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The crystal morphology and growth kinetic mechanisms of para-aminobenzoic acid

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The Crystal Morphology and Growth Kinetic Mechanisms of Para-AminoBenzoic Acid
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Needle-like crystal morphologies can cause problems during downstream unit processes assoicated with pharmaceutical and fine chemical product manufacture, due to their fragility under compaction, difficulties in filtering and tendency to block pipes. Tailoring a crystal morphology from solution requires an understanding of the molecular scale surface chemistry and the crystal growth kinetic mechanisms, forming the basis of the design of a solution environment.
α-para amino benzoic acid (pABA) crystallises as a needle-like morphology from most organic solvents, such as ethanol, water and acetonitrile1. Here the bulk solid-state intermolecular interactions (intrinsic synthons) are discussed in terms of the α-pABA stability, and the surface terminated intermolecular interactions of the major (101), (10-1) and (01-1) surfaces2, in terms of their interaction with the surrounding solution and crystal morphology.
The experimentally elucidated crystal growth kinetic mechanisms of the side (10-1) and capping (01-1) surfaces, in ethanol, are linked to the extrinsic synthons and crystal morphology observed3. The surface entropic α-factors are calculated to estimate the interfacial roughening of the individual faces in ethanol, and how this can affect the crystal growth kinetics. A model for the temporal evolution of a equilibrium crystal morphology of α-pABA at different supersaturation is presented, in terms of guiding the residence time for industrial batch crystallisation.
Finally, the effect of addition of nitromethane to the ethanol solutions on the crystal morphology of α-pABA is presented. This demonstrates that through a careful choice of solvent, based on a molecular and kinetic understanding of the crystal surface can successfully modify a crystal morphology from solution.
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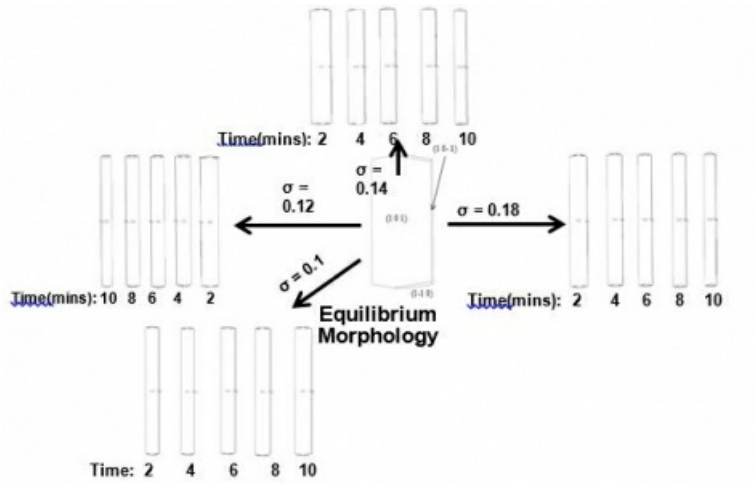

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