Halogen Bonding for Aromatic Hydrocarbon Assembly in the Solid State

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Strong intermolecular interactions serve as vital tools in cocystal assembly. Halogen bonding (XB) [1], a highly directional interaction, is most often observed between a halogen-atom donor and electron-rich acceptors, such as oxygen or nitrogen. However, XBs can also be used for the organization of arenes in the solid state through interactions with aromatic π-systems, as previously explored in the dichroic and pleochroic cocrystals of naphthalene or azulene, respectively. [2]

This presentation will outline our study of XB cocystal structures containing various polycyclic aromatic hydrocarbons (PAHs), and evaluate the reliability of halogen bonding to carbon as an overlooked tool for crystal engineering.


Keywords: Halogen bonding; cocystal; polycyclic aromatic hydrocarbons