Poster Presentation

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Polymorphism involving multiple molecules in asymmetric unit of trifluoromethylated phenylbenzamide

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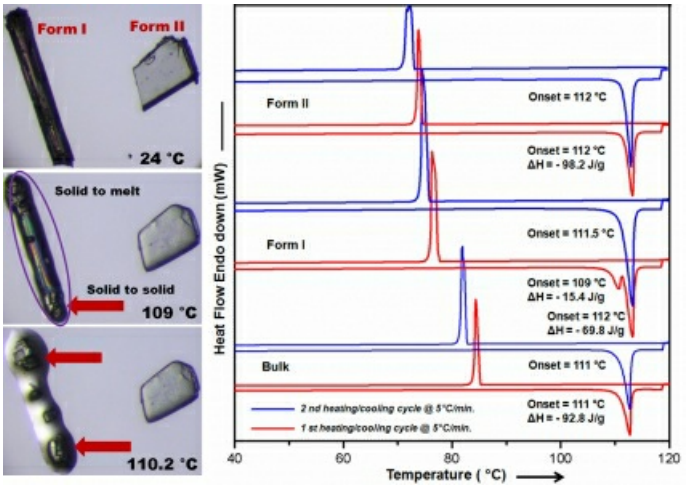
Compounds which crystallized with multiple number of molecules in the asymmetric unit (Z' > 1) have always been of interest in the crystallographic community [1]. However, the phase transition from a stable lower Z' polymorphic form to metastable higher Z' form is an important contribution towards our understanding of the processes which influence the formation of crystals with higher values of Z' [2]. In the current study, concomitant dimorphism has been observed from a solution phase crystallization of the compound 3-(trifluoromethyl)-N-[2-(trifluoromethyl)phenyl]benzamide [3]. The dimorphs, namely, form I (triclinic, P-1, Z' = 2) and form II (monoclinic, Cc, Z' = 4) exhibit nearly the same lattice energy as calculated from the atom-atom method in the CLP module and similarity in crystal packing involving mainly strong N-H•••O=C and weak C-H•••O=C hydrogen bonds. The Xpac analysis shows the presence of 2D isostructurality in between the two polymorphs while the difference in crystal packing arises from the presence of weak C-H•••F-C(sp3) hydrogen bond and C(sp3)-F•••F-C(sp3) interactions. Thermal studies [Fig. 1] revealed the rare occurrence of simultaneous melting and solid-to-solid phase transition from lower Z'>1 structure (form I) to higher Z'>1 structure (form II).

[1] (a) Desiraju, G. R. (2007). CrystEngComm, 9, 91–92. (b) Bond, A. D. (2008). CrystEngComm, 10, 411–415. (c) http://zprime.co.uk/ (d) Steed, K. M. & Steed, J. W. (2015). Chem. Rev. 115, 2895-2933.
[2] (a) Das, D. et al. (2006). Chem. Commun. pp. 555 – 557. (b) Long, S. et al. (2011). Cryst.Growth Des. 11, 414 – 421.
[3] Panini, P. et al. (2016). Cryst.Growth Des. 16, 2561-2572.



Keywords: Concomitant polymorphism, Crystal structures with Z'>1, Isostructurality and Phase transition.