Poster Presentation

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Mapping Structural Landscapes: Isomorphic mefenamic acid and tolfenamic acid forms

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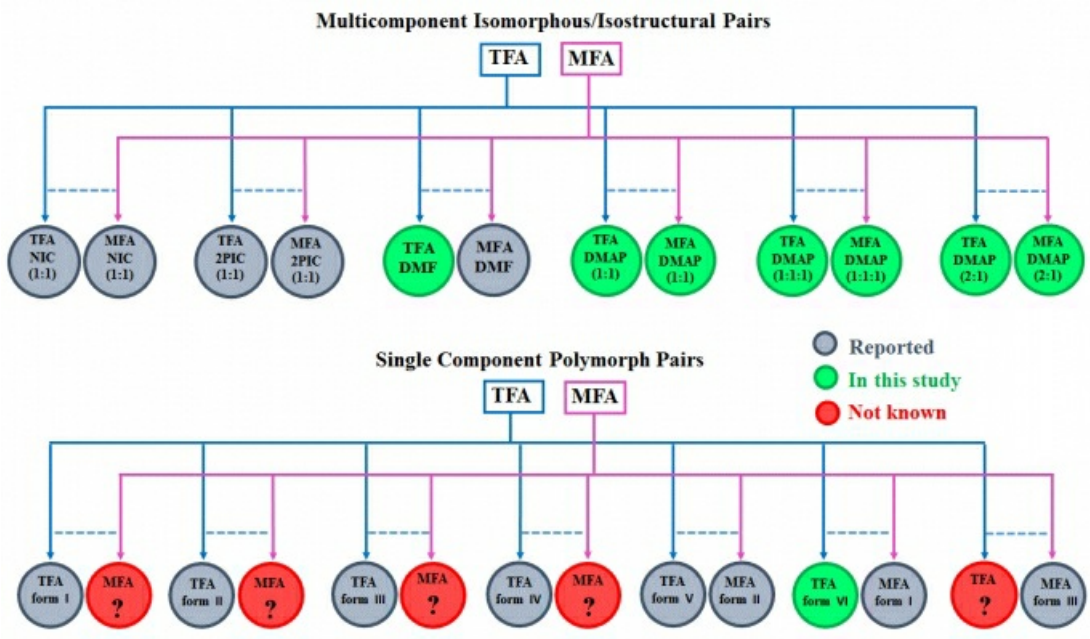
In crystal engineering, the isostructurality and isomorphism aspects are relatively unexplored compared to the common phenomenon, polymorphism. Two crystals are said to be isostructural if they have the same crystal structure, but not necessarily the same cell dimension nor the same chemical composition. On the other hand two crystals are said to be isomorphous if both have the same space group and unit-cell dimensions. In the family of fenamates, mefenamic acid (MFA) and tolfenamic acid (TFA) are isostructural and known to exist in multiple polymorphs. Amongst the polymorphs of these two fenamates, form-II of MFA and form-V of TFA are isomorphous. Herein, we explore the existence of this isomorphous nature in the multicomponent solids polymorphs of MFA and TFA by taking aid from their crystal structural landscape. In this process, we have synthesized three such new isomorphous multicomponent solid pairs with the commercially available MFA and TFA samples. The multicomponent solids include salt (1:1), co-crystal salt (2:1) and salt monohydrate (1:1:1) of MFA and TFA with 4-dimethylaminopyridine (DMAP). Thereafter the new solid forms were thoroughly characterized with several characterization techniques and their structural relationship was investigated. Among them the single crystal diffraction results show that the new solid form pairs of the same ratio (for e.g. 1:1 salts of MFA and TFA) possess same space group and structural packing, which implies that they retain isomorphous nature alike their parent APIs, MFA and TFA. In the course of this study, we realized a tremendous use of mapping the structural landscapes of the two isomorphic series, for instance to obtain the new (or hidden) polymorphs of isostructural pairs. In the quest to validate this utility, we discovered a sixth polymorph and a pseudopolymorph of TFA.

[1] International Union of Crystallography (2006) http://reference.iucr.org/dictionary/Isomorphous_crystals
[2] López-Mejías, V. et al. (2015) Cryst. Growth Des. 15, 3955-3962.
[3] Braga, D. et al. (2009) Chem. Eur. J. 15, 1508 – 1515.



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