

Intermolecular interactions involving fluorine in small organic molecules: A structural, computational and charge density analysis

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The study of weak interactions and their role in crystal engineering have been a major area of research in the past few decades.¹⁻⁴ Interactions involving organic C–X (X = F, Cl, Br and I) groups have attracted significant interest in controlling supramolecular architecture in the solid state.⁵⁻⁷ The interactions involving “organic fluorine” has always remind controversial due to its uncertain nature. Many simple organic compounds display biological activity when one or more fluorine atom is strategically inserted in the molecule, indicating that fluorinated molecules have biological importance compared to their non-fluorinated and chloro/bromo analogues.⁸ Hence, it is believed that the interaction of “organic fluorine” with biological receptors is different from that offered by other C–X (X = Cl, Br, I) groups. We have been involved in the systematic understanding of weak yet significant interactions offered by “organic fluorine” in crystal packing over the last decade.⁹⁻¹¹ Our combined structural, computational and experimental charge density studies¹² on a library of fluorinated small organic molecules will be highlighted in the presentation.

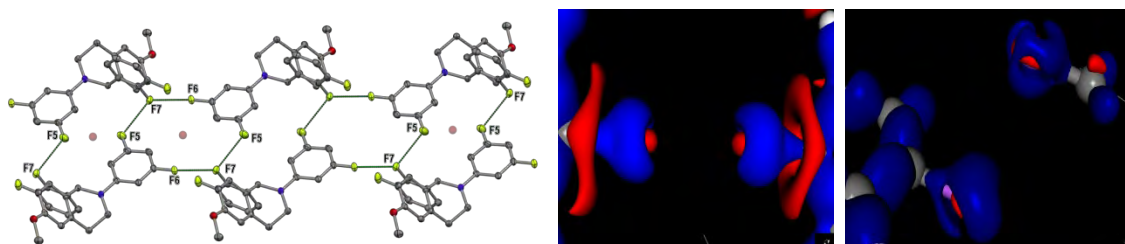


Figure 1. C–F...F–C interactions in small organic molecules, structure to 3D deformation density maps

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