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DFT-based prediction of geometric and thermodynamic parameters in the ATP to ADP hydrolysis reaction MARK C. PALENIK, JORGE H. RODRIGUEZ, Department of Physics, Purdue University — Studying covalent (chemical) and noncovalent (physical) mechanisms as well as key structural variations associated with ATP $\rightarrow$ ADP hydrolysis is of interest for understanding a multitude of biophysical and biochemical cellular processes. We have studied geometric variations of the ATP and ADP molecules during their hydrolysis reaction using density functional theory (DFT) with an implicit solvation model. We have computed the change in free energy, ΔG, associated with the hydrolysis reaction and established relationships between key geometric parameters and thermodynamic properties. Our computed values for ΔG were found in good agreement with available experimental data for two different sets of geometric conformations. A link is suggested between these values for ΔG and changes in geometry of the ADP molecule. Of methodological and computational interest, we also determined that, while the conductor-like solvation model in the framework of the polarizable continuum model (C-PCM) was capable of producing biochemically meaningful geometries for ATP and ADP, it also displayed a strong preference for binding between the H^+ and PO_4^{2-} ions formed during hydrolysis.

Jorge H Rodriguez
Department of Physics, Purdue University

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