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Supporting information for article:

Polymorphism of a widely used building block for halogen-bonded assemblies: 1,3,5-trifluoro-2,4,6-triiodobenzene

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Table S1 –Cohesion energies (kJ/mol) for Polymorphs **I** and **II** calculated using the CRYSTAL package with a B3LYP functional modified with a London-type correction term for long-range dispersive interactions, and different basis sets.

Basis set	Energy of polymorph I	Energy of polymorph II
6-31G** + Dolls	- 96.1	- 94.5
TZVP + Dolls	- 93.6	- 94.5
6-31G** + HAYWLC	- 102.4	- 104.1
TZVP + HAYWLC	- 102.0	- 104.9

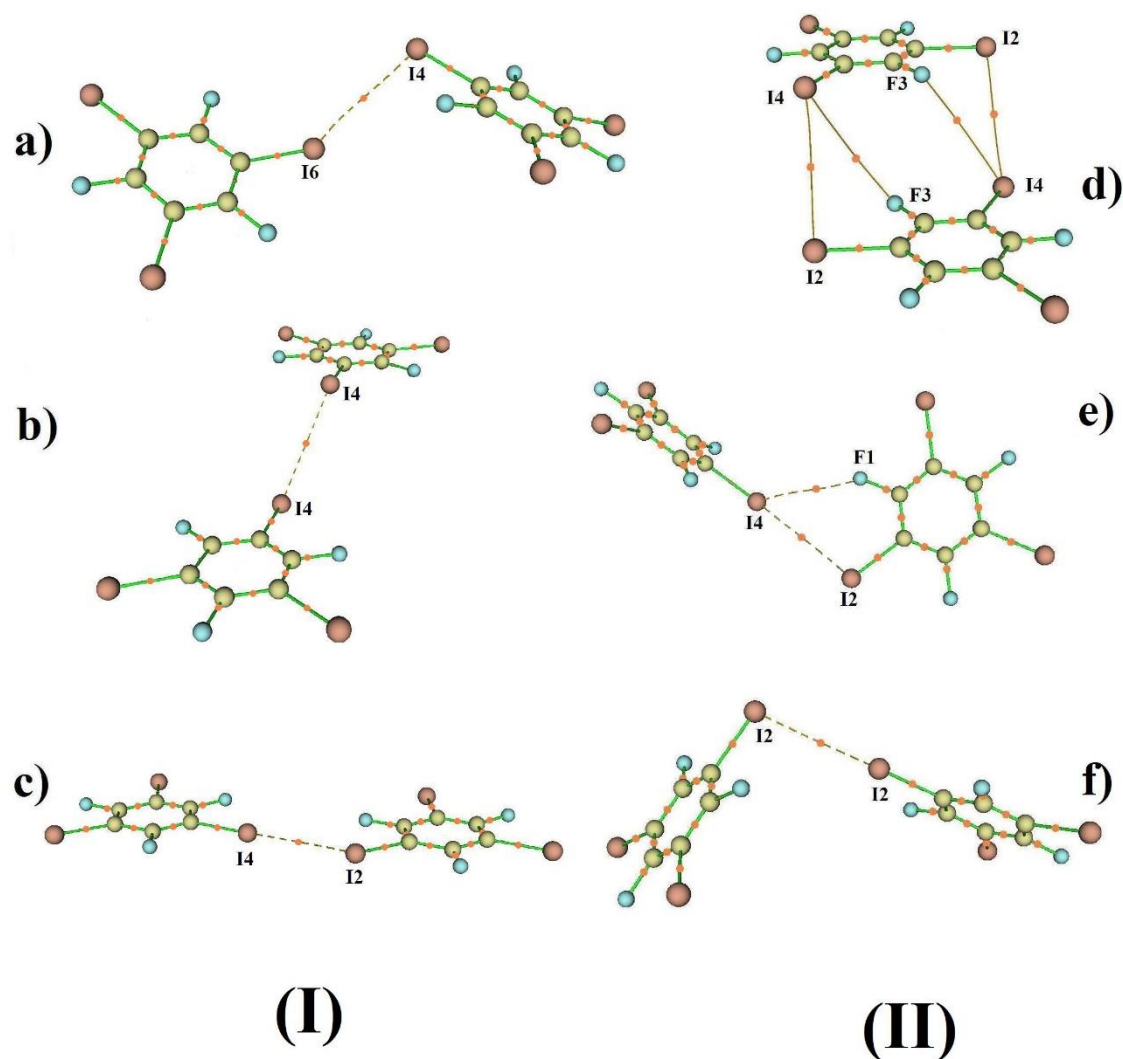


Figure S1. Selected X...X "dimeric" interactions showing "bond critical points" (as orange dots) and "bond paths" as broken lines.

(a), (b), (c): structure **I**. (d), (e), (f): structure **II**.

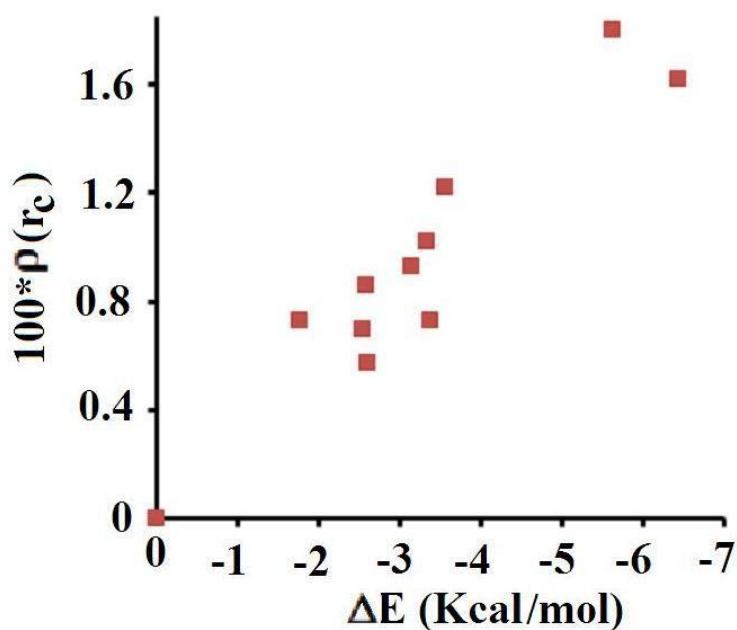


Figure S2. Correlation between DFT and AIM calculation for the dimeric systems. **NOTA BENE:** It is not always possible to individually analyse an interaction by DFT, since a dimer could involve more than one interaction. For this reason, dimer energy formations obtained by quantum-mechanical calculations were compared with the summation of the electron density at BCPs of each system. The obtained linear response indicates that both methods are in fact a complementary way to analyse the system: while DFT evaluates globally the energy involved in the dimer formation, AIM focuses individually on each interaction.