

Analytic First and Second Derivatives for the Fragment Molecular Orbital Method Combined with Molecular Mechanics

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Abstract

Analytic first and second derivatives of the energy are developed for the fragment molecular orbital method interfaced with molecular mechanics in the electrostatic embedding scheme at the level of Hartree-Fock and density functional theory. The importance of the orbital response terms is demonstrated. The role of the electrostatic embedding upon molecular vibrations is analyzed, comparing force field and quantum-mechanical treatments for an ionic liquid and a solvated protein. The method is applied for 100 protein conformations sampled in MD to take into account the complexity of a flexible protein structure in solution, and a good agreement to experimental data is obtained: frequencies from an experimental IR spectrum are reproduced within 17 cm⁻¹.

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