

Supramolecular synthons involving fluorine atoms in crystal structures of fluorobenzamides

Pradip Kumar Mondal¹, Deepak Chopra¹¹Department Of Chemistry, IISER Bhopal, Bhopal, India

E-mail: pradipm@iiserb.ac.in

The presence of both strong and weak intermolecular interactions has been observed to play a significant role in the crystal packing [1]. The systematic evaluation of the role of intermolecular interactions involving fluorine in crystal packing requires special mention, in particular, in the presence of other stronger intermolecular force(s) like strong hydrogen bonds [2]. In the present study, detailed crystallographic investigations (molecular conformation and crystal packing analysis) have been carried out on model compounds based on fluorinated benzamides. Herein we have synthesized a total of 46 benzamides containing multiple fluorine atoms, and these have been characterized using ¹H NMR, IR, single crystal, and powder X-ray diffraction techniques. In addition, the melting points were determined by DSC. A plethora of weak interactions, namely C(sp²)-H...F-C(sp²), C(sp²)-F...F-C(sp²) and C(sp²)-F...n are involved in crystal packing in the presence of strong N-H...O hydrogen bonds and π...π contacts. The energetics associated with these intermolecular interactions are quantitatively assessed using PIXEL calculations. Complete topological analyses were used to characterize these interactions and identify the frequently occurring supramolecular synthons [Figure 1A and 1B], involving the fluorine atom (C-H...F-C, C-F...F-C, and C-H...H-C). The deformation density and fingerprint analysis were performed to study the nature and evaluate the quantitative contribution of the interactions towards the crystal packing [3].

1. Chopra, D.; Guru Row, T. N. *CrystEngComm* 2008, 10, 54-67.

2. a). Chopra, D.; Thiruvengatam, V.; GuruRow, T. N. *Cryst. Growth Des.* 2006, 6, 843-845. b). Panini, P.; Mohan, T. P.; Gangwar, U.; Sankolli, R.; Chopra, D. *CrystEngComm* 2013, 15, 4549-4564. c). Kirchner, M. T.; Blaser, D.; Boese, R.; Desiraju, G. R. *CrystEngComm* 2009, 11, 229-231. d). Abad, A.; Agullo, C.; Cunat, A. C.; Vilanova, C.; Ramirez de Arellano, M. C. *Cryst. Growth Des.* 2006, 6, 46-57. e). Betz, R.; Klufers, P. *Acta Crystallogr., Sect. E, Struct. Rep. Online* 2008, 64, o2242.

3. Khan, I.; Panini, P.; Khan, S. U. D.; Rana, U. A.; Andleeb, H.; Chopra, D.; Hameed, S.; Simpson, J. *Cryst. Growth Des.* 2016, 16, 1371-1386.

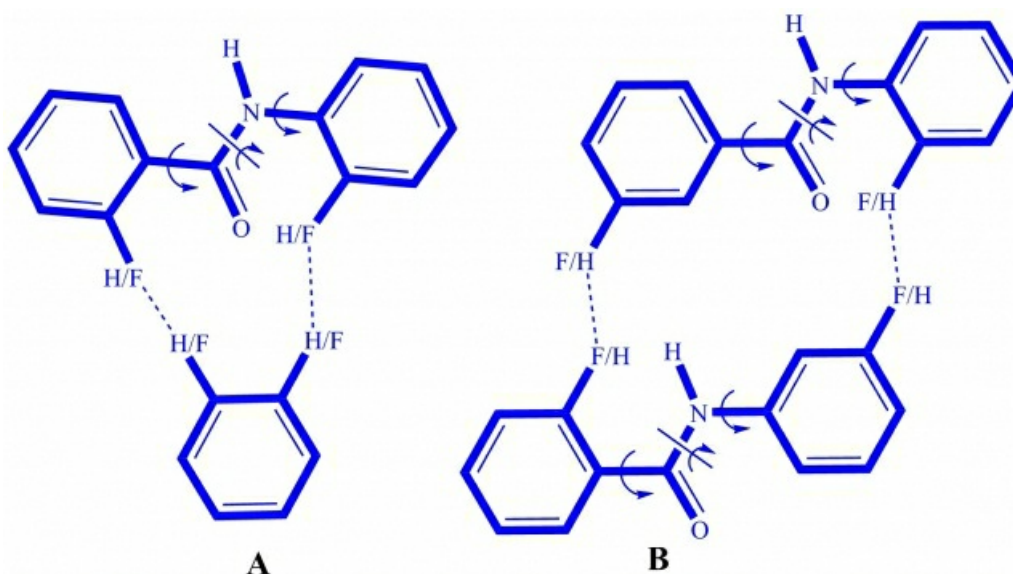


Figure 1: The twelve membered (A) and eighteen membered (B) ring synthons which consist of C-H...F-C, C-F...F-C, and C-H...H-C interactions.

Keywords: [Intermolecular Interaction](#), [Supramolecular Synthon](#), [Fluorobenzamide](#)