

Poster Presentation

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Synthon robustness by C-F groups in halogen substituted N-benzylideneanilines

G. Kaur¹, A. Roy Choudhury¹

¹Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, Punjab, India

The arrangement of the molecules in their crystal structure is controlled by the non-covalent intermolecular interactions other than the effectual space filling. The role of strong hydrogen bonds in guiding the crystal packing is well-known in the literature. But, how significant are the weak interactions in the field of crystal engineering, has yet not been fully understood. Our aim is to comprehend the nature and strength of the weak interactions involving fluorine in guiding the packing of small organic molecules in their respective crystal structure. The reason being the controversies, which are involved regarding the interactions offered by “organic fluorine”[1] and also due to the importance of these interactions in the pharmaceutical industry. Some of the research groups indicate the incapability of interactions offered by fluorine in the formation of supramolecular motifs, whereas other groups have indicated that substantial role is being played by fluorine in constructing the lattice through C-H \cdots F, C-F \cdots F and C-F \cdots π interactions in the presence and absence of strong hydrogen bond donor and acceptor groups. To understand more about these interactions, we have chosen a model system of halogen substituted N-benzylideneanilines[2]. In this system, we have analysed the impact of fluorine mediated interactions on the crystal packing by having fluorine as a substituent on both the phenyl rings. Then the robustness of the synthons offered by organic fluorine has been anticipated in the same system, but with one of the substituent as chlorine or bromine in either of the phenyl ring. It has been observed that the replacement of the non-interacting fluorine by its heavier analogue has not altered the supramolecular motif, which was formed by the other fluorine. But the crystal packing has been found to be completely altered in the molecules where the interacting fluorine was replaced by its heavier analogue. Salient features of our computational studies, which include the calculation of the stabilization energies of the studied dimers using MP2 method and their topological analysis using AIM2000, to support the experimental observations will also be presented to highlight the sturdiness of the synthons formed by so called “organic fluorine”.

[1] J. D. Dunitz, R. Taylor, *Chem. Eur. J.* 1997, 3, 89-98., [2] G. Kaur, P. Panini, D. Chopra, et al., *Cryst. Growth Des.* 2012, 12, 5096–5110.

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