The Use of Quantum Chemical Semiempirical Methods to Calculate the Lattice Energies of Organic Molecular Crystals. Part I: The Three Polymorphs of Glycine

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A method to calculate the lattice energies of organic molecular crystals is described. It is based on the semiempirical quantum chemical MINDO/3 approximation but might also be used within the framework of any other quantum chemical method. The lattice energy is approximated by the sum of dispersion-, induction-, exchange repulsion-, and electrostatic energy. Different, however, from other schemes employed in this field, like for example the atom-atom-potential method, the variables in the expression for the lattice energy have not been fitted to reproduce experimental values and, therefore, the single contributions retain their original physical meaning. Moreover, the method offers the advantage that it may be directly applied to all compounds that can be treated within the framework of the underlying quantum chemical method. Thus, time consuming readjustment of the entire parameter set upon extension of the group of target molecules by another class of compounds becomes obsolete.

As an example, the lattice energies of the three polymorphs of glycine are calculated.

Key words: Lattice Energy; Glycine; Semiempirical Methods.