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Title:	Quantitative characterization of new supramolecular synthons involving fluorine atoms in the crystal structures of di- and tetrafluorinated benzamides
Authors:	Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
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Abstract:	Strong hydrogen bonds play a significant role in crystal packing. In particular, the involvement of interactions involving fluorine in controlling the crystal packing requires appropriate attention, especially in the presence of other strong hydrogen bonds. In the present study, a detailed quantitative assessment has been performed of the nature, energetics and topological properties derived from the electron density in model compounds based on fluorinated benzamides (a total of 46 fluorine-substituted benzamides containing multiple fluorine atoms) in the solid state. The primary motivation in the design of such molecules is to enhance the acidity of the interacting H atoms in the presence of an increasing number of F atoms on the molecular scaffold, resulting in increased propensity towards the formation of intermolecular interactions involving organic fluorine. This exercise has resulted in the identification of new and frequently occurring supramolecular synthons involving F atoms in the packing of molecules in the solid state. The energetics associated with short and directional intermolecular Csp2—H···F—Csp2 interactions with significantly high electrostatic contributions is noteworthy, and the topological analysis reveals the bonding character of these ubiquitous interactions in crystal packing in addition to the presence of Csp2—F···F—Csp2 contacts.
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