Semiempirical Calculations on the Dipole Moment Enhancement in the Solid State*

Gerhard Raabe

Institut für Organische Chemie, Rheinisch-Westfälische Technische Hochschule Aachen,
Prof.-Pirlet-Straße 1, D-52074 Aachen

Reprint requests to Prof. Dr. G. R.; Fax: +49 241 80 92385, E-mail: gerd.raabe@thc.rwth-aachen.de

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The enhancement of the molecular dipole moment under the influence of the crystal lattice relative to the value for the corresponding isolated molecule has been calculated for the three low-pressure polymorphs of glycine using the semiempirical MINDO/3 *Hamiltonian*. In these calculations the influence of the lattice on an arbitrarily chosen reference molecule has been included by modifying the diagonal elements of the $\mathcal{H}^{\mathrm{core}}$ matrix. Starting from a set of atomic charges calculated for the isolated molecule an initial crystal lattice had been set up and included into the calculation of new self-consistent (SCF) charges for the reference molecule. The resulting set of new SCF charges was then used to replace the lattice charges from the preceding run, and a new SCF calculation was performed. This iterative process was continued until the difference between the electronic energies and the sum of the absolute values of the differences between the atomic charges from two subsequent SCF calculations was lower than 10^{-5} eV and 10^{-5} e_0, respectively. The results agree nicely with the experimental data obtained by other authors for α-glycine.

Key words: Dipole Moment Enhancement; Glycine; Calculations; Semiempirical Methods.