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Crystal Habit Modification of Vitamin C (L-Ascorbic Acid) due to Solvent Effects

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Abstract: Crystal morphologies are predicted for vitamin C (L-ascorbic acid) using attachment energy methods. The significant differences between predicted and observed morphologies when vitamin C is grown from water, isopropyl alcohol, acetone-water solution, and isopropyl alcohol-methanol solution are attributed to the effect of solvent on the growth rate of the various crystal habit faces. This effect, particularly the role of hydrogen bonding between solvent and crystal surface, is examined. Molecular modeling is combined with the results of simple experiments charting the habit shift of vitamin C as a function of the hydrogen bonding tendency of the solvent or solvent mixture. Attachment and slice energies can be determined from periodic bond chain (PBC) analysis or calculated directly from the crystal structure by partitioning the lattice energy calculated from each symmetrically independent molecule in the unit cell into slice and attachment energies. First in the PBC analysis of vitamin C the Cerius[2] molecular modeling package was used to search for connected nets in a given range of orientations (hkl).

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