The lattice energy of organic compounds: thermodynamic facts and computer simulation

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The nature of cohesive energies in organic crystals will be reviewed, with its expression in terms of enthalpy; lattice vibrational energies and lattice free energies will then be introduced. Relationships to heats of sublimation will be discussed. A special attention will be devoted to energy difference between crystal polymorphs. Modern methods (quantum chemical and force field, static and dynamic) for the computer simulation of solid state properties of organic compounds will be reviewed. Applications to possible crystal structure prediction and control will be described with a few practical examples.

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