

Free Energy Barrier for Dissociation of the Guanosine Monophosphate Anion in Water

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We report free energy barriers for the ground-state dissociation of the guanosine nucleotide anion in solution, employing implicit and explicit solvation models. The latter was based on the Free Energy Perturbation technique and Monte Carlo simulations. For the lowest-energy structure, both solvation models indicate a solvent-induced transition from a dipole-bound state in the gas phase to a π^* valence state in solution. The free barrier estimates obtained from explicit and implicit solvation are in fair agreement with each other, although significantly overestimated in comparison to a previously reported explicit solvation model based on *ab initio* molecular dynamics simulations. Accounting for corrections related to the different DFT functionals used in present and previous studies significantly improves the agreement.