](PF6)2·CH3CN, (where tptz is 2,4,6-tris(2-pyridyl)-1,3,5-triazine) have been prepared and characterized by elemental analysis, FT-IR and UV–Vis spectroscopies. Solid state structures of both complexes were determined by single crystal X-ray crystallography. Green crystals of [Cu(tptz)Cl2] were grown by ether diffusion into a methanol solution of the complex. In this complex, Cu(II) is five-coordinate and the tptz ligand is coordinated as a tridentate chelate, with one Ntriazine and two Npyridyl atoms. The FT-IR spectrum of this complex shows that the *ν*(C═N) and *ν*(C═C) shift to higher frequencies in comparison to the free tptz ligand. Electronic spectrum of this complex was taken in methanol. The intense absorption bands seen in the UV region are assigned to ligand-centered transitions and a weak absorption band seen in the visible region is assigned to *d*–*d* transition. Elemental analysis and ORTEP drawing of this complex shows that the [Cu(tptz)Cl2] complex is crystallized with two water molecules.

Air-stable green crystals of [Cu(tptz)2](PF6)2·CH3CN were grown by slow evaporation of an acetonitrile/toluene solution of the complex. In this complex, the tptz ligands are tridentate and linked to the Cu(II) *via* three N atoms and the CuN6 entity has a compressed octahedral geometry with the shortest Cu–N bonds that form the axial positions. It represents a Z-in distortion at 90(2) K. The shortness of the Cu–Ntriazine bonds compared to the Cu–Npyridyl bonds is suggested to be due to the stronger *π*-accepting properties of the triazine ring. ORTEP drawing and elemental analysis of this complex shows that the [Cu(tptz)2](PF6)2 complex is crystallized with an acetonitrile molecule. The lattice structure is further stabilized by a network of weak hydrogen bonds between the H atoms of the pyridyl rings of the tptz ligand and the F atoms of the PF6– anions. The FT-IR spectrum of the complex shows a sharp and intense absorption band around 840 cm–1 for the *ν*(P–F). The intense absorption bands seen in the UV region of the electronic absorption spectrum of this complex are assigned to ligand-centered transitions and a weak absorption band seen in visible region is a *d*–*d* transition.

Catalytic effect of Cu(II) in hydrolysis reaction of tptz was also studied. Hydrolysis of an aqueous solution of [Cu(tptz)Cl2]·2H2O produces a coordination polymer, [Cu(bpca)Cl]n , where bpca is bis(2-pyridylcarbonyl)amido ligand. The [Cu(bpca)Cl]n complex was characterized by elemental analysis, FT-IR and UV–Vis spectroscopies and X-ray crystallography. The structural determination shows that the [Cu(bpca)Cl]n complex is a 1D coordination polymer and the Cu(II) ions are five coordinate with distorted square-pyramidal geometry. A careful inspection of the packing pattern in the lattice of the complex reveals that non-covalent interaction of the C–H···O type is active in the lattice. The FT-IR spectrum of the [Cu(bpca)Cl]n complex exhibits a sharp band at 1716 cm–1 that is ascribable to the stretching frequency of the C═O bonds on the bpca ligand.

The qualitative observation of the hydrolysis reaction of [Cu(tptz)Cl2]·2H2O by UV–Vis spectroscopy in LF region shows an isosbestic point. The presence of this isosbestic point shows that the concentration of intermediate(s) is constant.

**Keywords:**

Cu(II) complexes, Polypyridyl ligands, 2,4,6-Tris(2-pyridyl)-1,3,5-triazine, Bis(2-pyridylcarbonyl)amido,Crystal structure, Z-in distortion, Isosbestic point.