Title:	Structural and Computational Analysis of Organic Fluorine-Mediated Interactions in Controlling the Crystal Packing of Tetrafluorinated Secondary Amides in the Presence of Weak C–H···O=C Hydrogen Bonds
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Abstract:	Hydrogen bonds play an important role in various parts of our life. Be it the hydrogen bonding in water or the DNA strands bonded by hydrogen bonds, its importance in every field is crucial. The hydrogen bonds may be strong, moderate, and weak depending upon the strength of the interaction energy. The strong hydrogen bonds play a significant role in defining the physical and chemical properties of the molecules and the moderate and weak hydrogen bonds play a crucial role in the packing and physical properties of the crystalline molecular compounds. Among the moderate and weak hydrogen bonds, a few interactions like C–H···N and C–H···O are extensively studied. Further, the interactions involving Fluorine have also been at the center of attraction for a long time. Fluorine being the highest electronegative element is supposed to be the strongest hydrogen bond acceptor but when fluorine is bonded to carbon, it becomes a very poor hydrogen bond acceptor. Various research groups across the globe are using various methods, like Single Crystal X-ray diffraction (SCXRD) experiment, indexing the Powder X-ray Diffraction (PXRD) data, computational methods, statistical analysis using Cambridge Structure Database (CSD), charge density analysis etc. on different systems in different environments to completely understand the nature of fluorine mediated interactions. This presentation will discuss different systems with changing environments to understand the fluorine-mediated interactions. We have used different methods like SCXRD study, ab initio methods, topological analysis, charge density analysis, and CSD study to look at different aspects of the interaction. The first system studied is the organic fluorine-mediated interactions in presence of strong N–H···O=C hydrogen bonds. The number and position of fluorine substitutions are varied in the studied system. The effect of these strong hydrogen bonds on the organic fluorine- mediated interactions will be discussed. Further, the second system studied has no tendency for strong N–H···O=C hydrogen bonds but is capable of having C–H···O=C and C–H···O–C hydrogen bonds. The computational analysis of these interactions along with the C–H···F–C and C–F···F–C will be highlighted. The third system studied only offers C–H···F–C and C–H···O–C interactions and no other hydrogen bonds. This system is studied using Gaussian09 and AIM studies to understand the nature and strength of the interactions. These studied systems will be followed by an experimental charge density analysis for one of the compounds in the second system. The high resolution and high-quality single crystal X-ray data are studied using the XD2006 package and the electronic properties of the molecule will be discussed. At last, a comparison study is done for C–H···F–C and C–H···O=C interactions using Hirshfeld surface area calculations using the database.
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