Poster Presentation

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Computational approaches towards crystal engineering in molecular crystals

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The investigation of a large number of crystal structures has resulted in the development of the area of crystal engineering, which involves the study of intermolecular interactions in crystalline solids [1]. It is now of importance to understand the nature and energetics associated with different interactions [2] which influence the crystal packing. In this regard, different computational approaches (utilizing PIXEL and TURBOMOLE) have been developed which aid in the understanding of intra- and intermolecular interactions (for example, hydrogen and halogen bonding) in molecular crystals. This approach has been successfully applied in different classes of molecules [3]. These approaches can be combined with topological analysis of the electron density using the quantum theory of atoms in molecules (QTAIM) (in absence of high quality crystals for experimental electron density studies). In order to validate the above-mentioned methodology, we have performed a comprehensive analysis of a series of synthesized fluoro-derivatives of N'-phenylbenzimidamide to gain quantitative insights into different interactions which accompany crystal formation. The packing of the molecules has contributions from strong N-H...N, weak N-H...π [Fig 1], C-H...N, C-H...F, and C-H...π intermolecular interactions along with π-π stacking. In addition to that, ubiquitous H...H contacts are also present in the solid state. This methodology can be extended to include cocrystals, polymorphs (including solvates) and protein-ligand interactions at the active site.

[1] *G. R. Desiraju, J. Am. Chem. Soc. 2013, 135, 9952.,* ***[2]*** *K. E. Riley, M. Pitonak, P. Jurecka, P. Hobza, Chem. Rev. 2010, 110, 5023.,* ***[3]*** *(a) G. Kaur, P. Panini, D. Chopra, A. R. Choudhury, Cryst. Growth Des. 2012, 12, 5096. (b) P. Panini, D. Chopra, CrystEngComm, 2013, 15, 3711.(c) P. Panini, T. P. Mohan, U. Gangwar, R. Sankolli, D. Chopra, CrystEngComm 2013, 15, 4549. (d) R. Shukla, T. P.*

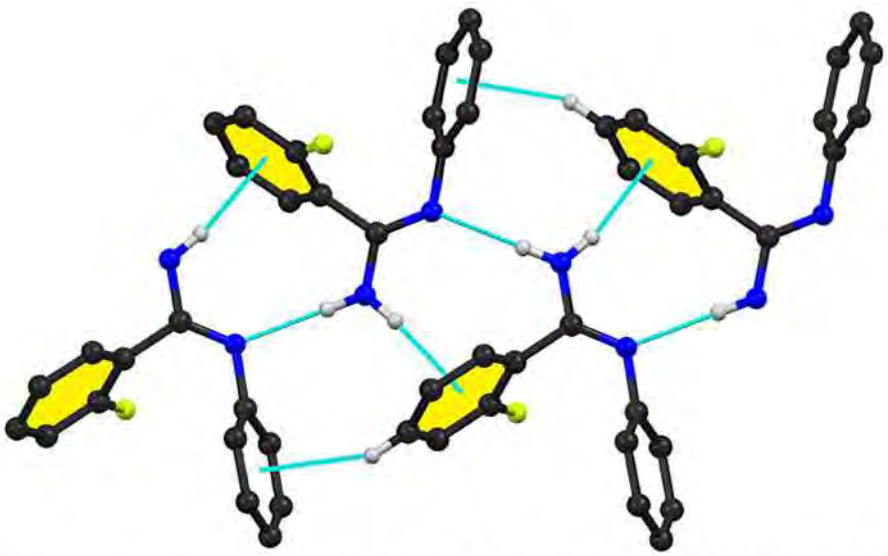

Figure 1: *Cis*-geometry in *ortho*-substituted fluorinated *N* '-phenylbenzimidamide depicting N-H...N, N-H...π and C-H...π intermolecular interactions

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