

## MS38-P6 The influence of oxime group substitution on hydrogen bonding patterns in pyridine-based complexes of Cd(II)

Ivan Kodrin<sup>1</sup>, Vedran Barbarić<sup>1</sup>, Ina Erceg<sup>1</sup>, Aleksandar Višnjevac<sup>2</sup>, Marijana Đaković<sup>1</sup>

1. Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A, 10000 Zagreb, Croatia

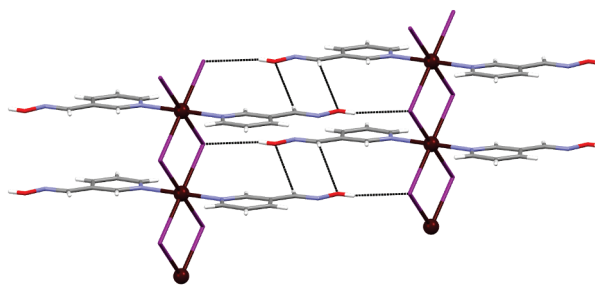
2. Laboratory for chemical and biological crystallography, Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

email: ikodrin@chem.pmf.hr

The synthesis and characterization of new materials together with the investigation of their physical properties represent areas of the greatest interest in chemistry today. Our knowledge about controlling the way in which metal-complexes, ligands and counter-ions assemble into more complex structures is rising every day. Even though each new discovery about the very intriguing and sometimes ambiguous relationship between a chemical structure of single molecules and non-covalent interactions that might govern their formation into higher-order structures is a one step closer to the successful design of new materials with desired properties. Moreover, even the simplest variations in chemical structure like exchange of hydrogen bond donors and acceptors, halide counter-ions may influence propensity toward specific hydrogen bond patterns.

Followed by the same idea, we have examined newly synthesized cadmium-based complexes linked to polymeric chains capable of acting as robust supramolecular synthons, yet enough flexible to accommodate to slight variations in molecular structure. Transformed pyridine-based ligands have at least two functionalities – they are able to complexate metals and form intermolecular interactions depending on substituents of aromatic ring. Therefore, they have already been well documented in literature as plausible building blocks and a logical joint between solely organic- and solely inorganic-based three-dimensional architectures.

This research work utilizes an experimental and theoretical approach in order to gain new insights about the supramolecular behavior of cadmium halide complexes with pyridine-based ligands functionalized in positions three and four with an oxime group. We report a synthesis of ligands and the derived complexes including description of crystallization techniques, spectral characterization, and determination of thermal properties. A computational study help us in further analysis of intermolecular interactions important for assembly of molecules in three-dimensional networks and to rationalize whether a dimeric supramolecular motif labeled as  $R^2_2(6)$  according to graph-set theory prevails over  $R^2_2(8)$ , or *vice versa*.



**Figure 1.** Intermolecular interactions between neighbouring polymeric chains,  $[CdI_2(3-oxpy)_2]_n$ .

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