Supporting Information

Effect of dehydration pathway on the surface properties of molecular crystals

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Thermogravimetric analysis

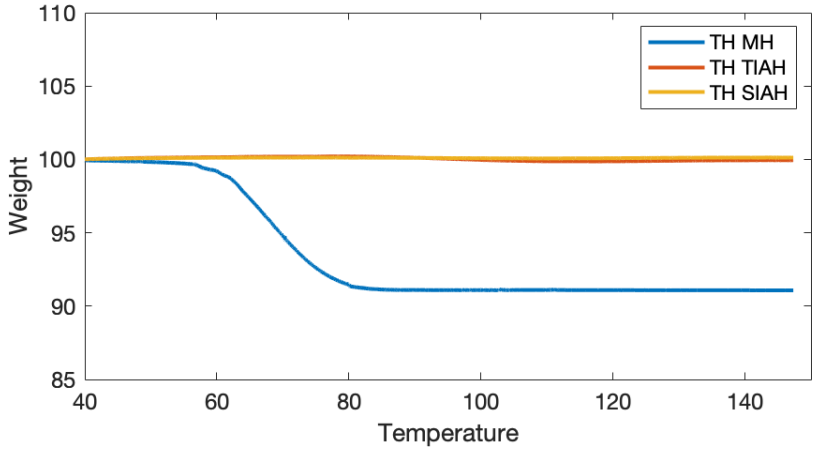

Figure S1. Thermogravimetric analysis of theophylline monohydrate (TH MH), a thermal induced anhydrate (TH TIAH) and a solvent induced anhydrate (TH SIAH).

Thermogravimetric analysis (TGA) of the three samples. The total mass loss after dehydration was approximately 8 %.

Contact potential measurements

The contact potential was initially measured with Kelvin probe force microscopy. Using highly oriented pyrolytic graphene (HOPG) as a reference, the work function of the three samples could be determined.

Potential (V)	TH MH	TH TIAH	TH SIAH	HOPG
Mean	-0.871	0.690	0.312	0.378
SE	0.002	0.025	0.074	0.112

Table S1. Contact potentials of the three samples and a highly oriented pyrolytic graphene (HOPG) reference sample. These values were used to determine the work functions.

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Dehydration kinetics

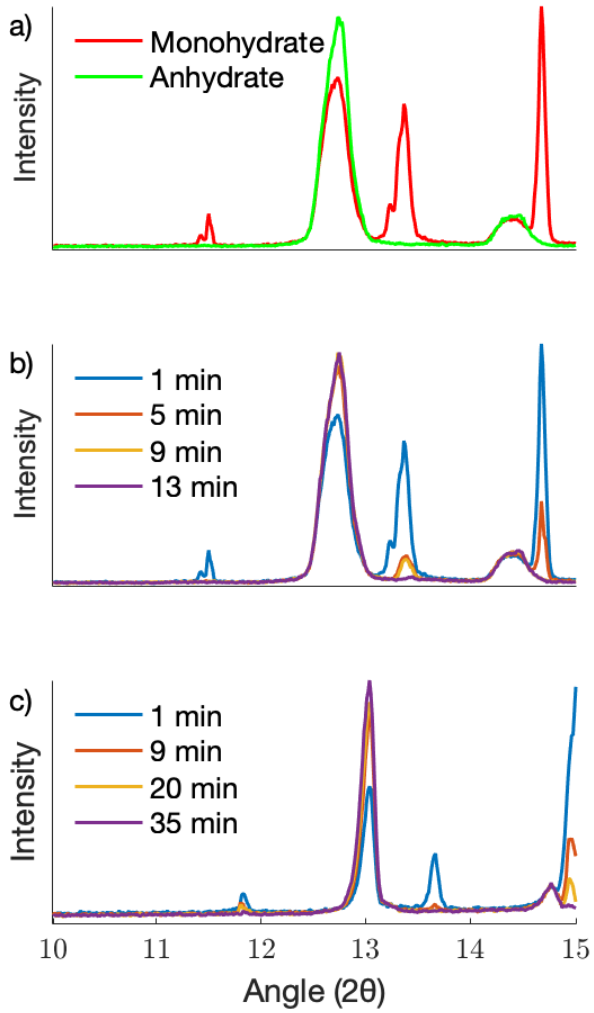

Figure S2. Powder X-ray diffraction of a) theophylline monohydrate and theophylline anhydrate b) in situ thermal induced dehydration of theophylline and c) in situ solvent induced dehydration of theophylline.

Powder X-ray diffraction (PXRD) was used to determine the dehydration kinetics of the transformations. The thermal induced dehydration took 13 minutes, and the solvent induced dehydration took 35 minutes. All transformations were measured with 1-minute intervals. The transformations occurred continuously.

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Scanning Electron Microscopy

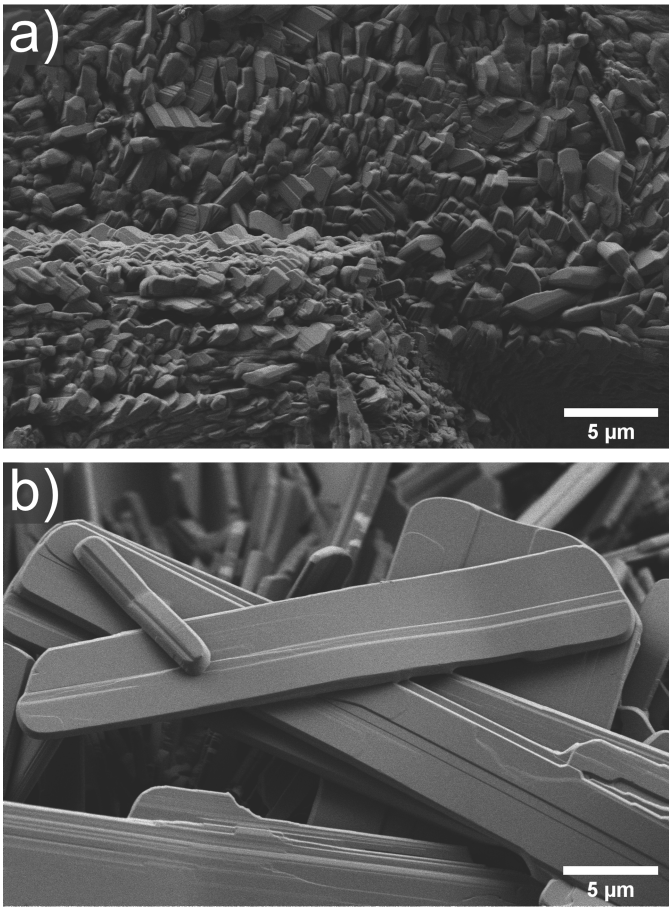

Figure S3. SEM micrographs of the surface of a) thermally induced and b) solvent induced theophylline anhydrate crystals.