Hydrogen bonding in DNA base pairs

Bởi:

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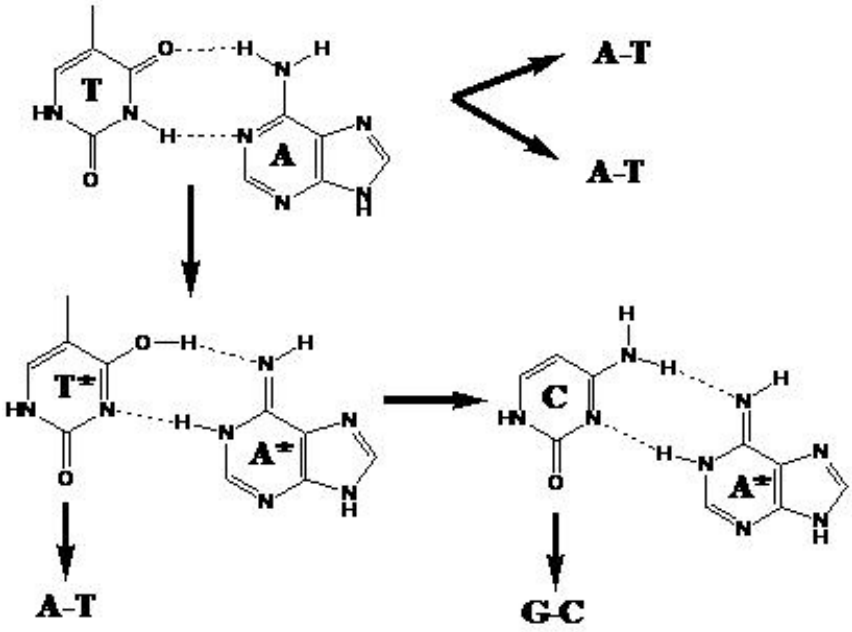
Hydrogen bonding is very important in biological systems, particular in DNA. One of the mechanism for point mutation in DNA is due to a double-proton transfer in A-T base pair to yield a rare tautomer form of adenine, denoted as A*. A* can form hydrogen bonding complex with Cytosine and thus will lead to the generation of a G-C pair at the original A-T location in the next cell division. Fortunately, DNA repair process can fix most of these changes before they become permanent mutations.

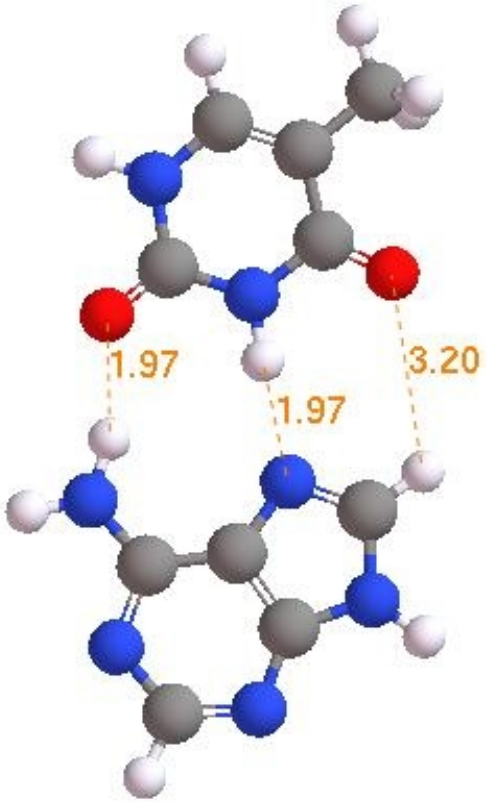


In this experiment, you will learn to compute the binding energies of these hydrogen bond complexes and thus to gain understanding on the nature of hydrogen bonding.

Procedure: Using tools in Avisto. You can download Avisto and its tools from Astonis.

- Use MolLib to send out to the workbench copies of adenine, thymine, cytosine, and guanine bases.

- Use MolDesign to edit thymine to make its T* tautomer and adenine to make A* tautomer. (See the figure above for its 2D structure).
- Use MolDesign to make the A-T, A*-T*, C-A*, and G-C base pair complexes. This is done by first open MolDesign then drag & drop the molecular data icons of these bases onto the graphic window of MolDesign. Note that these base pair complexes are nearly planar and have the hydrogen bond distances in the range of 1.8 - 2.0 Angstrom. An example of the A-T base pair is shown below.



- Use Basic QChem, Mopac GUI Cloud or Pro to search for stable structures of all bases and base pairs and record their heats of formation.

Properties	A	T	G	C	A*	T*	A-T	A*-T*	C-A*	G-C
Hf										

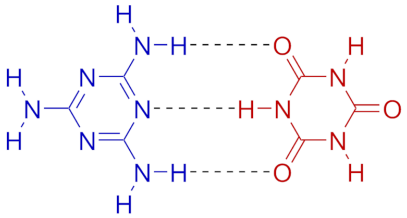
- Calculate the hydrogen bond energy for each complex.

Ehb (A-T) = Hf (A-T) - { Hf(A) + Hf(T)}

- Plot electrostatic potential ESP (isovalue = 0.1) to see possible hydrogen bond interactions (favorable electrostatic interactions) in each complex and draw a conclusion.

Related problem

Melamine has 66% nitrogen by mass and has been involved in a number of food recalls such as alulterated milk from mainland China. It is known that melamine forms strong hydrogen bond network with cyanuric acid to form crystalline complex melamine cyanurate which has been implicated as a causative agent for kidney damage in children in China in 2008 Chinese Milk incident.



Calculate the hydrogen bond energy for the melamine cyanurate complex and compare it with those from DNA base pairs above.