Estimation of Lattice Energies of Organic Molecular Crystals by Combination of Experimentally Determined and Quantum-Chemically Calculated Quantities: A New Value for the Lattice Energy of α-Glycine

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A new value for the lattice energy of α-glycine was determined by combination of the experimentally measured heat of sublimation taken from literature and the quantum-chemically calculated energy difference $E_{\mathrm{tot,gp}} - E_{\mathrm{tot,cry}}$, where $E_{\mathrm{tot,gp}}$ is the total energy of the most stable form of the compound in the gas phase (carboxylic acid) and $E_{\mathrm{tot,cry}}$ the total energy of the molecule as it occurs in its crystalline form (betaine). At the highest levels of *ab initio* theory employed in this study this energy difference is –(28±2) kcal/mol, indicating that older work overestimated this difference significantly. The reason for the overestimation of this energy difference was determined by means of additional *ab initio* calculations. The lattice energy of –(67±2)kcal/mol obtained using the new value for $E_{\mathrm{tot,gp}} - E_{\mathrm{tot,cry}}$ is significantly more positive than an older value of –103 kcal/mol frequently cited in the literature.