

[1] A. García-Raso, F.M. Albertí, J.J. Fiol, Y. Lagos, M. Torres, E. Molins, I. Mata, C. Estarellas, A. Frontera, D. Quiñero, P.M. Deyà, *Eur. J. Org. Chem.* **2010** 5171-5180 [2] M. Barceló-Oliver, C. Estarellas, A. García-Raso, A. Terrón, A. Frontera, D. Quiñero, I. Mata, E. Molins, P.M. Deyà, *CrystEngComm* **2010**, *12*, 3758-3767 [3] M. Barceló-Oliver, C. Estarellas, A. García-Raso, A. Terrón, A. Frontera, D. Quiñero, E. Molins, P.M. Deyà, *CrystEngComm* **2010**, *12*, 362-365.

Keywords: non-covalent interactions, nucleobase, crystal engineering

MS59.P03

Acta Cryst. (2011) **A67**, C601

Supramolecular assembly of hetero-halogen (F...X) or Homo-Halogen (X...X, X = F, Cl, Br, and I) interactions in substituted benzanilides

Susanta K. Nayak, M. Kishore Reddy and Tayur N. Guru Row *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, (India)*. E-mail: nksusa@gmail.com

A series of mixed halogen (F, Cl, Br, and I) substituted benzanilide crystal structures have been analyzed to evaluate the role of halogen involving interactions in regulating the molecular conformation and supramolecular packing [1-2]. The N-H...O H-bond is a key structure directing element acting in conjunction with C-H...O and C-H... π interactions in this series of compounds. It has been also observed that the halogen-halogen interaction plays a crucial role for polymorphic modification. It is of importance to note that organic fluorine prefers Type I F...F contacts, whereas Cl, Br and I prefer Type II contacts [3-4]. Hetero halogen...halogen interactions on the other hand are predominately of Type II geometry and this is due to the greater polarizability of the electron density associated with the heavier halogens [4-5]. This presentation will provide the importance to evaluate the contributing role of these interactions in crystal structure packing and the co-operativity associated with such interactions in the solid state.

[1] S.K. Nayak, M.K. Reddy, T.N.G. Row D. Chopra, *Crystal. Growth Des.*, **2011**, DOI: 10.1021/cg101544z and references therein. [2] P. Metrangolo, F. Meyer, T. Pilati, G. Resnati, G. Terraneo, *Angew. Chem., Int. Ed.* **2008**, *47*, 6114-6127. [3] G. Ramasubbu, R. Parathasarathy, P. Murray-Rust, *J. Am. Chem. Soc.* **1986**, *108*, 4308-4314. [4] T. Bui, T. Dahaoui, T.S. Lacomte, C. Desiraju, G.R. Espinosa, E. *Angew. Chem. Int. Ed.* **2009**, *48*, 3838-3841. [5] V.R. Hathwar, T. N. Row, *Cryst. Growth Des.* **2011**, DOI: 10.1021/cg1015862.

Keywords: halogen, supramolecular, interaction

MS59.P04

Acta Cryst. (2011) **A67**, C601

Halogen bonding towards assembling phosphorescent cocrystals and probing specific solvent effect

Wei Jun Jin, Qian Jin Shen, Hong Qing Wei, Hao Ling Sun, *College of Chemistry, Beijing Normal University, Beijing, (P. R. China)*. Email: wjjin@bnu.edu.cn

The abstract consists of two parts, one describes assembly of phosphorescent cocrystals by halogen bonding with other noncovalent interaction, and another is aimed to exploring possible specific solvent effect as encountering halogenated solvent.

Part one: two supramolecular cocrystals **1**, pyrene/1,4-diiodotetrafluorobenzene (1,4-DITFB) and **2**, pyrene/1,2-

diiodotetrafluorobenzene (1,2-DITFB) have been assembled by synergistical C-I...I interaction, π - π stacking and C-H...F contact. The x-ray single crystal diffraction data reveal the structural characteristics of two crystals and function of position of iodine atom in regulating cocrystal structure. Two cocrystals were also well characterized by element analysis, x-ray powder diffraction for homogeneity of samples, UV-vis absorption and FTIR. Furthermore, two cocrystals phosphoresce with well defined fine structure due to iodine acting as heavy atom perturber. They have 10^3 to 10^1 s⁻¹ phosphorescence decay rate.

Part two: halide and a dual fluorescence molecule 4-dimethylaminobenzonitrile (DMABN) are used to probe possible specific solvent effect, halogen bonding between halogen donor part (Cl-C) of the solvent and acceptor group (cyano-N) of the probe molecule or halide. The experiment and calculation show cyano-N...Cl-C and halide...Cl-C are compatible to cyano-N...H-C (hydrogen donor part of the solvent) and halide...H-C. The results enlighten that the halogen bonding as one specific effect parallel to hydrogen bonding should be considered habitually in explaining interaction between solute and halogenated solvent molecule.

Authors thank the National Natural Science Foundation of China (No.20675009, No.90922023 and No.20801006) for the support.

Keywords: halogen bonding, phosphorescence, specific solvent effect.

MS60.P01

Acta Cryst. (2011) **A67**, C601

Reversible Order-Disorder Phase Transition in a New Polymeric Metavanadate: {[Zn(Im)₄][V₂O₆]}_n

Samroeng Krachodnok,^a Kenneth J. Haller,^a Ian D. Williams,^b *^aSchool of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, 30000 (Thailand).* *^bDepartment of Chemistry, Hong Kong University of Science and Technology, Kowloon, (Hong Kong).* Email: ken.haller@gmail.com, dsk4610137@live.com

DSC measurements show that this compound undergoes a reversible first-order phase transition at 274.84 K (exothermic transition) and at 277.05 K (endothermic transition) with a hysteresis of ~2 K with the enthalpy $\Delta H = \sim 1$ kJ mol⁻¹ and entropy $\Delta S = \sim 4$ J mol⁻¹K⁻¹ upon cooling and heating rate of 5 °C min⁻¹. Single crystal X-ray diffraction shows an ordered triclinic *P*-1 phase at 100 (2) K and a disordered triclinic *P*-1 phase at 293 (2) K (the *c* axis half of 100 K). The structure consists of infinite anionic polymeric metavanadate chains which composed of the corner-sharing of VO₄ tetrahedra and the [Zn(Im)₄]²⁺ complex cations occupied between the anions. The 3-D supramolecular network between cations and anions through hydrogen bonding interactions.

As temperature increasing, the small reorientation of the polymeric anions with small expansion of their skeleton along *c* axis are driving force to the small rearrangement of a 3-D supramolecular network of the cations through observed significantly different weak C-H...O hydrogen bonding interactions between cations and anions and concerted aryl embraces of weaker *off* N-H... π , *off* C-H... π and *ef* C-H... π hydrogen bond interactions among the cations themselves. Good agreement with significantly different of infrared spectra at RT and at temperature of liquid nitrogen. In summary the order-disorder of polymeric anions can control the behavior of a phase transition in this work.

Keyword: reversible order-disorder phase transition, polymeric metavanadate, hydrogen bond interactions