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**Title:** Understanding the Influence of Fluorine in Crystal Packing of Organic Molecules in the Presence and in the Absence of Other Strong/Weak Hydrogen Bonds: A Structural Analysis

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**Abstract:** Understanding the Influence of Fluorine in Crystal Packing of Organic Molecules in the Presence and in the Absence of Other Strong/Weak Hydrogen Bonds: A Structural Analysis" consists of four chapters. Chapter 1 is a brief introduction to the field of intermolecular forces including the conventional strong and weak hydrogen bonds, other weaker interactions like C-H... and ... , and interactions involving halogens like C-H...X, C-X...X, and C-X... (X = F, Cl, Br). Chapter 2 evaluates the importance of organic fluorine in altering the crystal packing in the presence of strong N-H...O hydrogen bond in a series of mono and di-fluorinated phenylacetamides. Chapter 3 describes the structural features of tetrafluoro N-[2-(3-methoxyphenyl)ethyl]benzamide, in the absence of strong N-H...O hydrogen bond but with the possibility of weak C-H...O=C hydrogen bonds. Chapter 4 depicts the structural variations in tetrafluoro derivatives of diphenyl tetrahydroisoquinolines in the absence of strong hydrogen bonds like N-H...O hydrogen bond and weak hydrogen bonds like C-H...O=C. The intermolecular interactions are responsible for the state of existence of a compound at a given temperature and pressure. A combination of strong and weak intermolecular forces is known to dictate the physical properties of various compounds and materials. Therefore, the understanding of such forces is necessary to understand the properties of materials and compounds. Strong and weak hydrogen bonds are well known in the literature and its influence in guiding crystal structure has been established beyond doubt. The understanding of the role of weaker interactions in controlling the crystal packing is still a gray area in crystal engineering. Especially, the influence of fluorine in small organic molecules in guiding the packing leading to its crystallization has remained controversial, though few studies to understand the interactions involving fluorine have been made in the past. The systematic analysis of weak interactions involving organic fluorine based on three different but related molecular systems of fluorinated organic molecules is the theme of this thesis. The structural analyses of ten molecules (derivatives of phenylacetamide) containing a strong hydrogen bond donor (N-H group) and a strong hydrogen bond acceptor (O=C group) in addition to one or two C-F groups and a OMe group (Scheme 1) have been discussed in chapter 2. The role of C-F group(s) in altering the crystal structures of these molecules in the presence of strong conventional N-H...O=C hydrogen bond has been illustrated in this chapter. The influence of aromatic fluorine in bringing structural variation in these molecules has been highlighted. Chapter 3 illustrates the structural features arising due to the presence of four C-F groups in the molecule in the presence of C=O and OMe groups as hydrogen bond acceptors without the strong donor like N-H group (Scheme 2). These structures highlighted the cooperative effects of weak hydrogen bonds (C-H...O=C, C-H...OMe and C-H...F-C), C-H... $\pi$  and halogen...halogen (C-F...F-C) interactions. Various supramolecular synthons have been identified and rationalized in the thesis. Chapter 4 encompasses the structural variations of tetrafluoro derivatives of diphenyl tetrahydroisoquinolines (Scheme 3). These molecules are devoid of any strong hydrogen bond donor like N-H group and strong hydrogen bond acceptor like a C=O group. Therefore, crystal structures of all the compounds are governed majorly by weak interactions involving fluorine (C-H...F-C and C-F...F-C) and a few weak hydrogen bonds like C-H...OMe and much weaker C-H... $\pi$  interaction(s). Based on the observed structural features an attempt has been made to rationalize the interactions involving fluorine in the absence of strong hydrogen bonds in this chapter.

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