Ph.D. Viva Voce

Department of Chemistry, IISER Bhopal

Title of Seminar: Exploring Solid State Diversity in Molecular Crystals

Speaker: Pradip Kumar Mondal (Thesis advisor: Dr. Deepak Chopra) **Roll No**: 1210211

Date: 8 November 2018 **Time**: 11.00 AM **Venue:** AB2-401

The importance and characterization of intermolecular interactions in crystalline solids has undergone a major renaissance.[1a-1b] In this regard, the relevance of weak interactions, in particular those involving halogens, of the type **C–H···X**, **C–X···X–C**, and **C–X···π (X= -F, Cl, Br, I)** is of significance.[2] In the current work, systematic attempts have been made towards the synthesis, crystallization, and investigation of polymorphism in molecules containing organic halogens[3a,3b]. In addition, a quantitative assessment of the presence of different intermolecular interactions via inputs from Crystal Structure Prediction[3c] and *in situ* cryocrystallization[3d] (in case of organic fluorine only), alongwith PIXEL and QTAIM analysis have also been performed. The polymorphs obtained have been characterized via DSC and the mechanical properties have been established via the method of nanoindentation for polymorphs in a fluorinated amide.[4]

Furthermore, the solid-state diversity has been extended to understand the solution characteristics of a poorly soluble fluorinated drug, Riluzole via formation of cocrystals/cocrystal polymorph/salts obtained via cocrystallization with different carboxylic acids and pyridine derivatives acting as co-formers.[5] It is indeed noteworthy that a *metastable* state was characterized in riluzolium oxalate salt, which exhibits a spontaneous and reversible Single-Crystal-to-Single-Crystal phase transition.[6] Thus the current work unequivocally establishes the role of energetics and topological features, which contribute towards the formation of the organic solid state.

References

1. (a) Chopra, D. *Understanding Intermolecular Interactions in the Solid State: Approaches and Techniques;* Royal Society of Chemistry, UK, **2018**. (b) Desiraju, G. R. *J. Am. Chem. Soc.* **2013**, *135*, 9952-9967.
2. Chopra, D.; Guru Row, T. N. *CrystEngComm* **2011**, *13*, 2175 −2186.
3. (a) Mondal, P. K.; Yadav, H. R.; Choudhury, A. R.; Chopra, D. *Acta Crystallogr. Sect. B* **2017**, *73*, 805–819. (b) Mondal, P. K.; Shukla, R.; Biswas, S.; Chopra, D. *Acta Crystallogr. Sect. B* **2018 (In Press)**. (c) Mondal, P. K.; Chopra, D. *CrystEngComm* **2016**, *18*, 48–53. (d) Mondal, P. K.; Hathwar, V. R.; Chopra, D. *J. Fluor. Chem.* **2018**, *211*, 37–51.
4. Mondal, P. K.; Kiran, M. S. R. N.; Ramamurty, U.; Chopra, D. *Chem. - A Eur. J.* **2017**, *23*, 1023–1027.
5. Mondal, P. K.; Rao, V.; Mittapalli, S.; Chopra, D. *Cryst. Growth Des.* **2017**, *17*, 1938–1946.
6. Mondal, P. K.; Rao, V.; Chopra, D. *CrystEngComm* **2018**, *20*, 2079–2083.