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**Keywords:** MOFs, transformation, 3D compound

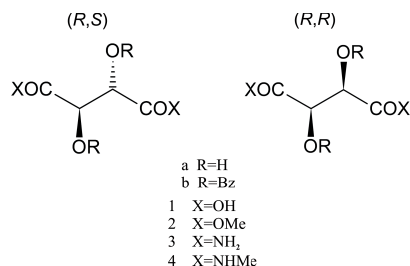
## MS24.P65

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### The many facets of tartaric acid its diesters and diamides

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Versatile possible chemical modifications, a variety of stereochemical forms and a great hydrogen bond capacity make tartaric acid and its derivatives interesting objects for structural studies. We have investigated the crystal structures of several derivatives of (*R,S*)-tartaric acid (the so called *meso* tartaric acid) and performed comparative analysis with their *R,R* counterparts. The obtained results have been analyzed in terms of chirality, conformation, molecular and crystal symmetry and supramolecular synthon robustness. Among the factors that affect molecular conformation local dipolar CH/CO interactions, intramolecular hydrogen bonds and a tendency to situate hydroxyl groups in mutually *gauche* orientation have been considered. The role of hydroxyl substituents as symmetry breaking elements will be illustrated. A link between hydrogen-bond synthons, as identified by X-ray analysis, and grow synthons present in solution as a consequence of thermodynamically driven self-association equilibria will be addressed. In this respect, a particular attention will be paid on formation of polyamide supramolecular ladder motifs, which in condensed media are by far more important than the maintenance of the preferred molecular conformation.



**Keywords:** tartaric acid derivatives, H-bond synthons, symmetry breaking

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

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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 endeavour 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-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-pi stacking interactions, N-Phenyl-2-pyrazine carboxamide was prepared and it's 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-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-pi stacking between pyrazine and Phenyl ring are the dominant factors. In [HgCl<sub>2</sub>(L)], the molecule contains One Hg(II) with distorted tetrahedral geometry, two chlorine and a carbonyl oxygen and pyrazine nitrogen atom. For [HgBr<sub>2</sub>(L)], the structure consists of two ligands and two Hg ions bonded to form dimeric complexes. Each metal is four coordinated 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-pi stacking to supramolecular entities.

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**Keywords:** carboxamide, mercury, crystal engineering

## MS24.P67

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### Synthesis and crystal structure of Ho(phen)<sub>2</sub>(NO<sub>3</sub>)<sub>3</sub>

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Rare earth metal cations are of growing importance for their

industrial, biochemical, and medicinal application [1]. Although rare earth metal cations are widely used, little is known about the stability and the structure of their complexes in solution. In the absence of strongly stabilizing ligands, the complex formation is often precluded by the competition for the coordination sites from the solvent molecules and the counteranions. Metal complexes of phenanthroline and other structurally related ligands are of increasing importance in studies with DNA. Obviously, investigation on rare earth metal complexes of phenanthroline are of significant value for modern coordination chemistry [2,3].

Herein, we report crystal structure of  $\text{Ho}(\text{phen})_2(\text{NO}_3)_3$ . The branched tube method was employed for the preparation of suitable single crystals.  $\text{Ho}(\text{phen})_2(\text{NO}_3)_3$  was synthesized from the mixture of  $\text{Ho}(\text{NO}_3)_3$  and phenanthroline in stoichiometric amount. The title compound was placed in one arm of a branched tube, methanol was carefully added to fill both arms, the tube sealed and the compound containing arm immersed in a bath at  $80^\circ\text{C}$ , while the other was at ambient temperature. After 2 days, crystals were deposited in the cooler arm which was filtered off, washed with ether, and air dried. The tencoordinate Ho(III) ion is chelated by four N atoms from two phenanthroline (phen) ligands and six O atoms from three bidentate nitrate groups. The environment around the Ho atom can be described as a distorted bicapped square antiprism. It is believed that the Phen ligand may displace the coordinated water molecules. Almost all of the complexes were crystallized in the monoclinic space group  $\text{C2}/c$  [4]. In the title compound, four nitrogen atoms (from two phen ligands) and six oxygen atoms from three bidentate nitrate groups are coordinated to the central Ho(III) ion. Bond lengths and angles have normal values. In the crystal structure, short intermolecular distances between the centroids of six-membered rings prove an existence of  $\pi$ - $\pi$  interactions, which link the molecules into stacks extended in direction. The crystal packing is further stabilized by the weak intermolecular C—H $\cdots$ O hydrogen bonds.

In conclusion, synthesis and crystal structure of  $\text{Ho}(\text{phen})_2(\text{NO}_3)_3$  has been investigated.

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**Keywords:** holmium, phenanthroline, rare earth elements

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### X-Ray diffraction and photophysical studies on new platinum complexes

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Non covalent interactions highly contribute to the arrangement of smaller molecules into more elaborate structures generating a diverse number of different architectures. They have also been recognized to play an important role in molecular recognition, crystal engineering, self assembly and molecular electronics [1-3]. Besides, some of these weak interactions ( $\pi$ - $\pi$  or Pt $\cdots$ Pt) can display rich photoluminescent properties fairly different from the observed in the single molecules.

We report the preparation of a new 2, 6-diphenylisonicotinic derivative, its mono- and bis-cycloplatination, using a slightly modified version of the Rourke's method [4]. Reactions of this new compound  $[(\text{EtO}_2\text{C}-\text{C}^{\wedge}\text{N}^{\wedge}\text{C})\text{Pt}(\text{DMSO})]$  with a range of monodentate

and bidentate ligands as well as with some metallic species gave rise to a brand new series of platinum (II) complexes which were analitically and spectroscopically characterized.

Solid state structures of these complexes have also been determined by X-ray diffraction studies, showing, the presence of weak inter- and intramolecular interactions (metal---metal,  $\pi$ --- $\pi$ , C-H--- $\pi$  and C-H---X). All these weak non-covalent interactions lead to the generation of different supramolecular bi- and tridimensional structures.

Photophysical studies have been performed on these complexes whether in solid state or in solution, showing a correlation between the crystalline structures and the emissive behaviour.

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**Keywords:** platinum, photophysics, X-Ray diffraction

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### Gel-based dimensionality control in multifunctional coordination polymers

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The use of gels as a crystal growth media of a wide range of compounds has been reported in the literature including inorganic salts, organic molecules, coordination compounds and also proteins. Gel media enables a mass transport in a convection-free diffusive regime, reducing the nucleation rate and generally improving crystal quality. In addition, higher degrees of supersaturation without instantaneous nucleation can be reached with crystallization in gels, enabling the access to metastable phases and inducing polymorphism. On the other hand, the use of gels can tune the ratio metal to ligand ratio when used in advanced crystallization techniques such as the counter diffusion method and thus lead to the formation of compounds with different dimensionalities [1].

The properties of metal-organic compounds depend to a large extent in the different dimensionality they may present (isolated complexes, 1D, 2D, or 3D coordination polymers). Moreover, the same ligands and metal atoms can form different dimensioned polymorphs and hydrates [2]. The aim of this research work is to control systematically the obtaining of the different polymorphs and hydrates of the coordination polymers prepared by diffusion through different gel media (varying the conditions), and in studying the nature and properties of the crystals obtained.

A family of coordination polymers with transition metals (Mn, Co, Ni, Cu, Zn) and mixed ligands (2,6-Naphthalenedicarboxylic acid: *NDC*, and 4,4'-bipyridine: *44bipy*) has been analyzed. Isolated (0D) structures and 1D paddle-wheel complexes of this family of compounds are found in the literature with Co, Ni and Zn, all of them obtained by hydrothermal synthesis [3-4].

