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The urea-barbituric acid polymorphic co-crystal system: characterization, thermodynamics and crystallization

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Polymorphism in co-crystals is known to have a dramatic effect on physiochemical properties. The current contribution covers the characterization, thermodynamic analysis, and cooling seeded crystallization investigation of the urea-barbituric acid (UBA) polymorphic co-crystal system including urea (UA), barbituric acid (BA), and two polymorphic UBA (Forms I and III). Supramolecular synthesis of UBA Forms I and III have been conducted by cooling crystallization in methanol and then systematically characterized by powder X-ray diffraction (PXRD), thermal analysis (DSC and TGA), Raman and IR spectroscopy. Compared to the TGA results, the exothermic and endothermic peaks shown in DSC curves represent the decomposition of UBA and the melting of BA, respectively. Using the measured solubility data, the UBA polymorphs were found to be an enantiotropic polymorphic system, and the transition points in the water and methanol were determined at 35 ^{o}C and 33 ^{o}C, respectively. Subsequently, the modified Apelblat equation and van't Hoff model were used to correlate the experimental data and to calculate the dissolution enthalpy and entropy of the different system. Moreover, cooling seeded crystallization of two

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