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Theoretical study of the properties of adenine amino acid tetomers with C_{60}

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Abstract

In this research at the Adenine tautomers and their fullerene derivatives were optimized. NBO calculations and NMR for the tautomers and their Fullerene derivatives were carried out at the B3lyp/6-31G*quantum chemistry level . The core and the valence electrons of atoms were compared. Other cases examined in this study, resonance energy, chemical potential (μ), chemical hardness (η) , Energy Gap, Chemical Hardness, Chemical Potential, Dipole moment parameters between Adenine tautomers and their fullerene derivatives were calculated .This organic base as a chemical component of DNA and RNA plays an important role in our body. In this study of fullerenes, we used a nano carrier. The data in tables and graphs and shapes were compared and discussed.

Keywords: adenine, fullerenes, NBO, NMR, IR

1. Introduction

Nanostructures can be categorized into following forms according to their structures: diamonds with sp^3 hybridization, Graphite with sp^2 hybridization, Hexagonal diamonds with sp^3 hybridization, fullerenes with SP^2 hybridization, Nanoparticles, Graphene, single-layer and multi-layer nanotubes, Crystal Nanostructures. All these forms of nanostructures produce unique Pharmaceutical and electronic properties. Graphenes have a two-dimensional structure of a single layer of carbon chicken wire [1-5]. A fullerene is any molecule composed of carbon in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical fullerenes are also called Bucky balls, and they resemble the balls used in football (soccer). Cylindrical ones are called carbon nanotubes or Bucky tubes. Fullerenes are similar in structure to graphite, which is composed of stacked Graphene sheets of linked hexagonal rings; but they may also contain pentagonal (or sometimes heptagonal) rings. The first fullerene molecule to be discovered, and the family's namesake, buckminsterfullerene (C_{60}), was prepared in 1985 by Richard Smalley, Robert Curl, James Heath, Sean O'Brien, and Harold Kroto at Rice University. The discovery of fullerenes greatly expanded the number of known carbon allotropes, which until recently were limited to graphite, diamond, and amorphous carbon such as soot and charcoal. Buckyballs and buckytubes have been the subject of intense research, both for their unique chemistry and for their technological applications, especially in materials science, electronics, and nanotechnology. Adenine is a nucleobase (a purine derivative) with a variety of roles in biochemistry including cellular respiration, in the form of both the energy-rich adenosine triphosphate (ATP) and the cofactors nicotinamide adenine dinucleotide (NAD) and flavin adenine dinucleotide (FAD), and protein synthesis, as a chemical component of DNA and RNA[1-2]. The shape of adenine is complementary to either thymine in DNA or uracil in RNA. Fullerene, a molecule composed of carbon atoms that form a hollow, cagelike structure. The arrangement of the atoms produces pentagonal and hexagonal shapes—that is, shapes with five or six sides, respectively [3].

Fullerenes are highly stable chemically and have a variety of unusual properties. Chemists have been able to add branches of other molecules to them, place atoms inside of them, and stretch them into rods and tubes. Fullerenes can be made to be magnetic, act as superconductors, serve as a lubricant, or absorb light [4-7]. The aim of this study was to evaluate the effect of fullerene on chemical properties of Adenine Tautomers by density functional theory (DFT) method.

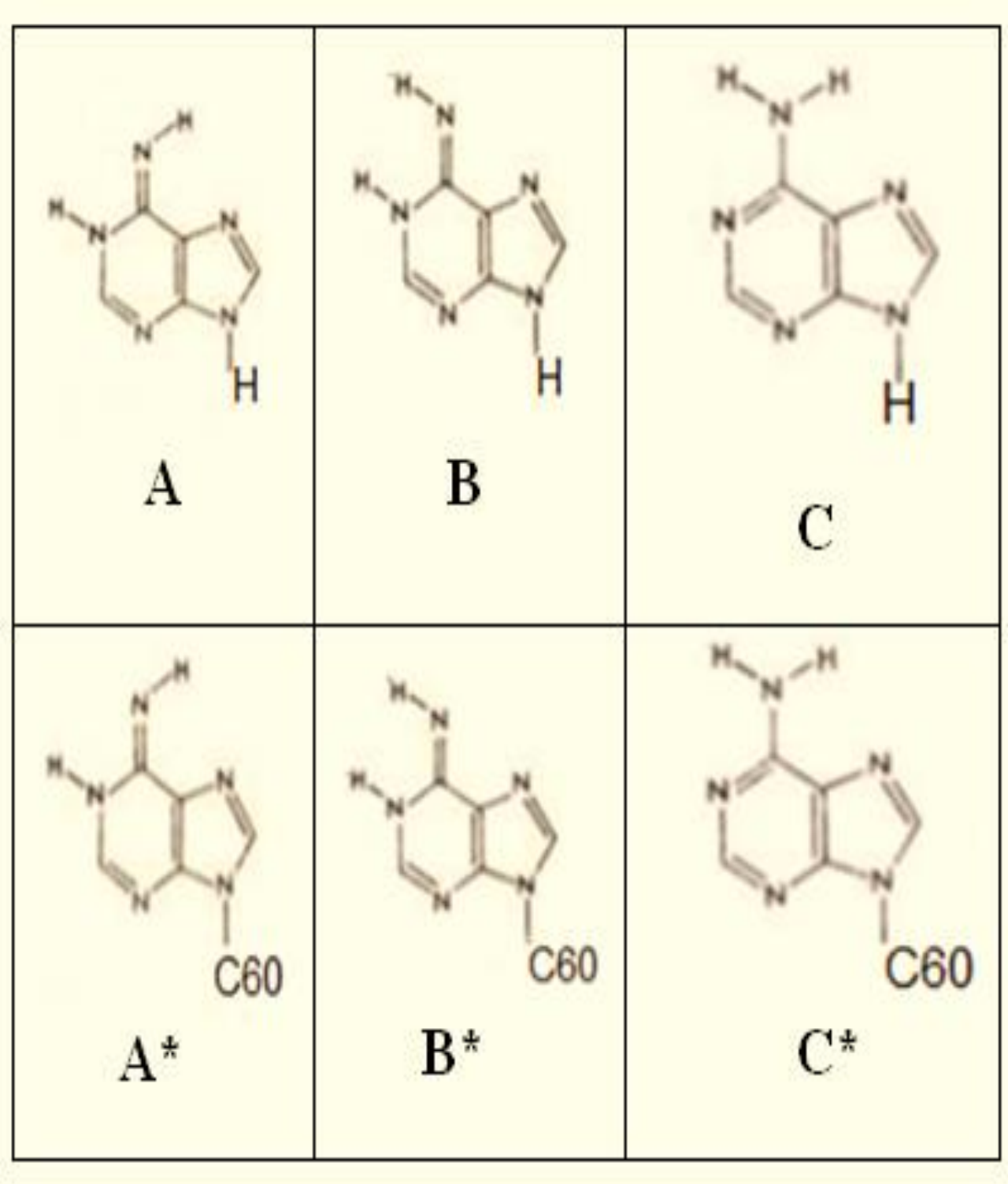

Fig 1. View of Adenine tautomers & Nano fullerene derivatives

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [8-9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter

functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of Adenine tautomer's on Fullerene were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Adenine tautomer's on Fullerene were investigated through attachment to three different base positions. All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor. In this study, fluoxetine drug and its 3 fullerene derivatives investigated. The related structures are named in the following way all structures relating to structures of Adenine tautomer's and their fullerene derivatives were designed primarily with use of Gauss view 5.0.8. In order to do final optimization, Gaussian 98 program of package HF method were used. However, for this purpose, 6-31G basis set was used. Computation were done in gas phase [10-16].

3. Apparatuse:

Total computations were done with use of Pentium III with processor Intel cor i5 with memory of 4 gigabytes and inside the operating of windows SEVEN. All computations were performed under gas phase, 1 atmosphere and 298 Kelvin temperature.

4. Result and discussion:

In this work adenine tautomers were linked to the fullerene, adenine tautomers and their fullerene derivatives investigated. then compare Gap Energy, Hardness, Chemical Potential, Dipol moment parameters between Adenine tautomers and fullerene derivatives.

compound	Energy HLG	dipole moment	chemical hardness	chemical potential	Average of resonance energy
A	0.4523	3.3409	0.22615	0.00254	68.955
B	0.45379	4.3166	0.226895	0.001195	68.21
C	0.47302	2.8282	0.23651	-0.04262	64.67
A*	0.28184	4.1228	0.14092	-0.04919	30.978
B*	0.30721	4.6165	0.153605	-0.048495	30.492
C*	0.30715	2.4414	0.153575	-0.047915	29.538

5. Conclussion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structures of Adenine tautomers and their Fullerene Derivatives was done separately and only when the structures of Adenine tautomers were attached to Fullerene and the results of this computation can be classified as follows:

- The investigation of all the parameters show that the attachment of Fullerene structure to Adenine Tautomers structure will influence the energy levels and dipole moment changes and these changes are able to be investigated in the electrical and chemical parameters of Fullerene Derivatives structure.
- The results showed that energy gap of A are the highest and C* is the lowest. It should be noted that conductivity of C*is the highest and A is the lowest.
- Chemical potential of A* is the highest.
- Chemical hardness of B is the highest and the lowest value is related to A*
- Dipole moment of B*is first and B is the second.
- Resonance energy of A is the highest.

In this study, adenine tautomer's its 6 fullerene derivatives investigated. The related structures are named in the following way:

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