[MS25-P02] Probing Halogen Bonding in Porphyrin Assemblies

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Halogen bonding is one of the most investigated fields in crystallography in recent years. [1] Halogen bonds have been exploited as a significant tool for crystal engineering with molecular and coordination compounds. Halogen interactions are specific and directional, and they have been proven to play a crucial role in supramolecular materials. However, only a few examples of porphyrin structures based on halogen-pyridyl linkers are available.[2] The expression of halogen bonds in organic crystal structures is often affected by the presence of other non-covalent interactions. In this work, we explored a series of six-coordinate Sn-porphyrin complexes with various substitutions of the halogen and pyridyl functions on the porphyrin and the axial ligands (Figure-1). It was aimed to explore the mutual effect of the competing non-covalent interactions in the analyzed assemblies. Theoretical investigations have probed the electrostatic potentials of a number of halogen bonded complexes, to study the fundamental features of these interactions in the porphyrin environment. The results led to interesting observations regarding the competitive nature of the halogen and hydrogen bonding interactions.

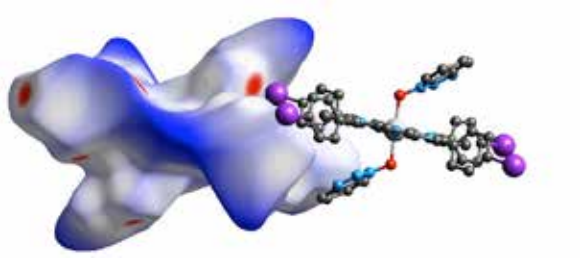

Figure-1: The Hirshfeld surface exhibits direct I···N halogen bonds. The molecule on the left is represented by its Hirshfeld surface.

Keywords: porphyrins, halogen bonds, molecular recognition.

References:

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[2] Hatem M. Titi, Anirban Karmakar and Israel Goldberg, *J. Porphyrins Phthalocyanines*, **2011**; 15, 1250-1257. Sankar Muniappan, Sophia Lipstman and Israel Goldberg, *Chem. Commun.*, **2008**, 1777–1779.