

MS31-P2 *q*-GRID: a new method to calculate lattice and interaction energies for molecular crystals from electron densities

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Mapping of intermolecular interactions is a useful tool to obtain packing motives and insights in the relative stability of different crystal structures. Obtaining quantitative information on these interactions is, however, not straightforward. Often, the gas phase conformation and charge distribution of an isolated molecule are used as a starting point - for instance in the PIXEL method[1] - although many examples exist in which this approximation is not applicable. Here we present *q*-GRID[2], a newly developed and freely accessible tool (www.theochem.ru.nl/qGRID) that is designed to calculate intermolecular interactions directly from conformations and the charge distribution as obtained within the crystal. The charge distribution on a grid is partitioned over the different molecules. For the electrostatic interactions, simply the Coulomb energy is determined by a summation over the grid points of the different molecules. Added to this are empirical dispersion and repulsion contributions. The sum of the three components leads to pairwise intermolecular interactions that perform very well in all three test systems studied; anthracene, isonicotinamide and DL-methionine.[2]

Two ways in which *q*-GRID can be used are, ranking the stability of different crystal structures on the basis of the lattice energy[3] and zooming in at specific interactions within a crystal. Fig. 1 is an example of the latter, it shows the dominant interactions in the five known polymorphic forms of isonicotinamide. Two different classes of dimer configurations can be clearly seen. The strongest one is an amide-connected dimer which is only present in the thermodynamically stable polymorph, Form I. Interestingly, metastable polymorphs only crystallize from solution when these amide-connected dimers are absent from the solution.[4] This can be understood with the results of Fig. 1, since this particular dimer has a stronger interaction energy than the other leading interactions. Currently, we are further developing *q*-GRID by more precisely treating the dispersion and repulsion energy terms. In the future we aim to use *q*-GRID for morphology and nucleation rate predictions.

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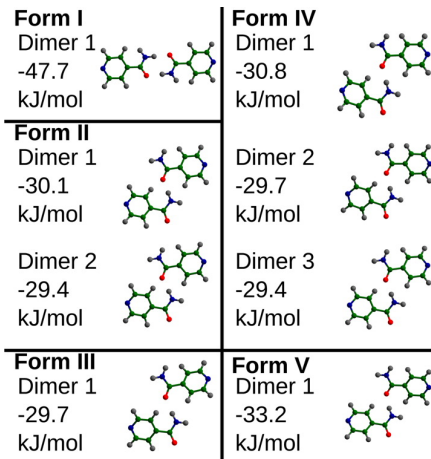


Figure 1. The strongest intermolecular interactions within the five different polymorphic forms of isonicotinamide as obtained with the *q*-GRID method. The strongest dimer in the thermodynamically stable polymorph, Form I, is much stronger than the strongest dimers in the metastable polymorphs.

Keywords: intermolecular interactions, computational tool, molecular crystals, charge distribution, polymorphism