

PhD Open Seminar
Department of Chemistry, IISER Bhopal

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Title of Thesis: A Quantitative Investigation of Intermolecular Interactions in the solid state in multi-functional organic compounds

Date: 21 February 2016

Time: 11.00 AM

Venue: AB-II 401

Abstract

The ability to predict and control the formation of supramolecular assembly involving organic fluorine into ordered networks is now well-recognized in the context of crystal engineering.¹ The understanding of the cooperative effects of various structural motifs associated with the presence of different intermolecular interactions involving organic fluorine has been investigated in a series of fluorinated benzoyl chlorides (liquids at room temperature, determined via *in situ* cryocrystallization²), phenyl benzamidines and phenyl benzoates. In this study, the crystal structures are analyzed based on the molecular conformation and the supramolecular architectures in the absence or presence of any strong H-bonds. All the supramolecular building blocks associated with similar or different intermolecular interactions were analyzed in terms of their nature and energetics using PIXEL and topological analysis using the approach of QTAIM.³ In fluorinated benzoyl chlorides, the diatropic ring current establishes the existence of aromaticity in the five-membered ring associated with the presence of intramolecular C-F \cdots O=C contact which locks the molecular conformation in the presence of an intramolecular C-H \cdots Cl-C contact.^{4a} In addition, the weak C-H \cdots O/F/Cl interactions are instrumental in tuning the growth of the primary building blocks associated with $\pi\cdots\pi$ stacked columns *via* changing the mode of fluorine substitution.^{4b} It is interesting to observe that fluorinated benzamidines exhibit different phenomena like *E/Z*-isomerisation, polymorphism, solvatomorphism, isostructurality and quasi-isostructurality in the presence of either N-H \cdots N chain or N-H \cdots N dimers associated with intermolecular N-H \cdots F, N-H \cdots π , C-H \cdots N, C-H \cdots F, C-H \cdots π interactions and $\pi\cdots\pi$ stacking.⁵ The change in substitution of the fluorine atoms in phenyl benzoates exhibits supramolecular packing with 3D, 2D and 1D structural similarity wherein the robustness of the 1D C-H \cdots O chain plays an important role in the occurrence of isostructurality.⁶ Furthermore, a series of trifluoromethylated phenyl hydrazones exhibit structural diversity, namely the occurrence of isostructurality and polymorphism associated with different supramolecular architectures.⁷ Hirshfeld surface analysis and the associated fingerprint plots⁸ helps to understand the similarities and the differences between the polymorphic forms and the compounds which exhibit isostructurality.

Reference:

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