MOLECULAR MECHANICS FORCE FIELDS FROM *AB INITIO* CALCULATIONS

T. Sundius, K. Palmö[1], L.-O. Pietilä, and S. Krimm[1]

University of Helsinki, Dept. of Physics, Accelerator Laboratory,
SF-00170 Helsinki, Finland

[1]Biophysics Research Division and Dept. of Physics, University of Michigan
Ann Arbor, Michigan 48109, U.S.A.

The improved speed and availability of modern supercomputers has made it possible to use high level *ab initio* calculations on increasingly complex molecules as a standard means to obtain molecular data, such as structures and force fields, that otherwise would be difficult to determine reliably. *Ab initio* calculations have therefore become an important tool in the construction of empirical potential energy functions used in molecular mechanics, molecular dynamics, and Monte Carlo calculations. Major applications involve protein and drug design, and composition of new polymer based materials.

A new method for the utilization of scaled *ab initio* force fields and structures in the construction of the energy functions, has recently been developed. The *ab initio* calculations have been performed with the Gaussian program at the MP2/6-31G* level, followed by a calculation of scaling factors according to Pulay's method from observed spectra using a modified version of the program MOLVIB [1]. So far we have studied some olefins and alkanes, and a set of silyl ethers.

The scaled *ab initio* force field was then transformed into the corresponding molecular mechanics force field using a previously developed procedure [2-3]. This transformation yields molecular mechanics force constants and reference geometry parameters [4] that retain the *ab initio* minimum structures and vibrational frequencies and modes.

The study of olefins showed that the torsions cannot be described in terms of quadratic force constants, so these parameters have to be converted to periodic potentials. For the methyl torsions this is relatively simple, but the double bond torsions require special attention if one wants the potential to reproduce correctly the torsion barriers, including that of cis...trans 2-butene, as well as the torsional vibrations. It was found that the double bond torsion potentials can be sufficiently well represented with two electrons in two orbitals MCSCF calculations. The calculated torsion barrier is then about 65 kcal/mol both for ethene and propene.

References:

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