

Poster Presentation

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Decoding conformational polymorphism in organic substances

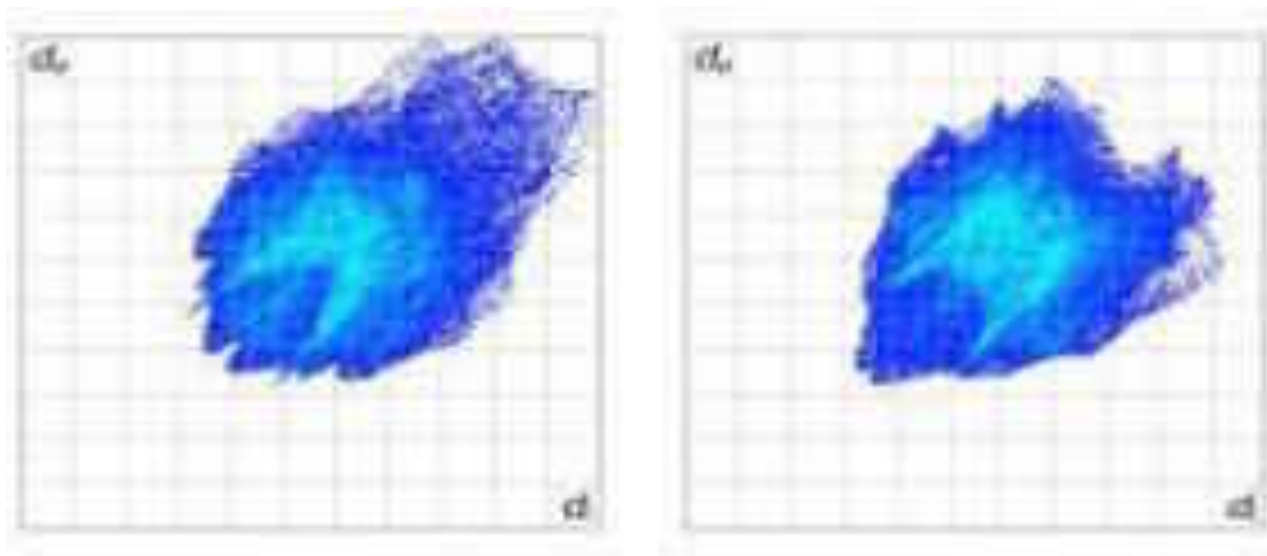
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Different polymorphs have different intensive physical properties and it is still impossible to predict from scratch if a change in the crystallization conditions will result in different crystal structures or not. In this contribution, possible correlations are highlighted among charge density features, molecular conformation and interaction energetics in the two known polymorphic forms of (DTC)[1,2], an isothiazole β -sultamic derivative. A tentative rationale is provided for the relative stability of the two forms on the basis of their different self-recognition patterns. Both polymorphs crystallize in the same $P2_1/n$ space group and show very different non-covalent networks of weak C-H \cdots X (X = N,O, π) interactions due to the dissimilar conformation of the asymmetric units (ASU). Accurate multi-temperature (100 K \leq T \leq 298 K) single-crystal X-Ray diffraction experiments were carried out and the evolution of crystal packing and self-recognition energetics were monitored through periodic quantum-mechanical calculations at fixed geometries. Preliminary results show that dispersive/repulsive and electrostatic non-covalent interactions dominate the crystal packing in both polymorphs. At T=100 K the form A have a tighter packing, as it shows a greater propensity in being involved in H bonds than B (see the Hirshfeld surface fingerprint plots[3] of forms A -left- and B -right- here reported). This reflects in greater density, whereas the estimated DFT cohesive energies of the two forms are similar. DTC has enough molecular flexibility to access various favourable arrangements during the nucleation, as the interconversion between the A and B conformers in the gas phase takes place with a very small activation energy. The possible role of the solvent in favouring either of the two observed conformations is discussed.

[1] F. Clerici; M. L. Gelmi; R. Soave; et al *Tetrahedron* 2002, 58, 5173-5178, [2] A. M. Orlando, L. Lo Presti, R. Soave *Acta Cryst.* 2010, E66, o2032-o2033, [3] M. Spackman, D. Jayatilaka *CrystEngComm* 2009, 11, 19-32



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