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[1] R.Pavan, P. Maia, S.Leite, S. Deflon, V. Batista. *European Journal of Medicinal Chemistry* **2010**, *45*, 1898-1905. [2] P. Yogeewari, D. Sriram, V. Veena, R.Kavya, K.Rakhra. *Biomedicine & Pharmacotherapy* **2005**, *59*, 51-55.

Keywords: semicarbazone, single-crystal X-ray diffraction, DFT.

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Crystal engineering of hydroxybenzoic acids. Influence of solvent in the synthon diversity and crystal packing

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Systematic analysis of intermolecular interactions formed between various molecular building units is an interesting topic in the area of crystal engineering. [1] Although the acid-pyridine interactions are well known in literature, the studies pertaining to triazines are relatively rare. Melamine is an interesting candidate due to its symmetry and the availability of several hydrogen bond donor and acceptor functionalities. Further, it is an important compound from the industrial and economical perspective. The recognition patterns of melamine with a series of substituted hydroxybenzoic acids have been studied with the assumption that the OH and COOH groups can make a cooperative influence in the recognition process and results in diverse synthons and supramolecular architectures. All these complexes form solvated assemblies and the solvent of crystallization plays an important role in the structure stability. The molecular adducts exhibit a salt-cocrystal continuum and the formation of the salts cannot be predicted on the basis of ΔpK_a values, as most of the molecular candidates have similar pK_a values.[2] The synthon diversity and the crystal packing in terms of intermolecular interactions provide useful inputs for crystal design.

[1] G.R. Desiraju, *Crystal Engineering. The Design of Organic Solids*, Elsevier, Amsterdam, **1989**. [2] V.R. Hathwar, R. Pal, T.N. Guru Row, *Crystal Growth & Design*. **2010**, *10*.

Keywords: crystal engineering, supramolecular synthon, salt-cocrystal continuum

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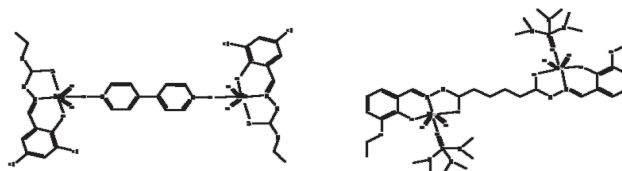
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Synthesis and structures of binuclear dioxomolybdenum schiff base complexes

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Two types of binuclear dioxomolybdenum Schiff base complexes were synthesized and their X-ray crystal structures were determined. In the first instant, the reaction of bis(acetylacetonato)dioxomolybdenum with 3,4-dichlorosalicylaldehyde 4-ethylthiosemicarbazide in the presence of 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide gave a binuclear *cis*-dioxomolybdenum complex in which the bidentate ligand, 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide formed a bridge between the two

molybdenum atoms. The overall geometry at each molybdenum site can be regarded as a distorted octahedron, with the equatorial plane formed by the imino nitrogen, phenoxyl oxygen, hydroxyl oxygen of the Schiff base and one of the terminal oxygen atoms of the dioxomolybdenum cation. The other terminal oxygen and the donor atom from the 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide ligand occupy the apical position. In the case of the binuclear dioxomolybdenum complex containing the 4,4'-bipyridine *N*-oxide ligand, the molecules are linked by N-H \cdots O hydrogen bonds into a polymeric chain.



The second type of binuclear dioxomolybdenum(VI) Schiff base complexes was formed by the reaction of bis(acetylacetonato)dioxomolybdenum with 1,4-bis(3-ethoxy-salicylaldehyde carbohydrazonato)butane in the presence of ethanol or hexamethylphosphoramide. In this case, the two molybdenum atoms are not bridged directly by a bidentate ligand, but coordinated at each end to the O,N,O donor atoms of the symmetrical hexadentate Schiff base ligand. Each of the molybdenum atoms also adopts the distorted octahedral configuration with the equatorial plane formed by the imino nitrogen, phenoxyl oxygen, hydroxyl oxygen of the Schiff base and one of the terminal oxygen atoms of the dioxomolybdenum cation. The other terminal oxygen and the donor atom from either ethanol or hexamethylphosphoramide molecule occupy the apical position. In the case of the complex containing the ethanol molecule, adjacent molecules are linked by O-H \cdots N hydrogen bonds into a polymeric chain that runs along the *a*-axis of the monoclinic unit cell.

Keywords: Schiff base, dioxomolybdenum

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Is molecular adduct formation predictable?

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The purpose of our study was to check the predictability of the formation of molecular adducts using the recently developed hydrogen bond propensity method^{1,2}. Six new drug forms **1a-1f** of the anti-malarial drug pyrimethamine, **1** were synthesized with trans-cinnamic acid, **a**; ibuprofen, **b**; aspirin, **c**; glycolic acid, **d**; 4-methylbenzenesulfonic acid, **e** and carbamazepine, **f** respectively. Their crystal structures will be described. Salt formation (by the transfer of the proton from the cofomer to the most basic heteroaromatic nitrogen of pyrimethamine) was observed in all the complexes except **1f**. The attempted cocrystallization reactions (**1g-1h**), of pyrimethamine, with hexachlorobenzene; **g**, and 1,4-diiodobenzene; **h**, respectively were unsuccessful in yielding adducts. Hydrogen bond propensity calculations [1], [2] were carried out to check the predictability of formation/non-formation of these molecular adducts. For **1a-1f**, the bonds of highest propensity were calculated between **1** and the corresponding cofomers rather than self-association, predicting the formation of adducts. In contrast the bonds of highest propensity were calculated for self-association of molecules of **1**, for **1g-1h**, in agreement with the unsuccessful reactions.