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Condensation of isonicotinic hydrazide and acetylacetone resulted in the formation of novel V-shape organic ligand (L) that consists of a six-membered pyridine and five-membered hydroxyl, dimethylsubstituted diazole cycles joined via carbonyl bridge [1]. The metathesis reaction between [Co(DfgH)2Br(H2O)] (DfgH2=diphenylglyoxime) and L resulted in mononuclear octahedral complex [Co(DfgH)₂BrL] (1) with the substitution of water molecule in apical position by L ligand (Fig. 1). The dihedral angle between the cycle units is equal 49.5° in L in 1. The reaction starting from $[Co(DmgH)_2Cl(H_2O)]$ (DmgH=dimethylglyoxime) and Lresulted in the mononuclear octahedralCo(III) complex again with the composition [Co(DmgH)₂ClL'] (2), were unexpectedly L' represent the dehydrated derivative of L (Fig. 2). The dihedral angle between pyridine and diazole rings is equal 88.8° in L' in **2**. While the organic molecules L/L' have several donor centers, both ligands act as monodentate ligands and coordinate with metal atom by nitrogen atom of pyridine fragment.





Acknowledgements: This work was supported by the 10.819.05.03F project.

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Keywords: cobalt(III), coordination compound, X-ray

MS24.P59

Acta Cryst. (2011) A67, C379

Influence of ligand substituent on molecular architecture; Very large changes in structural assembly and coordination geometry <u>Hamid Reza Khavasi</u>, Maryam Mehdizadeh, Mahmood Azizpoor Fard. Department of Chemistry, Shahid Beheshti University, G.C.,

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The planning in coordination crystal engineering, construction of the structures of crystalline coordination compounds, [1] depends on a number of experimental variables such as the solvent, time of reaction, reagent ratio, temperature, pH, guest molecules and counterions. In this regard, chemical structure of the organic ligand [2] -eventh slight of the substitute position- and preferred coordination geometry of the metal [3] play an important role on the formation of different molecular architecture of complexes in the assembly processes. To make progress in controlling specific interactions in the solid state of coordination compounds requires systematic investigations of the effects of different factors on the final structures. Despite to the potential utility, from crystal engineering point of view, there has been little attention to systematic studies that examine the effect of the substituent variation of the ligand on the supramolecular aggregation of coordination complexes.

In this study, *N*-(aryl)-2-pyrazinecarboxamide ligands with two different aryl groups (o-anisidyl, L1, and o-phenitidyl, L2, groups) have been employed for the synthesis of six Hg (II) complexes, $[HgCl_2(L1)_2]_n$, $[HgBr_2(L1)]_n$, $[HgI_2(L1)]_n$, $[Hg_3Cl_6(L2)_3$ -HgCl_2(L2)], $[HgBr_2(L2)]$ and $[HgI_2(L2)]$ in order to get insights to the substituent effects on the molecular architecture of complexes. Structural analysis of mercury (II) halides containing L1 ligand demonstrated that the assembly process produced infinite 2D structures. For mercury (II) halides containing L2 ligand, the assembly processes are involved weak interaction between monomeric Hg(II) coordination compounds.

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Keywords: carboxamide, mercury, crystal engineering

MS24.P60

Acta Cryst. (2011) A67, C379-C380

New supramolecular dimer and 2D-supramolecular layers formation through hydrogen bonds

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Coordination compounds with both donor A–H and acceptor B groups and forming hydrogen bonds are used as building block for construction of supramolecular networks. Some copper(II) carboxylate complexes have shown that the intermolecular H-bonds can alter their magnetic properties. We have recently published mononuclear molecular complex [1], binuclear molecular complex [2] and more coordination polymers [3,4] which exhibit similar magnetic properties. These very similar magnetic properties of mononuclear, binuclear as well as polymeric complexes could be explained by the presence of very similar H-bond systems, supramolecular synthons, that are pathway for antiferromagnetic interactions.

In this report we present new supramolecular dimer [Cu(3-Brbz)₂(dena)(H₂O)₂] (3-Brbz is 3-brombenzoate, dena is *N*,*N*-diethylnicotinamide as terminal ligand) and series of 1D-coordination polymers of general formula [Cu(RCO₂)₂(μ -dena)(H₂O)]_n (RCO₂ are 3-chlorbenzoate, 4-chlorbenzoate or 3,5-dichlorbenzoate, and dena as bridging ligand) with similar system of hydrogen bonds and properties. The hydrogen bonds described by $R_2^2(10)$ and $R_2^2(12)$ supramolecular