

Structural and chemical details of the title compound will be reported.

[1] Alexander Hübner, Thomas Bernert, Inge Sängler, Edith Alig, Michael Bolte, Lothar Fink, Matthias Wagner, Hans-Wolfram Lerner, *in preparation*. [2] David, W. I. F., Shankland, K., Van de Streek, J., Pidcock, E. & Motherwell, S. (2004). DASH Version 3.0. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, England. [3] Coelho, A. (2007). TOPAS-Academic Version 4.1. Coelho Software, Brisbane, Australia.

Keywords: Mesityllithium, powder data, Rietveld refinement

FA4-MS34-P19

Crystal structure of Cu complex with pyridine-2,6-dicarboxylic acid and 9-aminoacridine.

Jafar Attar Gharamaleki^a, Zohreh Derikvand^b and Helen Stoeckli-Evans^c, ^aYoung Researchers Club, Islamic Azad University, North Tehran Branch, Tehran, Iran, ^bDepartment of Chemistry, Faculty of Science, Islamic Azad University, Khorramabad Branch, Khorramabad, Iran, ^cInstitut de Physique, Université de Neuchâtel, Rue Emile-Argand 11, C.P. 158, CH-2009 Neuchâtel, Switzerland

E-mail: attar_jafar@yahoo.com

Recently, we have defined a plan to prepare water soluble proton transfer compounds as novel self-assembled systems that can function as suitable ligands in the synthesis of metal complexes [1,2]. In this regard, we prepared new (AacrH)₂[Cu(pydc)₂] · 3H₂O compound in which (pydcH₂) is pyridine-2,6-dicarboxylic acid and (Aacr) is 9-aminoacridine. Cu^{II} compound crystallized in triclinic crystal system with two molecules per unit cell. The anion was six-coordinate complexes with distorted octahedral geometries around the Cu^{II} centers. The negative charges of [Cu(pydc)₂]²⁻ species in this compound were neutralized with (AacrH)⁺ cations, protonated at the endocyclic nitrogen atom, as counter-ions. Extensive π-π stacking interactions between two aromatic rings of 9-aminoacridine with distances ranging from 3.3498(18) to 3.8718(17) Å, were observed in the title compound. Non-covalent interactions such as hydrogen bonding (consisting O—H...O, N—H...O and C—H...O hydrogen bonds), π-π and C=O...π stacking interactions (with O...π distances ranging from 3.564(2) to 3.834(2) Å) play important roles in stabilizing the structures.

[1] H. Aghabozorg, J. Attar Gharamaleki, M. M. Olmstead and Z. Derikvand, S. Hooshmand, *Acta Cryst.*, 2009, E65, m186. [2] H. Aghabozorg, Z. Derikvand, M. M. Olmstead and J. Attar Gharamaleki, *Acta Cryst.*, 2008, C64, m372.

Keywords: crystal structure, Cu(II) complex, π-π stacking interactions

FA4-MS34-P20

Synthesis, molecular structure, spectroscopic studies of cyanide-bridged Mn(III)Ni(II) Complex.

Elif Gungor^a, Hulya Kara^a, Mairi F. Haddow^b, ^aDepartment of Physics, Balikesir University, Balikesir, Turkey, ^bThe School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK

E-mail: elifonly@gmail.com

The cyanide bridged complex [Mn₂(L1)₂][Ni(CN)₄]₃ (C₂H₆O) 3H₂O (**1**) (L1=(3,5-di tert-butyl-2 hydroxybenzaldehyde-1,2-diaminopropane) has been prepared and characterized by spectroscopic and single crystal X-ray analysis. Single crystal X-ray structure analyses have shown that the crystal structures of **1** is ionic and are built up of [Mn(L1)]²⁺ cations, [Ni(CN)₄]²⁻ anions, water and ethanol molecule. In the complex, two quadridentate ligands are bonded to the Mn(III) ion in a distorted octahedral arrangement and the Ni(CN)₄²⁻ anion remains outside the coordination sphere.

Keywords: Cyano-bridged complex, X-ray diffraction, Schiff Base Ligand

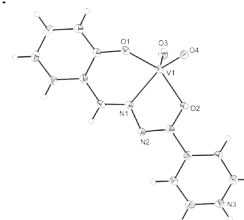
FA4-MS34-P21

Synthesis and crystal structure of a vanadium(V) complex with salicylaldehyde

isonicotinoylhydrazone. Liudmila Gusina^a, Ion Bulhac^a, Diana Dragancea^a, Yurii Simonov^b, Sergiu Shova^b, ^aInstitute of Chemistry, Academy of Sciences of Moldova, Chisinau, Moldova, ^bInstitute of Applied Physics, Academy of Sciences of Moldova, Chisinau, Moldova

E-mail: lgusina@gmail.com

The catalytic properties of vanadium compounds and their effects in biological systems or as therapeutic agents have led to an increasing interest in the coordination chemistry of this element. In this paper we report the synthesis and single-crystal X-ray diffraction study of mononuclear vanadium(V) complex [VO₂(HL)] with salicylaldehyde isonicotinoylhydrazone H₂L. The crystal is monoclinic, space group P2₁/n, *a* = 7.14930(10), *b* = 14.5150(2), *c* = 11.9411(2) Å, β = 94.410(2)°, *V* = 1235.48 Å³, *Z* = 4 for C₁₃H₁₀VN₃O₄. The vanadium(V) atom adopts a square-pyramidal geometry coordinated by the tridentate Schiff base ligand stabilized in E form and two oxygen atoms in *cis* positions. The N1–N2 = 1.395(3), N2–C8 = 1.308(3) and C8–O2 = 1.299(3) (Å) bond distances put in evidence the enolate form of the amide functionality. X-ray diffraction study has demonstrated the protonation of the pyridine ring, which was also observed earlier in Fe^{III} and V^V complexes with a related ligand [1,2]. The crystal structure is stabilized by a strong intermolecular N–H...O H-bonds, involving the protonated pyridinic nitrogen and the equatorial oxo ligand (N3–O4', 2.61(2) Å; ∠N3–H...O4' = 164.5°).



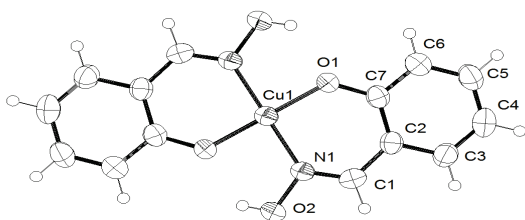
[1] Richardson D.R., Bernhardt P.V., *J. Biol. Inorg. Chem.*, 1999, 266. [2] Yu, Q., Li, Ch.-Y., Bian, H.-D., Liang, H., Song, H.-B., Wang, H.-G. *Chinese. J. Struct. Chem.*, 2007, 37.

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

FA4-MS34-P22

Redetermination of Crystal Structure of bis(salicylaldoximato)copper(II). Mehmet Kabak, *Ankara University, Faculty of Engineering, Department of Engineering Physics, 06100 Tandoğan, Ankara, Turkey*
E-mail: kabak@eng.ankara.edu.tr

The crystal structure was determined by using oscillation photographs method with the space group and lattice constants of $P2_1/n$, $a=27.61 \text{ \AA}$, $b=6.00 \text{ \AA}$, $c=7.86 \text{ \AA}$ and $\beta=98.17^\circ$ 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 $a=13.98(1) \text{ \AA}$, $b=6.08(1) \text{ \AA}$, $c=8.00(1) \text{ \AA}$, $\beta=97.35^\circ$ [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-1H-imidazole) Copper(I) Iodide. Hadi Kargar^a, Reza Kia^b, Islam Ullah Khan^c, ^a*Department of Chemistry, School of Science, Payame Noor University (PNU), Ardakan, Yazd, Iran*, ^b*Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran*, ^c*Materials Chemistry Laboratory, Department of Chemistry, GC University, Lahore 54000, Pakistan*
E-mail: hkargar@pnu.ac.ir

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 bidentate 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-1H-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.; Ramaswamy, B. S.; Simonsen, S. H.; Thompson, L. K. *Cand. J. Chem.* 1970, 48, 3076. [3] Kia, R.; Fun, H. -K.; Kargar, H. *Acta.Cryst.* 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]. Reza Kia, *Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran*
E-mail: zsrkk@yahoo.com

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 simple 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 2,3,6,7-tetra-phenyl-1,4,5,8-tetraazaphenanthrene (Ph₄TAP) ligands (distorted tetrahedral) and a star-like hepta- μ -iodocuprate(I) anion. There are two possible orientations of the copper(I) pentahedron which results in partial occupancy of the crystallographic copper(I) sites.

[1] 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.

Keywords: halocuprate(I), tetraazaphenanthrene, ionic adduct