

*Do halogen bonds dictate the packing preferences in solid solutions?*Titas Pramanik¹, Tayur N. Guru Row¹¹Solid State And Structural Chemistry Unit And Indian Institute Of Science, Bengaluru, India

E-mail: titaspramanik1990@gmail.com

The isomers 4-bromo-2-chloro benzoic acid (4Br) and 2-bromo-4-chlorobenzoic acid (2Br), crystallize in space groups, P21/n and P-1 respectively. Strong O-H...O hydrogen bond generates a carboxylic acid dimer along with an unusual triangular halogen bonded motif in 4Br with two type II Br...Cl and Cl...Br and one type I Br...Br contact with the halogen atoms located at the vertices (Pavan & Row, 2016) which is different from the X3 synthon characterized purely based on type II interactions. (Bui et al., 2009). However, in 2Br a well-defined type II Br...Cl contact holds the molecular assembly in the crystal structure. Charge density analysis establishes the nature of halogen bonds in the two structures bringing out significant changes in the packing features of the two structures. Cocrystallization experiments generate solid solutions of varied stoichiometric ratios among these different crystalline forms dictated mainly by the halogen triangular motif observed in 4Br as proved by accurate single crystal diffraction studies with difference Fourier maps providing the evidence. Additional supporting evidence is given by Powder diffraction analysis (PXRD) and differential scanning calorimetric (DSC) studies verifying the formation of the solid solution (Shemchuk et al., 2016). Indeed, a systematic evaluation of the spectrum of solid solutions establishes the dominance of the variability in halogen bonded motifs and the directional capability in the formation of supramolecular assembly.

[1]. Pavan, M. S. & Row, T. N. G. (2016) J. Chem. Sci. 128, 1579–1587.

[2]. Bui T T T, Dahaoui S, Lecomte C, Desiraju G R & Espinosa E (2009). Angew. Chem. Int. Ed. 48, 3838.

[3]. Shemchuk, O., Braga, D. & Grepioni, F. (2016). Chem. Commun., 52, 11815- 11818.

**Keywords:** [Solid Solutions](#), [Halogen Bonding](#), [Isomers](#)