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DIADORIM: a Monte Carlo Program for Liquid Simulations including Quantum Mechanics and Molecular Mechanics (QM/MM) Facilities: Applications to Liquid Ethanol

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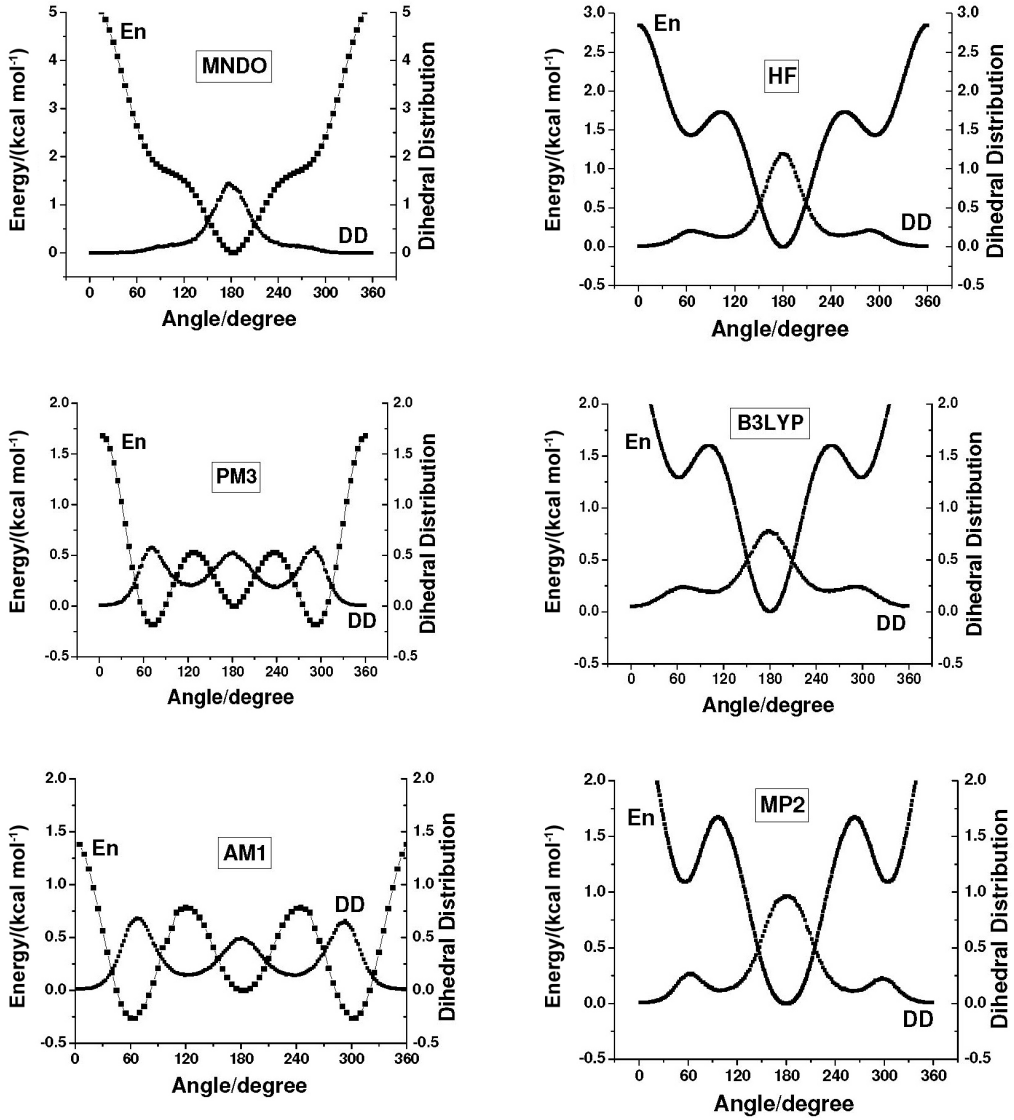

En = energy as a function of dihedral angle; DD = Dihedral angle distributions obtained in corresponding pure liquid Monte Carlo simulation.

Figure S1. The rotational energy profiles for an isolated ethanol molecule calculated as a function of the dihedral angle defined by atoms H–O–C–C using different quantum chemistry methodologies. The dihedral angle distribution obtained in the corresponding Monte Carlo simulation is also shown.

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Comments

The rotational energies profiles obtained with the semiempirical methods are qualitatively different from the ones calculated with Hartree-Fock, second order Moller-Plesset (MP2) theory and B3LYP functional using 6-31g* basis set. The qualitative disagreement between the semiempirical and the others methodologies are clear. These differences are mainly related to the small values of the barriers to internal rotation as well as to the inadequacy of semiempirical methods in reproducing conformational analysis.[34,37] For each rotational energy profile the corresponding dihedral angle distribution obtained in the Monte Carlo simulation is also shown. As expected from the Boltzmann distribution, minima in the potential energy curve are correlated with maxima in the corresponding distribution. This correspondence explains the predominance of *gauche* populations obtained with AM1-OPLS and PM3-OPLS models as well as of the *trans* population observed in the MNDO-OPLS results.