Assessing Lattice Energy Minimisation for Crystal Structure Prediction

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The goal of reliable crystal structure prediction has been a driving force for the development of methodologies in modelling molecular organic crystals. The first step in crystal structure prediction involves a search for all low energy structures on the potential energy surface. Such searches usually generate far more energetically feasible structures than are known or are likely to be observed and the energy differences between possible structures are typically very small. Therefore, the ordering of energetic stability requires a high quality model for the lattice energy.

Several options for modelling the energies of predicted crystal structures are examined: empirical atom-atom potentials with atomic charges and multipoles; the recently developed semiclassical density sums (SCDS or "Pixel") method [1]; and periodic density functional theory calculations. The models are assessed on a test set of small organic molecules [2] and results of the most recent (third) blind test of crystal structure prediction are also examined. Advantages and shortcomings of the various methods are discussed.

[1] a) Gavezzotti A., *J. Phys. Chem. B,* 2002, **106**, 4145-4154; b) Gavezzotti A., *J. Phys. Chem. B,* 2003, **107**, 2344-2353. [2] a) Day G. M., Chisholm J., Shan N., Motherwell W. D. S., Jones W., *Crystal Growth & Design,* 2004, **4**, 1327-1340; b) Day G. M., Motherwell W. D. S., Jones W., *Crystal Growth & Design*, 2005, *in press*.

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