A New Halogen Bond Donor: 1,2,3-Trifluoro-4,5,6-Triiodobenzene

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Halogen bonding is well studied, yet numerous organoiodine-heterocycle systems lack structural characterization. The arrangement of electron-withdrawing fluorines around three highly polarized iodine sites in 1,2,3-trifluoro-4,5,6-triiodobenzene represents a unique organoiodine donor with no reported crystal structures in the Cambridge Structural Database. This work investigates its cocrystallization with a diverse set of nitrogen heterocycles to determine whether halogen bonding emerges and how these assemblies organize. Together, these results will establish the interaction patterns that govern these systems and enable more reliable design of future supramolecular architectures.

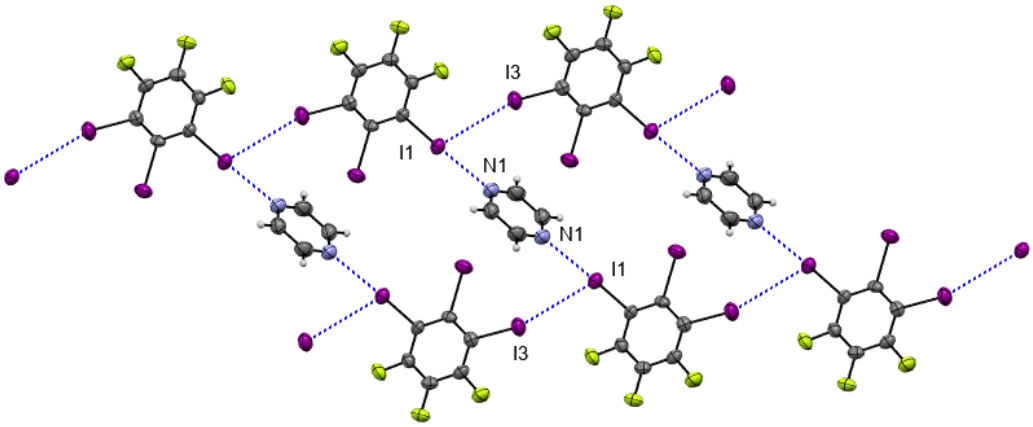

Figure 1. Novel cocrystal of 1,2,3-trifluoro-4,5,6-triiodobenzene and pyrazine