MS29-P13 Atom interaction propensities between atom types in crystal packings assessed by Hirshfeld surface analysis. The best partners and behaviors of several chemical functions, including oxygen , hydrogen, halogens and water are investigated.

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The partitioning of space with Hirshfeld surfaces enables to analyze and fingerprint molecular interactions in crystalline environments [1]. The decomposition of the crystal contact surface between pairs of interacting chemical species enables to derive an enrichment ratio [2]. This descriptor yields information on the propensity of chemical species to form intermolecular interactions with themselves and other species. The enrichment ratio is obtained by comparing the actual contacts in the crystal with those computed as if all types of contacts had the same probability to form.

The enrichments and contacts tendencies were analysed in several families of compounds, based on chemical composition and aromatic character. As expected, the polar contacts of type H•••N, H•••O and H•••S, which are generally hydrogen bonds, show enrichment values larger than unity. In aromatic compounds, C•••C contacts can display large enrichment ratios due to extensive p•••p stacking occurrence in the crystal packings of heterocyclic compounds. The crystal packings of several families of halogenated compounds also highlights that hydrogen, notably the lowly polar H-C atoms are a preferred interaction partner for halogens [3].

In alcohols, the systematic large enrichment ratios of some interactions like the O-H…O hydrogen bonds suggests that these contacts are a driving force in the crystal packing formation. The same statement holds for the weaker C-H…O hydrogen bonds in ethers, esters and ketones, in the absence of polar hydrogen atoms. The over-represented contacts in crystals of oxygenated hydrocarbons are generally of two types: electrostatic attractions (H-bonds) and hydrophobic interactions between lowly polar groups. It was found in several cases that, in the presence of several oxygenated chemical groups, cross-interactions between different chemical groups (e.g. water/alcohols; alcohols/phenols) are often favored in the crystal packings.

While general tendencies can often be derived for many contact types, the outlier compounds are instructive as they display peculiar or rare features. The methodology allows also detecting outliers which can be structures with errors. The behavior of water in monohydrate compounds was also investigated

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[3] Jelsch, Soudani & Nasr (2015). *IUCr J.* **2**, 327-340.

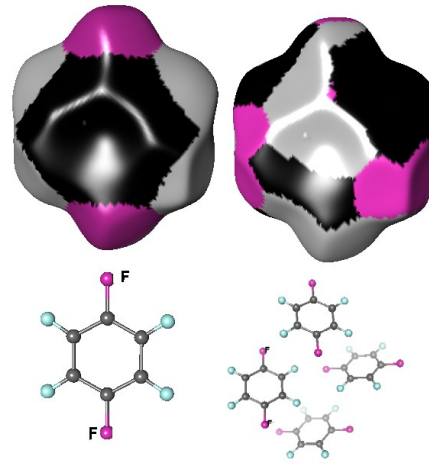

Figure 1. C6H4F2 compound and its crystal packing. The Hirshfeld surface is colored according to the inner (left) and outer contact atom (right).

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