Crystal engineering in mercury (II) coordination compounds based on pyrazine carboxamide ligand

Ali Reza Azhdari Tehrani, Hamid Reza Khavasi, Department of Chemistry, Shahid Beheshti University, G. C., Evin, Tehran 198396113, (Iran). E-mail: a_azhdari@sbu.ac.ir

Crystal engineering is a flourishing field of research in modern chemistry. Contemporary crystal engineering involves the design and synthesis of crystals. The aim of this endeavor is the development of new crystalline materials with a variety of properties, functions, and applications.

Among the non-covalent motifs, hydrogen bonding, metal-ligand coordination, and pi-stacking have been employed as synthetic paradigm to rationally design superstructures.

Herein, we report crystal engineering of mercury (II) halides of N-Phenyl-2-pyrazine carboxamide, which are obtained of N-Phenyl-2-pyrazine carboxamide with mercury (II) chloride & Bromide.

In this regards, To explore the supramolecular trends exhibited by molecules that can engage simultaneously in metal-ligand coordination, hydrogen bonding, and pi-stacking interactions, N-Phenyl-2-pyrazine carboxamide was prepared and its coordination chemistry and crystalline packing behavior was investigated. This ligand consists of three structural parts: (1) a pyrazine group that can coordinate to a metal, (2) a carboxamide group, which can have hydrogen bonding interactions through the amide nitrogen atom as well as via the carbonyl oxygen atom, and (3) a phenyl group, which can be involved in pi-stacking interactions.

In our design, the metal center assemble the ligand into the required geometrical orientation. From the packing diagram of carboxamide ligand , it is clear that hydrogen bonding between amide moiety and (Ph)C-H and pi-stacking between pyrazine and Phenyl ring are the dominant factors. In [HgCl2(L)], the molecule contains One Hg(II) with distorted tetrahedral geometry, two chlorine and a carbonyl oxygen and pyrazine nitrogen atom. For [HgBr2(L)], the structure consists of two ligands and two Hg ions bonded to form dimeric complexes. Each metal is four coordinated as bridging and bonded to two halogen atoms, one pyrazine nitrogen atom, and one carbonyl oxygen atom from the second ligand. All two complexes have been expanded by Hydrogen Bonding and pi-stacking to supramolecular entities.

Keywords: carboxamide, mercury, crystal engineering

MS24.P67

Synthesis and crystal structure of Ho(phen)(NO3)3

Taraneh Hajiahsrafi,1 Ali Nemati Kharat,2 Ali Reza Ghanbarpour,3 Hamid Reza Khavasi,4* School of Chemistry, University College of Science, University of Tehran, Tehran. 3Department of Chemistry, Shahid Beheshti University, G. C., Evin, Tehran 198396113, (Iran). E-mail: t_estafanii@khayam.ut.ac.ir

Rare earth metal cations are of growing importance for their

Keywords: carboxamide, mercury, crystal engineering