

The Structural Stability of Enzymatic Proteins in the Gas Phase: A Comparison of Semiempirical Hamiltonians and the GFN-FF

Autorzy

Jarosław J. Panek

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Streszczenie

The study of the gas-phase behavior of proteins has recently gained momentum due to numerous prospective applications in, e.g., the construction of molecular sensors or nano-machines. The study of proteins outside their standard water environment, necessary to arrive at their successful applied use, is, however, limited by the loss of the structure and function of the macromolecules in the gas phase. We selected two enzymatic proteins with great potential for applied use, the digestive enzyme trypsin and the cytochrome sterol demethylase, for which to develop gas-phase structural models. The employed levels of theory were semiempirical, density functional tight binding, and polarizable force-field techniques. The convergence of the self-consistent field equations was very slow and in most cases led to oscillatory behavior, encouraging careful tuning of the convergence parameters. The structural optimization and molecular dynamics simulations indicated the parts of the proteins most prone to structural distortion under gas-phase conditions with unscreened electrostatics. This problem was more pronounced for cationic trypsin, for which the stability of the simulation was lower. The fate of the hydrogen bonding network of the catalytic triad in the gas phase was also investigated.

Słowa kluczowe

protein structure, gas phase, semiempirical methods, force fields, trypsin, sterol demethylase

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