

MS29 Crystal engineering: structural flexibility, phase transitions and non-standard manipulation of synthons

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More thoughts on the (un)predictability of supramolecular interactions in molecular crystals¹

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Abstract

We report the use of real-time and *in situ* X-ray diffraction monitoring of thermal and mechanochemical cocrystallisation reactions (using a modified differential scanning calorimeter and an adapted ball mill) to discern hierarchies of supramolecular synthons in multi-component molecular crystals.² The cocrystallisation experiments uncovered a series of solids with unexpected supramolecular structures (along with peculiar and previously unobserved mechanochemical crystallization phenomena³), thus highlighting limitations of our current abilities to understand, engineer, and maintain molecular crystals.⁴

This presentation aims to critically assess a range of concepts and ideas that form the basis of contemporary crystal engineering research,⁵ with the aim to prompt a community-wide conversation about the current state of the art.

References

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