Mapping halogen bonds and other interactions in iodoperfluoroalkylimidazoles: An experimental and theoretical charge density study

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Halogen bonding, namely any noncovalent interaction involving halogens as electrophilic sites, is a relatively new item in the supramolecular toolbox and shares numerous properties with the better known hydrogen bonding. The topological analysis of the X-ray multipole refined charge density proved to be an effective tool to elucidate the nature of halogen bonding [1] and in general of intermolecular interactions responsible for molecular crystals formation.
We present here the results obtained on two iodotetrafluoroethylimidazole derivatives, whose crystal structure is dominated by formation of I···N halogen bonds between equivalent molecules, and stabilized by the presence of F···F, C–H···F, π···π and other weak interactions. The experimental charge densities have been derived from X-ray data collected at 100 K, using the aspherical atom formalism of Stewart [2] as implemented in VALTOPO [3], as well as by accurate DFT and MP2 molecular modeling calculations. Information such as the topological features and nature of the involved interactions, as derived from topological analysis of electron density and its Laplacian, and the interaction energies associated to halogen bonding and the weaker interactions, will be presented.

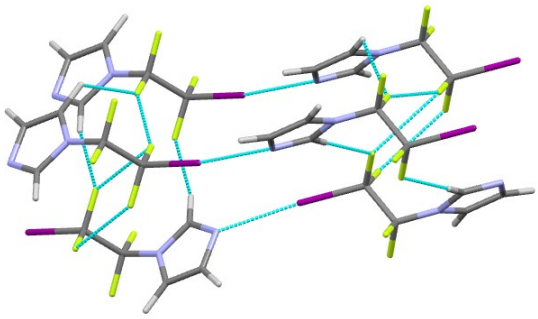

Figure 1: Interactions Network in Iodotetrafluoroethylimidazole (C, gray; H, light gray; N, blue; F, green; I, magenta).

References

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