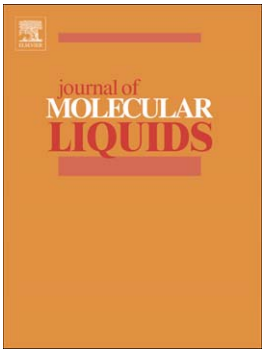

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INVESTIGATION OF SOLVENT EFFECT ON ADENINE-THYMINE BASE PAIR INTERACTION

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Abstract

In this research, the nature and properties of hydrogen bond interactions in adenine- thymine complex have been investigated using density functional (B3LYP and M06-2X) and perturbative (MP2) methods. All calculations have been carried out by the aug-cc-pVDZ basis set. The existence and nature of the weak C-H…O hydrogen bond, in adenine-thymine complex in the gas phase and different solvents, have been investigated. As the solvent effect, the correlation between atoms in molecules (AIM) parameters and geometrical properties of the considered complex have been studied. In addition, solvent effect on the frontier orbitals energies, hardness and dipole moment of adenine- thymine complex have been investigated.

Keywords: Adenine-Thymine Base Pair; Solvent Effect; DFT; Energy Decomposition Analysis; QTAIM.

1. Introduction

Hydrogen bonding and van der Waals interactions play key roles in the structure and properties of biological macromolecules such as DNA and proteins.[1-5] Although experimental and computational methods have been widely used to investigate the nature of H-bonds,[6-9] description of hydrogen bond effects on biochemical phenomena is challenging, yet.

The building blocks of DNA polymer are the nucleotides. Each nucleotide is constructed by three elements; including deoxyribose, the nitrogen base and phosphate group. The DNA bases are classified into two types: purines (including adenine and guanine) and pyrimidines (including cytosine and thymine). The DNA backbone is formed by the phosphodiester bonds; the covalent bond between sugar and phosphate units. Two DNA strands, located in opposite directions, construct a helical spiral structure. The bases of each strand perch inside the mentioned helix. Two helical chains of nucleotides are held together by pairing the purine nucleic bases of one strand, with pyrimidine nucleic bases of the other strand. So that, cytosine connects to guanine; and adenine pairs with thymine. [10]

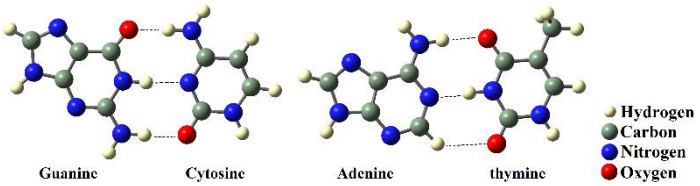

Fig. 1: Triple hydrogen bonds in adenine- thymine and cytosine- guanine complexes.

As it has been shown in the Figure 1, cytosine and guanine base pairs connect together by three hydrogen bonds, including two N-H...O type and one N-H...N interactions. On the other hand, adenine- thymine base pair forms as a result of two typical N-H...O and N-H...N hydrogen bonds. In addition, there is a weak, but non negligible, C-H...O hydrogen bond in the adenine- thymine complex.[11] However, some researchers question the existence of this hydrogen bond in the adenine-thymine base pair.[12,13] Some others believe that the extremely weak C-H...O interaction in the adenine- thymine base pair is not stable enough to be known as a hydrogen bond.