Supplementary Materials

Analysis of Co-Crystallization Mechanism of Theophylline and Citric Acid from Raman Investigations in Pseudo Polymorphic Forms Obtained by Different Synthesis Methods

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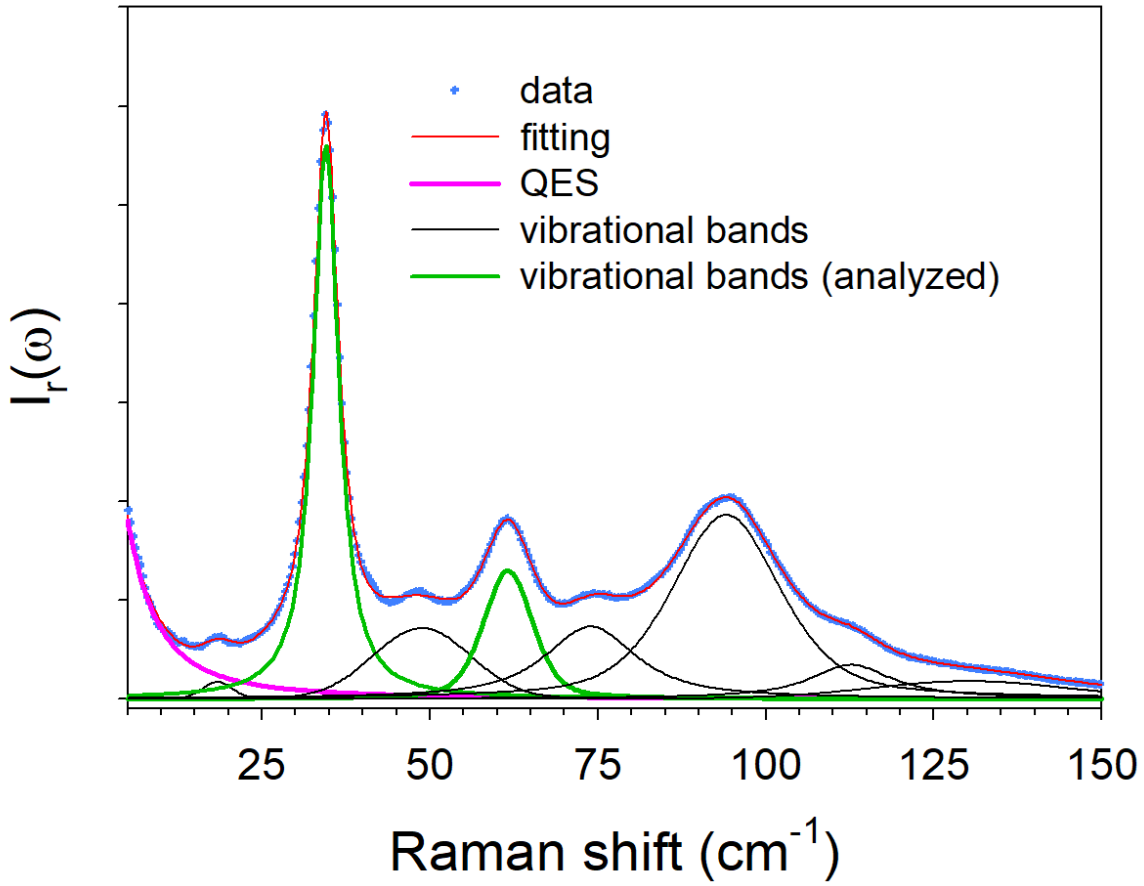

Figure S1. Fitting procedure of the low-frequency spectrum in co-crystals. Bands plotted in **green thick lines** and the quasielastic scattering (QES) have been analyzed in anhydrous and hydrate forms.

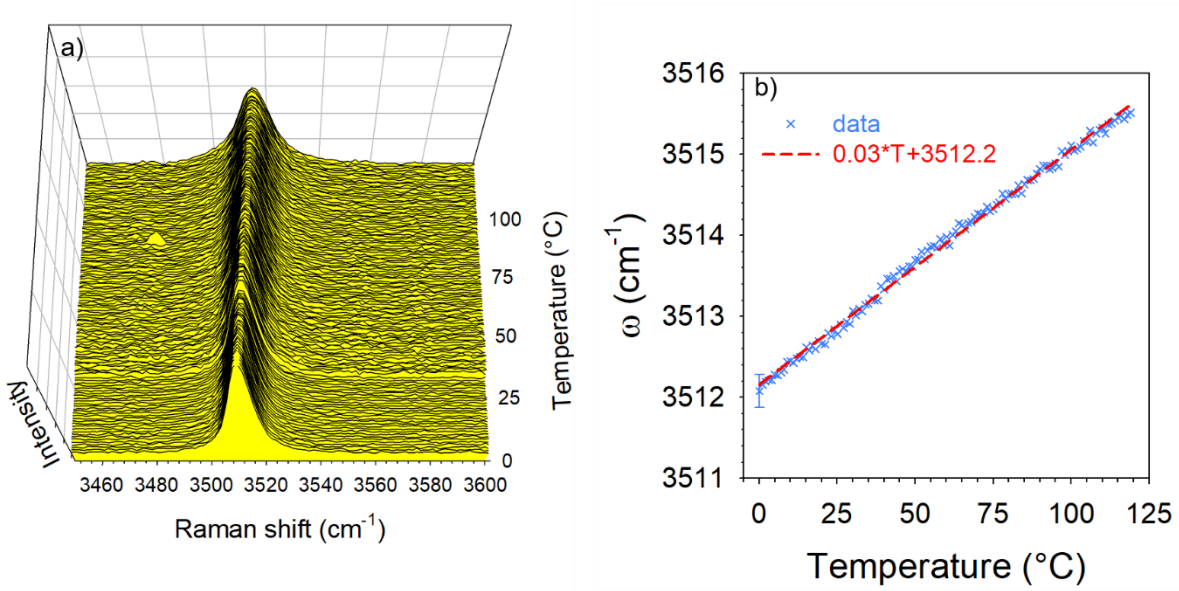

Figure S2. Temperature dependence of the O – H stretching band in the anhydrous co-crystal, typical of vibrations of OH groups within citric acid molecules involved in π-H-bonding with TP molecules; **a**) temperature dependence of the spectrum; **b**) temperature dependence of the position of the O – H stretching band obtained by fitting the band with mixed Gaussian-Lorentzian peak – the dashed line corresponds to the fit of data with a linear regression.

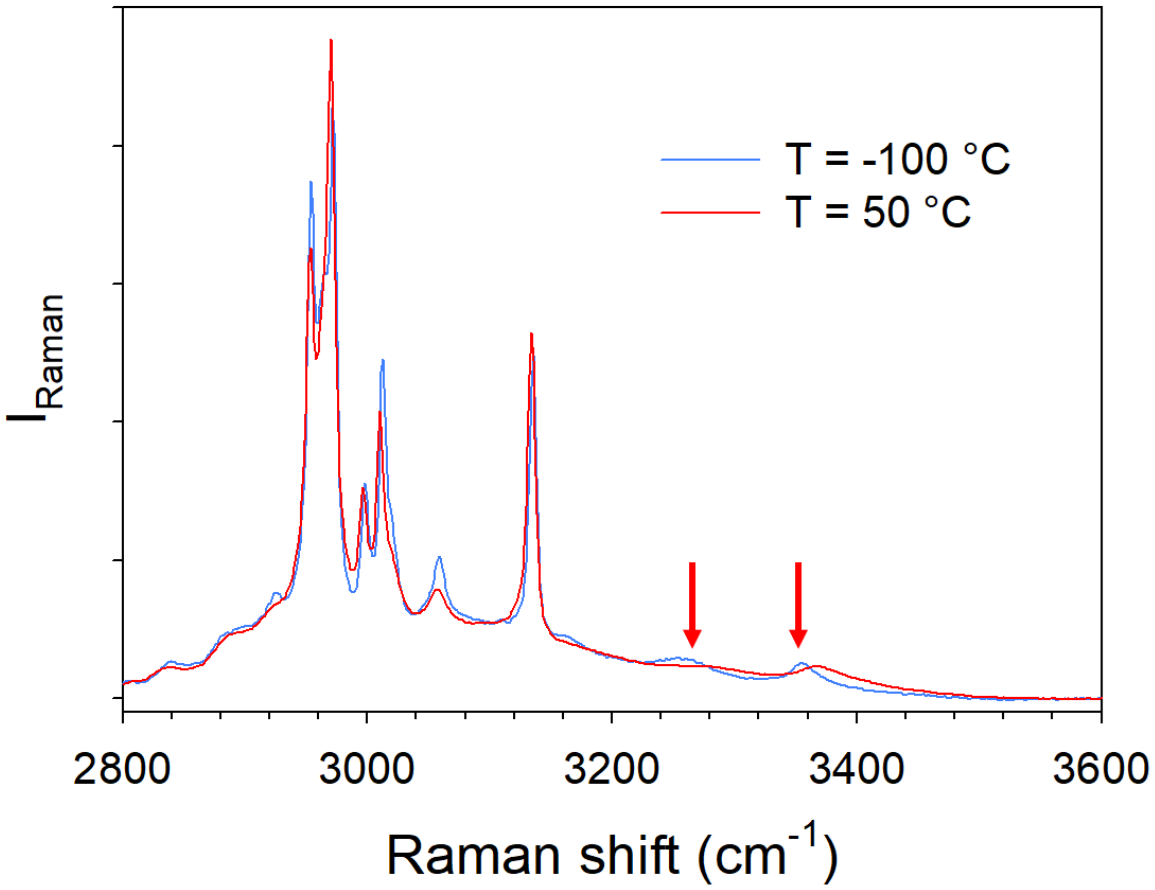

Figure S3. Temperature dependence of the high frequency spectrum taken in the co-crystal hydrate. The arrows show the two O – H stretching bands which exhibit a signature of H-bonding, i.e. a positive temperature dependence of the position. These bands have assigned to vibrations of OH groups within water molecules bound interacting with TP and CA molecules