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On the mechanism of cocrystal mechanochemical reaction via low melting eutectic: a time resolved in-situ monitoring investigation

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Cocrystals, namely crystalline compounds made of different chemical entities, are typically synthetized in bulk via mechanochemistry. Whereas the macroscopic aspects of grinding are becoming clear,[1] the fundamental principles that underlie mechanochemical cocrystallisation at the microscopic level remain poorly understood.
Time-resolved in situ (TRIS) monitoring approaches have opened the door to exceptional detail regarding mechanochemical reactions.[2–4] We here report a clear example of cocrystallisation between two solid coformers that proceeds through the formation of a metastable low melting binary eutectic phase. The overall cocrystallisation process has been monitored by TRIS-XRPD with a customized ball milling setup and low-energy synchrotron beam. The reaction is complete in less than 5 seconds and the metastable formation of the amorphous-like phase is clearly spotted thanks to a fast data acquisition time of 500 ms.[5]
An insight on the details of the TRIS-XRPD data analysis for the real-time structure and microstructure investigation, generally applicable to all chemistry, will be also provided.[4]
The binary system and the low melting eutectic phase were further characterized via DSC, HSM, and VT-XRPD.

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