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Title: A comprehensive understanding of the synthons involving C-H···F-C hydrogen bond(s) from structural and computational analyses Authors: Kaur, Gurpreet (/jspui/browse?type=author&value=Kaur%2C+Gurpreet) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.) Keywords: C-H···F-C hydrogen synthons hydrogen 2015 Issue Date: Royal Society of Chemistry Publisher: Citation: CrystEngComm, 17 (15) pp. 2949-2963. Abstract: The studies of weak interactions involving "organic fluorine" have resulted in a number of conflicts in the literature. Although the involvement of a C-F group in influencing the crystal packing has been demonstrated in various compounds, no one has emphasized the consistency of the synthons formed by C-H···F-C hydrogen bonds. Herein, we have attempted to draw a correlation between the formation of a particular synthon and the positions of the fluorine substitutions from the structural analyses of a model system of tetrafluoro substituted N-benzylideneanilines. A few frequently occurring supramolecular synthons involving C-H···F-C hydrogen bonds have been identified in these and related molecules, and have been quantified by ab initio calculations using the MP2 level of theory and the 6-31+G* basis set in the gas phase. The topological properties of these C-H···F-C hydrogen bonds have been calculated using AIM2000. The nature, strength,

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directionality and synthon reproducibility of the C-H···F-C hydrogen bonds are the key features

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