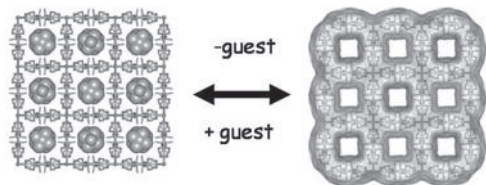


methanol, ethanol, propanol) the guest molecules dramatically effects the SCO properties [1].

In further studies using parallel *in situ* variable temperature single crystal and powder X-ray diffraction, the desorption and resorption of these guest was followed over the SCO temperature range and revealed distinct correlations, including steric and electronic effects, between the solvates [2]. Thus we have made a large step towards rationally tuning guest-dependent SCO behaviour in such systems.



[1] Neville et al. *Angew. Chem.* **2007**, *46*, 2059-2062. [2] Neville et al. *J. Am. Chem. Soc.* **2009**, *131*, 12106-12108.

**Keywords:** coordination polymers, magnetism, guest sensor

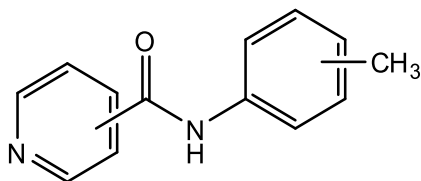
## MS24.P27

*Acta Cryst.* (2011) A67, C366

### Structural systematics and conformational analyses of a 3×3 isomer grid and three chlorinated relatives

John F. Gallagher, Pavle Mocijac, *School of Chemical Sciences, Dublin City University, Dublin 9, (Ireland)* E-mail: john.gallagher@dcu.ie

A 3×3 isomer grid of nine *N*-(tolyl)pyridinecarboxamides (C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O) as **NxxM** (*x* = *para*-/*meta*-/*ortho*-) was examined to evaluate structural relationships from both *ab initio* calculations (*gas-phase*, PCM-SMD solvation models) and the solid-state. The effect of the pyridine N atom (**Nx**) and methyl group (**xM**) substitution patterns on molecular conformations from calculations and in terms of molecular organization is evaluated for comparison with related **Mxx** and **NxxF** isomer series [1-2]. The **NxxM** isomers aggregate via N-H...N or N-H...O=C hydrogen bonds, while the intramolecular N-H...N interaction influences co-planarity in the aromatic rings of **NoxM**. In addition three 5-Cl-**NoxM** derivatives have been characterised as minor components in the **NoxM** syntheses.



**NmpM** forms catemeric chains via N-H...N interactions in space group P2<sub>1</sub>/c in contrast to **NmpF** which forms tetramers in P1̄ (No.2). The mixed 50:50% **NmpFM** crystalline solid solution forms catemeric chains in Pna2<sub>1</sub> that differ from **NmpM** at the secondary hydrogen bonding level.

Calculations demonstrate that most crystallographic dihedral angles correlate with their computational counterparts by having similar conformations with an average offset of torsion angles of ±20-40° though with some exceptions. Analysis of melting point data reveals a general trend of melting point decrease from the symmetrical **NppM** (162°C) to the unsymmetrical **NomM** (50°C), a trend which follows Carnelly's rule where *high molecular symmetry is associated with higher melting points* [3].

[1] P. Mocijac, M. Tallon, A.J. Lough, J.F. Gallagher, *CrystEngComm* **2010**, *12*,

3080-3090. [2] P. Mocijac, A.J. Lough, J.F. Gallagher, *CrystEngComm*, **2011**, *13*, 1899-1909. [3] T. Carnelley, *Philos Mag*, 5th series, **1882**, *13*, 112-130 & 180-193.

**Keywords:** systematics, isomers, computation

## MS24.P28

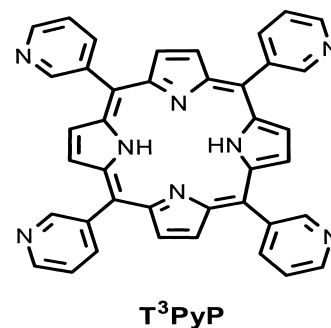
*Acta Cryst.* (2011) A67, C366

### Reactivity of tetra(3-pyridyl)porphyrin in crystal engineering

Sophia Lipstman, Israel Goldberg. *School of Chemistry, Sackler Faculty of Exact Sciences, Tel-Aviv University, 69978 Ramat-Aviv, Tel-Aviv, (Israel)*. E-mail: lipstman@post.tau.ac.il

Formulations of porphyrin-based hybrid coordination networks with metal ion connectors are of particular interest due to the relative robustness of metal-organic-frameworks and their potential utility in practical applications. The chemical and structural diversity of porphyrins allows us to reasonably control their self-assembly process and to alter systematically the composition, topology and porosity of the supramolecular arrays that form. This approach represents an attractive "bottom-up" strategy to tailoring ordered lattice materials from suitably functionalised tetraarylporphyrin building blocks.

In this work we have explored the versatile molecular recognition features of the tetra(3-pyridyl)porphyrin (T<sup>3</sup>PyP) scaffold, and its utility in the construction of porphyrin based supramolecular assemblies via coordination as well as hydrogen bonding interaction synthons. The diversified supramolecular reactivity of T<sup>3</sup>PyP can be attributed to the conformational flexibility of this porphyrin framework, namely the possibility of the four *meso*-substituted 3-pyridyl arms to align in different orientations with respect to the rigid porphyrin plane. Only a small number of T<sup>3</sup>PyP-based supramolecular ensembles have been reported thus far. In order to demonstrate the important role that this building block can play in crystal engineering of framework solids, we report in this study on the preparation and structural characterization of a series of new T<sup>3</sup>PyP network materials.



T<sup>3</sup>PyP

[1] S. Lipstman, I. Goldberg, *Cryst. Growth Des.*, **2010**, *10*(10), 4596-4606.

[2] S. Lipstman, I. Goldberg, *Cryst. Growth Des.*, **2010**, *10*(11), 5001-5006.

**Keywords:** supramolecular, crystal engineering, porphyrin

## MS24.P29

*Acta Cryst.* (2011) A67, C366-C367

### Synthesis and characterization of pharmaceutical cocrystals from polymorphic constituents

Heba Abourahma, Devon Cocuzza. *Department of Chemistry, The College of New Jersey, PO Box 7718, Ewing, NJ 08628 (USA)*. E-mail: abourahm@tcnj.edu

The objective of this project is to investigate the polymorphic tendencies of cocrystals synthesized from polymorphic active pharmaceutical ingredients (APIs). Furthermore, the objective extends to evaluate the potential use of these cocrystals as a means