Keywords: vanadium compounds, X-Ray crystallography, hydrogen bonds

FA4-MS34-P22

Redetermination of Crystal Structure of

bis(salicylaldoximato)copper(II). <u>Mehmet Kabak</u>, Ankara University, Faculty of Engineering, Department of Engineering Physics,06100 Tandoğan, Ankara, Turkey

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The crystal structure was determined by using oscillation photographs method with the space group and lattice constants of $P2_1/n$, a=27.61 Å, b=6.00 Å, c= 7.86 Å an =98.17° for the first time [1]. Later, same crystal structure was solved by Weissenberg photographic method with the space group of $P2_1/c$ and the lattice parameters as a=13.98(1) Å, b=6.08(1) Å, c=8.00(1) Å, β =97.35° [2]. Because of the large standard deviations of the unit cell and atomic parameters and fairly large *R* values at the previous works the crystal structure of bis(salicylaldoximato) copper(II) was redetermined. The precise and corrected unit cell parameters were given by using X-Ray single crystal diffractometer [3,4] and the structure was solved with SHELXS-97 [5] and refined to *R*=0.057 value with SHELXL-97 [6].



[1] Cox, E.C. & Webster, K.C. J. Chem.Soc.. 1935, 731.[2] Jarski,
M.A. & Lingafelter, E.C. Acta Cryst., 1964, 17, 1109–1112.[3] Frenz,
B.A. Enraf-Nonius Structure Determination Package. Enraf - Nonius,
Delft, The Netherlands, 1985.[4] Stoe & Cie REDU4. Data Reduction
Program. Version 6.2. Stoe & Cie, Dramstadt, Germany, 1988.[5]
Sheldrick, G.M. Acta Cryst. 1990, A46, 467–473.[6] Sheldrick, G.M.
SHELXL97:Program for the refinement of crystal structures.
University of Goettingen, Germany, 1997.

Keywords : redetermination, salicylaldoximato

FA4-MS34-P23

Syntheses and Crystal Structure of bis(2-(2-Thienyl)-4,5-dihydro-1*H*-imidazole) Copper(I) Iodide. <u>Hadi</u>

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Imidazoline derivatives are of great importance because they exhibit significant biological and pharmacological activities

including antihypertensive, antihyperglycemic, antidepressive, antihypercholesterolemic and antiinflammatory properties [1]. The metal complexing ability of some bidentat ligands containing imidazoline rings reported previously [2]. Coordination chemistry of copper(I) complexes has received increased attention over the last decades. The steric, electronic, and conformational effects imparted by the coordinated ligands play an important role in modifying the properties of the prepared metal complexes. We have reported the crystal structure of (2-(2-Thienyl)-4,5-dihydro-1*H*imidazole) [3]. Here we report the crystal structure of new copper (I) iodide complex with thienylimidazoline ligand.

[1] Vizi, E. S. Med. Res. Rev. 1986, 6, 431.[2] Lever, A. B. P.;
 Ramaswamsy, B. S.; Simonsen, S. H.; Thompson, L. K. Cand. J. Chem. 1970, 48, 3076. [3] Kia, R.; Fun, H. -K.; Kargar, H. Acta.Crtst. 2009, E65, o301.

Keywords: Imidazoline, Copper (I) Complex, Crystal structure

FA4-MS34-P24

A star-shaped iodocuprate(I) cluster anion crystallizing with a bulky Cu(I)-tetraazaphenanthrene cation complex: crystal structure of [Cu(Ph₄TAP)₂]₂[Cu₅I₇]. <u>Reza Kia</u>, Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran E-mail: <u>zsrkk@yahoo.com</u>

Reaction of copper(I) halides, CuX, with nitrogen-based ligands (L) yields CuXL_n adducts. These halogenocuprate(I) complexes exhibit a wide variety of stoichiometries, with structures mainly based upon a tetrahedral copper coordination [1]. The structural richness in halogenocuprate(I) crystallizing with different cations has been rationalized in term of the cation size [2]. A series of systematic studies on halogenocuprate(I) indicates that the anion configuration, i.e. the coordination number of copper(I) and the tendency of the anion to form polymeric structures, depends on the degree of dilution imposed on the halides by the cation [4]. The simples rule that, with decreasing cation size and also changing from Cl through Br to I, the tendency to attain a high coordination number and towards catenation in crystalline halogenocuprate(I) increases provides a facile framework for understanding a range of observation [2]. In this study, the solid-state structure of the title complex, reveals ionic complexes containing a cation of copper(I) coordinated to four nitrogen atoms of the two 2,3,6,7tetraphenyl-1,4,5,8-tetraazaphenanthere (Ph₄TAP) ligands (distorted tetrahedral) and a star-like hepta-µ-iodopentacuprate(I) anion. There are two possible orientations of the copper(I) pentahedron which results in partial occupancy of the crystallographic copper(I) sites.

 Kiechner, R. M., Mealli, C., Bailey, M., Howe, N., Torre, L. P., Wilson, L. J., Andrews, L. C., Rose, N. J., Lingafelter, E. C., *Coord. Chem. Rev.* 1987, 77, 89. [2] Jagner, S. *Adv. Inorg. Chem.* 1991, 37, 1.

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