

# Quantum-Mechanical Analysis for the Accurate Prediction of Noncovalent Interaction Energy Contributions of H-Bonded DNA Base Pairs

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**Abstract:** Understanding the function of bio-macro-molecules such as DNA or RNA and proteins requires a deep knowledge of non-covalent interactions (NCIs). In this respect, quantum chemical studies of non-covalent complexes provide key steps in this direction. Herein, we report a quantum-mechanical analysis of the interaction energy contributions of H-bonded biomolecules. Coupled-cluster theory through perturbative triples [CCSD(T)] extrapolated to the complete basis set (CBS) limit and SAPT2+(3)(CCD) $\delta$ MP2/aug-cc-pVXZ (X=D, T) level of theory are considered to estimate very accurately (the so-called "gold-standard" of quantum chemistry) NCI energies. Investigated biomolecules with the SAPT variant of intermolecular perturbation theory, yielding a rigorous decomposition of the interaction energy into electrostatic, dispersion, induction, and exchange contributions. Total interaction energies extrapolated to the CBS limit are compared with corresponding MP2 and CBS and estimated CCSD theory results. Further, a comparison of the NCI energy contribution of H-bonded biomolecules is done. This study could significantly change the present view on the importance of specific non-covalent H-bonding interactions, for instance, in DNA. Present stabilization energies for H-bonding energies represent the most accurate and reliable values and can be considered as new reference data for future studies.