

**Keywords:** pharmaceutical co-crystallization, hydrogen-bond propensity calculations, supramolecular chemistry

[1] Propensity calculations were carried out by a newer version of mercury software which is under development by CCDC. [2] P.T.A. Galek, L. Fabian, W.D.S. Motherwell, F.H. Allen, N. Feeder, *Acta Crystallogr., Sect. B* **2007**, B63, 768.

### MS17.P06

*Acta Cryst.* (2011) A67, C315

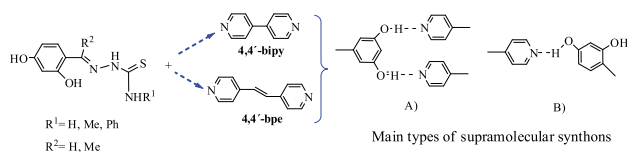
**O-H...N Heterosynthons in co-crystals. Assemblies based on resorcinol derivatives**

Ara Núñez-Montenegro, Rosa Carballo, Ezequiel M. Vázquez-López. *Inorganic Chemistry Department, University of Vigo, Vigo-Galicia (Spain)*. E-mail: aranu@uvigo.es

Multicomponent molecular crystals usually referred to as co-crystals, have recently become into a focus since their potential applications in e.g. synthetic chemistry and pharmaceutical industry. The fact that a co-crystal is obtained reflects that is possible to analyse a few significant intermolecular interactions between chemically distinct components. Such idea leads directly to the concept of heterosynthons, which can describe as hydrogen bonded recognition unit between dissimilar molecules [1].

We have selected a series of pyridines (4,4'-bipyridine and trans-1,2-bis-(4-pyridyl)ethylene) with different derivatives of resorcinol (2,4-dihydroxybenzaldehyde and 2,4-dihydroxyacetophenone thiosemicarbazone) to explore the robustness of hydroxyl-pyridyl heterosynthons. Clearly, by choosing appropriate resorcinols as templates, a rational design of crystals can be achieved. We have used the graphics sets introduced by Etter for motifs generated from intermolecular hydrogen bonds in order to define a hydrogen-bond pattern [2].

The organizational consequences of hydrogen-bonds in the hydroxyl-pyridine heterosynthons in the presence of competitive hydrogen-bonding functional groups were elucidated. Co-crystallization produces discrete structures due to intermolecular hydrogen bonds between O-H...N orienting the pyridine molecules parallel to each other, and the pyridil rings are further stabilized by  $\pi$ - $\pi$  interactions at a distance around 4Å. The ability of resorcinols derivatives to assemble pyridines yields also infinite 1D arrays. The stoichiometric of these co-crystals and the presence of any solvent in the crystallographic net are responsible for the polymorphs found.



[1] A. Mukherjee, G.R. Desiraju, *Chem. Commun.* **2011**, 47, 4090-4092. [2] M.C. Etter, *Acc.Chem.Res* **1990**, 23, 120-126.

**Keywords:** assembly, H-bridge, ayridine, lower cases

### MS17.P07

*Acta Cryst.* (2011) A67, C315

**Two in one: A fréchet-type dendron manifesting conformational duality**

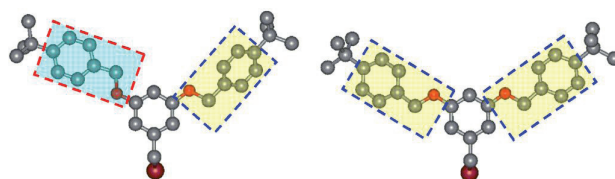
Lydia Brelot,<sup>a</sup> Adrian-Mihail Stadler,<sup>bc</sup> Corinne Bailly,<sup>a</sup> <sup>a</sup>*Service de Radiocristallographie, Institut de Chimie de Strasbourg, France.* <sup>b</sup>*Institut de Science et d'Ingénierie Supramoléculaires, Université de Strasbourg, France.* <sup>c</sup>*Karlsruhe Institute of Technology (KIT), Forschungszentrum Karlsruhe (FZK), Institute for Nanotechnology (INT), (Germany)*. E-mail: brelot@unistra.fr

The molecular structure of a Fréchet-type dendron revealed two different conformers present in the same crystal. This case of conformational duality is described and a detailed analysis is carried out to understand this phenomenon.

The difference of conformation lies in the *m*-di(methyleneoxy)benzene motifs of the dendron, which are oriented in a different way. The low energy difference between the two types of conformation is discussed.

The solid state intermolecular interactions and the crystal packing are also investigated in order to rationalize this conformational duality. Indeed, the structure shows the presence of CH- $\pi$  interactions between the molecules and generates a layered stacking with more or less coplanar molecules.

A comparative analysis is also done on other reported Fréchet-type dendritic structures existing in the Cambridge Structural Database (CSD) and showing conformational duality or diversity. This analysis shows that dendrimers and dendrons based on the *m*-di(methyleneoxy)benzene motif are flexible and this flexibility generates the formation of different conformers despite the existence of some preferred conformations [1].



[1] A.-M. Stadler, L. Brelot, *Crystal Growth & Design* **2010**, 10, 2285-2290.

**Keywords:** conformers, crystal engineering, dendrimer

### MS17.P08

*Acta Cryst.* (2011) A67, C315-C316

**Inclusion compounds as secondary building units for supramolecular chemistry**

José A. Fernandes, Ana I. Ramos, Paulo J. A. Ribeiro-Claro, Susana S. Braga, Filipe A. Almeida Paz, *CICECO, Department of Chemistry, University of Aveiro, Campus de Santiago, 3810-193 Aveiro (Portugal)* E-mail: jafernandes@ua.pt

In last few years the field of coordination chemistry has seen a great rebirth due to the intense research concerning the synthesis, isolation and structural characterisation of Metal-Organic Frameworks (MOFs).