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The theoretical study on complexes of the nucleic acid bases with a water

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Introduction

Since Franklin and Gosling examined the first fibers of DNA, it has been known the DNA occurs in vivo in the hydrated form. Numerous experimental studies using different methods have led to the conclusion that DNA is heavily hydrated. The hydration layer is known to play a crucial role in promoting nucleic acid base stacking and helix stabilization [1].

Computational Method

B3LYP/6-311++(2df, 2pd) calculations were performed to obtain the geometries of the complexes involving water and nucleic acid bases (Adenine, Guanine, Cytosine, Thymine and Uracil). Full geometry optimization is performed for the A-H_2O, G-H_2O, C-H_2O, T-H_2O and U-H_2O. Figure 1 shows the U+H_2O the results for the geometry of the optimized cluster. Using the optimized structures, binding energies, dipole moment and rotational constants were obtained for all these complexes. Analysis of the vibration frequencies was made to ensure that the calculated structures are true minimal of the energy surfaces and to obtain the zero-point vibration energies. All calculations were carried out with the Gaussian 03 ab initio package.

Results

Figure 1 shows the system considered here and give the optimized hydrogen bond distances. These are summarized in Table 1 that also shows the calculated dipole moments, rotational constants, energies and binding energies. The mutual positions of bases and water molecules in local energy minima for single base-single water systems are obtained. The calculation results show that there are several such minima for each base. The deepest minimum has a geometry in which the water oxygen locates on the base plane and forms two nonlinear hydrogen bonds.
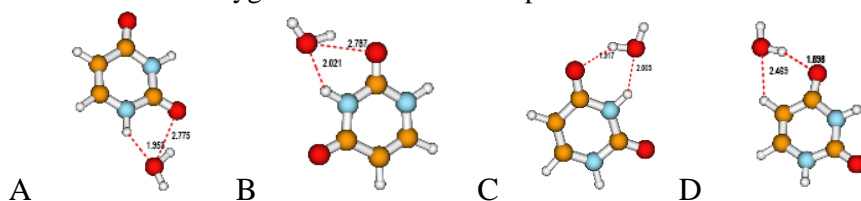

A B C D

Figure 1 Optimized structures of Uacial-H_2O complexes A, B, C and D.
Table 1. Calculated dipole moment (Debye), rotational constants (GHz) E(Hartree), Binding energy (Kcal/mol) for the H_2O, Uracil and Uracil+H_2O

	μ	I_A	I_B	I_C	E (total)	*Binding energy*
H_2O	1.949	827.69	430.72	283.29	-76.442	
Uracil	4.484	3.90	2.02	1.33	-414.885	
A	3.824	3.71	0.98	0.77	-491.338	-6.42
B	4.819	2.23	1.34	0.84	-491.335	-4.46
C	4.259	2.26	1.33	0.84	-491.336	-5.04
D	2.907	3.79	0.89	0.72	-491.334	-3.63

[1]. Saenger, W. Principles of Nucleic Acid Structure; Springer-Verlag: New York, 1988.