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.