

Controlling the Crystal Packing Feature by Weak C–H···F Hydrogen Bond(s) in the Absence of Strong Hydrogen Bond

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Abstract:

Hydrogen bond is the most important tool for the molecular recognition to design the materials in crystal engineering¹, and it plays a vital role in various biological activities and pharmaceuticals industry.² Strong hydrogen bond like N–H···O, N–H···N, O–H···O, O–H···N etc have been extensively studied in the literature and they are being fully utilized in building desired crystalline supermolecular architecture.³ The study of weak hydrogen bonds involving “organic fluorine”⁴ (C–H···F–C type hydrogen bonds) have been the focus of the crystal engineering community for the last few years.⁵ The structural feature(s) that may arise due to the presence of one or more fluorine atoms in a molecule is still unpredictable and a rationale for their use in crystal engineering is farfetched. Therefore, a better understanding of the weak interactions involving organic fluorine is required for their successful application in crystal engineering to develop new materials with desired structural features. In the last few years, it has been demonstrated that organic fluorine through weak C–H···F–C hydrogen bond is capable to modulate the crystal packing and molecular conformation in structural chemistry and biology.⁶



Scheme 1: Chemical Scheme of the molecules studied

To understand and elucidate the role of C–H···F–C hydrogen bonds in small organic molecules, we have selected a series of tetrafluorinated N, N-disubstituted amides. It has been observed that C–H···F–C hydrogen bond(s) sequentially alter the packing mode of the compounds through the alteration of torsion angle(s) on varying the position of fluorine substitution in the aromatic ring. Molecules utilize these C–H···F–C interactions to generate different supramolecular synthons. These have been found to generate different three-dimensional arrangement of molecules in crystal lattice.

References:

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