Understanding and Using Solution Chemistry to Direct Crystal Nucleation

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Our understanding of non-covalent interactions which determine crystal packing in the solid state has progressed enormously over the last years due largely to the explosion in numbers of crystal structure determinations and their availability via the Cambridge Structural Database. In the context of *controlled* building of crystals however, this information is not enough, we also have to consider the interactions which exist in the solution phase at the time of nucleation. Such information can be gleaned from a number of sources: thermodynamic and colligative data (eg solubility, freezing point depression);

UV/vis spectroscopy; vibrational spectroscopies; NMR; and neutron scattering.

This paper reports on the use of these techniques in understanding the key interactions in highly concentrated solutions of urea, benzoic acid, tetrolic acid, sulfamerazine and 2,6dihydroxybenzoic acid. In many cases there is a clear link between solvent mediated self assembly and the resulting crystal structures.

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