

**Figure 1.** Cadmium(II) 1D coordination polymer with chloride and isoniazid (a) and 2D coordination polymer with thiocyanate and isoniazid (b)

**Keywords:** coordination polymer, cadmium, isoniazid, niazid, crystal structure, weak interactions

## MS30-P22 Structural, spectroscopic and activity studies of biomimetic resorcinarene-based zinc and copper complexes

Aleksandar Višnjevac<sup>1</sup>, Jérôme Gout<sup>2</sup>, Olivia Bistri<sup>2</sup>, Olivia Renaud<sup>2</sup>

1. Institut "Ruđer Bošković", Bijenička 54, 10000 Zagreb, Croatia  
2. Université Paris Descartes, CNRS UMR 8601, 45, Rue des Saints Pères, F-75006 Paris, France

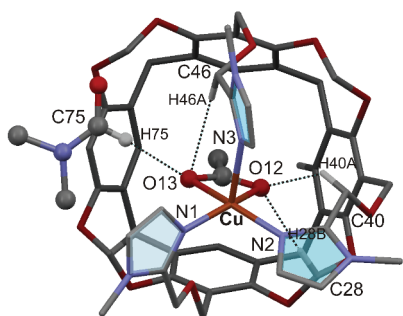
email: aleksandar.visnjevac@irb.hr

The syntheses, chemical characterizations, and activity studies of Zn(II), Cu(I) and Cu(II) "bowl" complexes, based on the resorcin[4]arene scaffold with three imidazole-containing coordinating arms at the large rim, is presented. These complexes are biomimetic models of a mononuclear active site where cofacial triade of amino-acid residues holds the metal coordinated. The trisimidazole ligand RIm3 was prepared in a seven-steps procedure. The complexes of Zn(II), Cu(I) and Cu(II) were prepared by simple reactions of the ligand with stoichiometric amounts of corresponding salts. Spectroscopic studies [and X-ray single crystal analysis in case of the Cu(II) acetato complex] revealed a 5-coordinate SBP environment for the Zn(II) and Cu(II) centres provided by three imidazole arms, and two extra donors, one embedded inside the resorcinarene cavity, the other in exo position. These two labile sites are occupied by solvent molecules or residual water, and are readily displaced by carboxylate donors, the position of which (endo or exo) is under tight control of the cavity. The reaction of RIm3 ligand with Zn(II) or Cu(II) acetates led to the formation of the acetato complexes with the acetate irreversibly embedded inside the cavity. The molecular structure of the Cu(II) acetato complex features a rigidified resorcinarene bowl. The isolated resorcinarene basket possess a non-crystallographic,  $4mm$  point symmetry, and can easily host small guest molecules. Three methylimidazole-containing coordinating arms at the large rim coordinate the Cu(II) ion. Its coordination sphere is completed by two O atoms from the intra-cavity bound acetate. The electron donors form a distorted square pyramide, where one of the nitrogens is at the apical position. The endo-coordination of the acetate is supported by an extensive network of intramolecular C-H $\cdots$ O and C-H $\cdots$  $\pi$  interactions. Complex crystallizes in  $P2_1/c$  space group;  $a = 32.3310(4)$  Å,  $b = 11.5490(1)$  Å,  $c = 21.6020(2)$  Å,  $\beta = 102.281(3)^\circ$ .

[1] Višnjevac, A.; Gout, J.; Ingert, N.; Bistri, O.; Renaud, O. (2010) *Org. Lett.* **12**, 2044 - 2047.

[2] Gout, J., Višnjevac, A., Rat, S., Bistri, O., Le Poul, N., Le Mest, Y. & Renaud, O. (2013) *Eur. J. Inorg. Chem.* 5171 – 5180.

[3] Gout, J., Višnjevac, A., Rat, S., Parrot, A., Hessani, A., Bistri, O., Le Poul, N., Le Mest, Y. & Renaud, O. (2014) *Inorg. Chem.* **53**, 6224 – 6234.



**Figure 1.** Structure of  $[\text{RIm}_3\text{Cu(II)CH}_3\text{COO}]\text{ClO}_4$ , top view

**Keywords:** resorcinarene, biomimetic, zinc, copper, X-ray single crystal diffraction, IR, NMR, EPR

## MS30-P23 Through the looking glass: anomalies and packing

Alice Brink<sup>1</sup>

1. University of the Free State, Chemistry Department, P.O. Box 339, Bloemfontein, 9301, South Africa

email: [alice.brink@gmail.com](mailto:alice.brink@gmail.com)

The formation and substitution of mono-, bi- and tridentate ligand substituted organometallic complexes to tailor the reactivity and biological activity of potential radiopharmaceuticals is filled with unexpected developments. X-ray crystallography grants undeniable advantages to “peer through the looking glass” in understanding the chemical trends in Group 7 (I) tricarbonyl complexes.

Our interest in the variation induced by ligand systems on *fac*- $[\text{M}(\text{CO})_3]^+$  complexes allows for interesting solid state as well as solution mechanistic studies utilising a range of spectroscopic techniques in addition to crystallography. The mixed ligand concept supports the platform of labelling the bioactive molecules to the transition metal complex utilising various bifunctional chelators. The solid state behaviour and the kinetic rate of substitution are widely influenced by the charge of the coordinated ligand system and the effects of the substituted monodentate incoming ligand. Isostructural and polymorphic crystallization effects will be described in addition to the substitution effects caused by incoming ligands with various acid/ base characteristics.

**Keywords:** Radiopharmaceutical design, substitution kinetics