Title:	Computational Study of C-H·· ·F Hydrogen Bonds in Aromatic System
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Abstract:	Hydrogen bond is a non-covalent type of interaction which is a crucial phenomenon for almost everything on Earth. Stronger hydrogen bonds (N-H· · ·O, O-H· · ·N, N-H· · ·N, O-H· · ·O etc.) are responsible for various chemical, biological and physical properties of matter. The weaker hydrogen bonds also have immense importance in controlling various chemical and biological phenomenons. The weakest hydrogen bonds are found when a C-F group acts as hydrogen bond acceptor in chemical and biological molecules. The understanding of these weak hydrogen bonds involving a C-F group is of significant importance as fluorine is an important element in pharmaceutical compounds and fluorinated molecules has better drug activity than its non-fluorinated analogue. Fluorine mediated interactions have variety of applications in protein-ligand binding, supramolecular chemistry, pharmaceutical chemistry etc. Though fluorine has highest electronegativity, the role of C-H·· ·F hydrogen bonds in crystal engineering and supramolecular chemistry is debated over the years. We attempted to establish the role of C-H·· ·F hydrogen bonds in crystal engineering by understanding the strength and directionality of the supramolecular synthons offered by “organic fluorine” using aromatic model systems. For that, a set of fluorinated dimers involving aromatic systems were studied computationally to investigate the structural parameters and energetics which lead the formation of structure stabilizing C-H·· ·F hydrogen bonds, using Gaussian09. The molecules have been studied in MP2 level of theory using aug-cc-pVDZ basis set and performed the frequency calculations. To study the effect of additional fluorine(s) in the same system of dimers, fluorine atom has been added in the ortho-, para- and meta- positions of both acceptor and donor molecule. Study of topological properties using AIM approach of each synthon by AIM calculation provided evidences in favour of the nature and strength of the C-H·· ·F hydrogen bonds. All the C-H·· ·F hydrogen bonds were validated by Koch-Popelier’s criteria for weak hydrogen bond. The stabilization energy has been decomposed into its all meaningful components to understand the physical origin of these bonds using localized molecular energy decomposition analysis (LMO-EDA).
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