Poster Presentation

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Investigation of intra- and intermolecular F...O contacts in crystals

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Non-covalent interactions have contributed enormously towards the understanding of structure-property relationships in all fields of natural sciences [1]. In particular, interactions involving organic fluorine deserve special mention. Due to the high electronegativity and lesser polarizability of the fluorine atom, the existence of a possible interaction between F and O is deemed questionable. The existence of halogen bonding involving the heavier halogen atoms Cl/Br/I•••N/O (intramolecular) is well known in the literature [2].

The current investigation [3] involves a detailed and systematic exploration of the structural and electronic features associated with the presence of a unique intermolecular C(sp3/sp2)-F···O contact in the crystal structure of 1-(3-nitrophenyl)-2, 2, 2-trifluoroethanone (A1) and (E)-4-((4-fluorophenyl) diazenyl)phenol (A2). These contacts have been observed to play a significant role in the crystal packing. These contacts were investigated using inputs from theoretical charge density analysis, energy decomposition analysis using PIXEL, QTAIM, Hirshfeld surface analysis, delocalization index, reduced density gradient (RDG) plot, electrostatic potential surface and distributed atomic polarizability. The intermolecular energy decomposition (PIXEL) and RDG-NCI analysis of the F•••O contacts establish the interaction to be dispersive in nature. The mutual polarization of an oxygen atom by fluorine and vice-versa provides real physical insights into the role of atomic polarizability in interacting atoms in molecules in crystals.

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