

Fitting of torsional force field parameters as an analytic linear least squares problem

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Abstract

We present an improved computational approach to simultaneous fitting of force field dihedral parameters for multiple dihedral angles to target conformational energies. This type of fitting has traditionally been treated as a non-linear least squares type fit, using the requisite iterative or heuristic search methods in order to arrive at an optimal parameter set that best fits the target data. We show that the conventional functional form for the dihedral potential energy in the major force fields can be recast in a linear form, and thus the fitting problem can be solved analytically via a linear least squares solution. We then compare the analytic solution of dihedral parameters to the method of a genetic algorithm, in terms of computational time and quality of parameters, for two simple molecules.