Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 18 (4) 63-70: Winter 2022
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

Computational Study of Drug Pimagedine on Carbon Nanotubes (8,0) by DFT Method

Morteza Keshavarz *

Department of Chemistry, Shahreza Branch, Islamic Azad University, Shahreza, Iran

Received June 2022; Accepted August 2022

ABSTRACT

In this research the role of carbon nanotubes as carrier of pimagedine drug have been investigated. These drugs have been used in cure of diabetes. For this purpose nanotubes (8, 0) with different length have been used. To perform of quantum calculation we used Gaussian software and DFT/B3LYP method and 3-21G BASIS SET. In this research first of all pimagedine drug from head and other time by azo methane elide agent has been connected to each nano structures. Calculation have been done in 2 phases, liquid and gas, and parameters like electron energy, adsorption energy, HOMO,LUMO and dipole moment have been calculated and results showed that the best nitrogen in drug is N_1. Because the dipole moment of N_1 in connection time is larger than other nitrogen. Furthermore the dipole moment of drug and nano tube complex with the length of 10 A° aqua phase have the largest value moment between drug and other complexes and it value is 14.99 Debye that it's larger dipole moment in aqua solution show the ability of better solubility and investigation of adsorption energy also show that the best adsorption energy was in the case of nanotube with the length of 8 A° and with higher length the adsorption energy have been reduced. Investigation of dipole moment also show that the highest solubility is drug with agent and nanotube complex and the best support for this calculation is Nanocone support with 180 degree and 8 length.

Keywords: Carbon Nano tube, Carbon Nanocone, Adsorption, Amino guanidine, pimagedine

1. INTRODUCTION

Nanoparticles link the two domains between nano science and nanotechnology, and these definitions are very appropriate [1-2]. The particle size range of nanotechnology that shows the most capability is less than 100 nanometers, but it should be noted that larger particles that can have high benefits are still needed [3].

Carbon nanotubes are the first generation of nano-products to be discovered and introduced to the world in 1991. Nanotubes are obtained by wrapping graphite sheets with a honeycomb-like structure [4]. These pipes are very long and thin and have stable, durable and flexible structures [5]. In fact, they are graphite pipes. These nanotubes come in a variety of shapes and sizes and can be single-walled or multi-walled [6-7] .Single-walled nanotubes are composed of

*Corresponding author: Keshavarz@iaush.ac.ir

cylindrical graphene walls with a diameter of 1 to 2 nanometers [8]. The multi-wall type has thicker walls and is composed of several co-axis graphene cylinders separated by a distance of 34 nm. The structure of multi-walled nanotubes is such that several nanotubes are centered and nested together [9]. Are located and show a microscopic property whereby the inner nanotube core slides on its top layer without friction [10]. The outer diameter of the multi-walled nanotube is 2 to 25 nanometers and the inner hole is in the range of 1 to 8 nanometers, and there is no three-dimensional order between the individual layers of graphite [11]. Nanotechnology has provided a wide range of new techniques in the field of drug delivery [12]. Medication is the delivery of a drug at a specific time and in a controlled dose to specific drug targets, which reduces the side effects of faster and specific treatment for patients [13]. For treatment to be effective, the drugs must be delivered to the desired location [14].

Drugs can be loaded into nanoparticles by a variety of methods, including dissolution, entrapment, and binding to a polymer matrix [15]. Among the available nanoparticles, Nano capsules and Mislay nanoparticles are more efficient. Mislay nanoparticles slowly release the drug into the body due to the drug interacting with the central hydrophobic portion of the nanoparticle, while the Nano capsules release the drug much faster due to its thin polymer shell [16]. Quantum computing is at the common border between physics, computer science, information technology, and nanotechnology [17-18]. This emerging field has received special attention from governments and large-scale industrial investments over the past ten years [19]. Thermodynamic parameters and dielectric effect in different solvents have been investigated for one of the well-known anti-cancer drugs called cisplatin and its combination with single-walled nanotubes [20]. The calculations are performed using the Monte Carlo method and the density function theory, and the base series 6-31G ** is used [21]. And the main result in both methods is that single-walled nanotubes and cisplatin are suitable combinations for drug transport in different environments [22]. Activated carbon and fullerene nanotubes have been used as nano-carriers for the delivery of anti-tuberculosis compounds. In this research, density theory calculations are used to study the effect of ISO covalent bonding as an anti-tuberculosis compound with functionalized nanotubes and fullerenes, and the bond energy, solvent energy, and chemical quantum of the molecule are calculated [23]. The bond energy has been shown to be thermodynamically binding of the drug to the nanotube and fullerene, and this binding to fullerene is better than that of the nanotube. Solvent energy values indicate that the solubility of the functionalized nanotubes is higher than that of fullerene, and in general the solubility of both in water is thermodynamically possible [24-25].

2. COMPUTATIONAL METHODS

In this research, the structure of the drug and the substrates required for the study have been created with the help of Modeler nanotube, Gauss view3 and Gaussian 03 software. All instructions are based on DFT / B3LYP method and 3-21G BASIS SET. We have considered the interactions between the nanotube and the drug in both the gas and liquid phases. In general, in this study, first, because the structure of the drug has 4 different nitrogen, in the first study, the effect between the bonding interaction of each of these nitrogen to the nanotube to select the best nitrogen to bind to the substrate and then the select of nitrogen, the length of

the nanotube and fully reported the effect of the type of substrate as well as the effect of the presence of a factor between the drug and the nanotube. Two different substrates of nanotube and Nanocone were used. The zigzag nanotube was used in three different lengths along with chiral nanotubes. Zigzag nanotubes were used in three different lengths of 6, 8, 10 angstroms and chiral nanotubes were used along 7 angstroms. The angle is 180 ° and the length of 8 angstroms is considered, is a total of five modes under study, which are introduced in Figure (1) of each of these substrates.

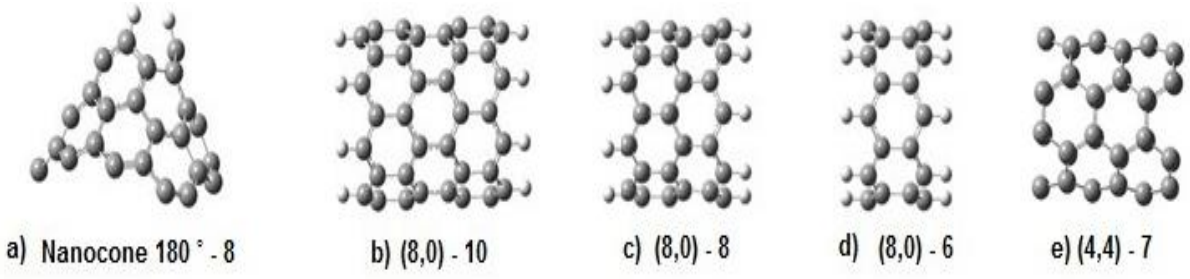


Fig. 1. Case carbon substrates used.

Pimagdine is one of the newest drugs used in diabetes, with the chemical composition CH6N4 and a molecular mass of 74.109 g/ mol, also known as amino guanidine; it is the first drug of choice in type 2 diabetes, especially in obese people. Its effect is by reducing glucose production in the liver, reducing insulin resistance and increasing glucose fuel in peripheral tissues. The drug molecule has four nitrogen atoms and is able to bind through each of these nitrogen. The amount of angles between the nitrogen and carbon atoms in the drug molecule is defined in Figure (2).

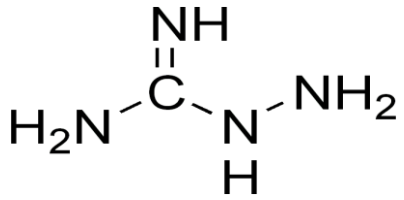


Fig. 2. Geometric structure of the drug Pimagdine (Amino guanidine).

3. RESULTS AND DISCUSSION

Figure (3) to (6) shows the different methods of binding the drug molecule to the nanotube surface in the vacuum phase and Figure (7) to (10) shows the binding methods in the aqueous phase.

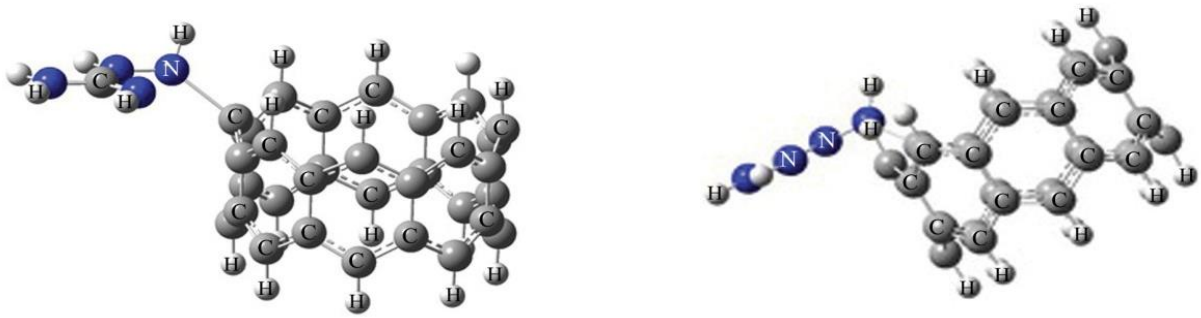


Fig. 3. Effect of nitrogen binding from N1 on the gas phase of image (a) before optimization and image (b) after optimization.

Fig. 4. Effect of nitrogen bonding of N2 on the gas phase Image (a) before optimization and Image (b) after optimization.

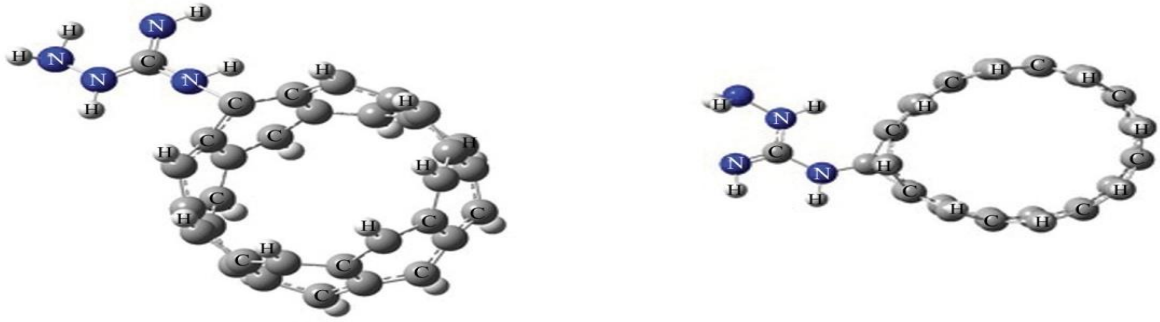


Fig. 5. Effect of nitrogen binding of N3 on the gas phase Image (a) before optimization and Image (b) after optimization.

Fig. 6. Effect of nitrogen bonding of N4 on the gas phase Image (a) before optimization and Image (b) after optimization.

Fig. 7. Effect of nitrogen binding of N1 on the liquid phase of image (a) before optimization and image (b) after optimization.

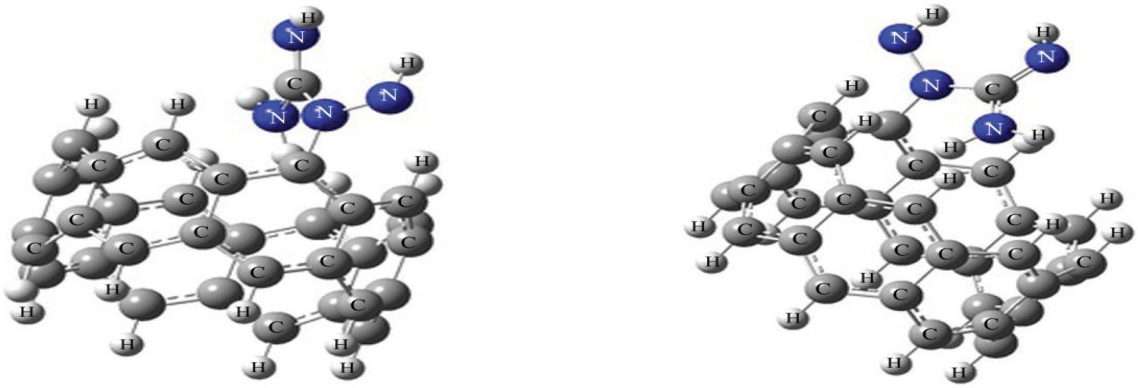


Fig. 8. Effect of nitrogen binding of N2 on the liquid phase of image (a) before optimization and image (b) after optimization.

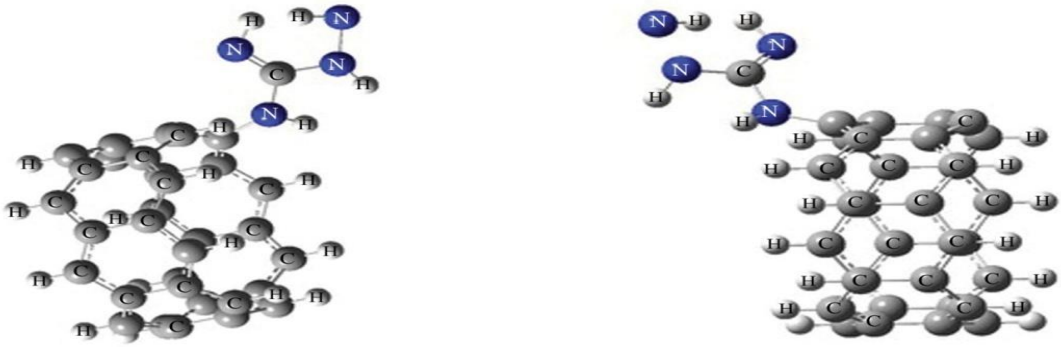
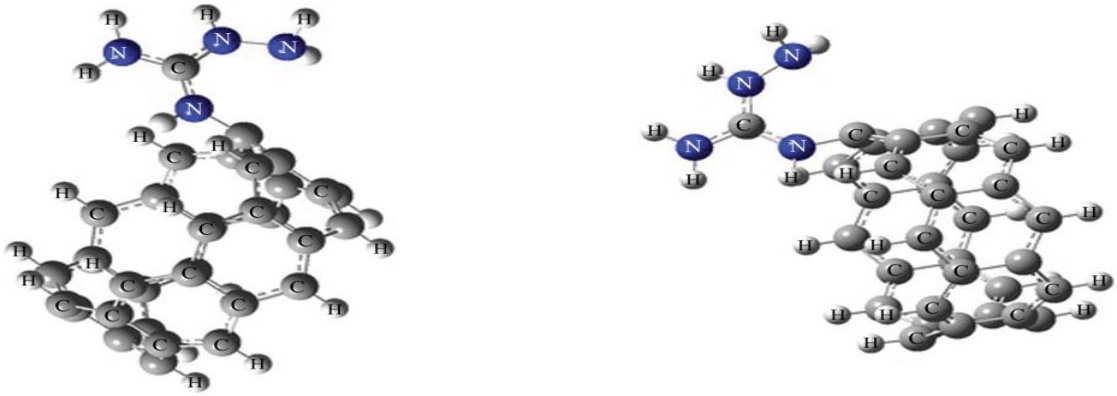


Fig. 9. Effect of nitrogen binding of N3 on the liquid phase of image (a) before optimization and image (b) after optimization.



a) before optimization b) after optimization

Fig. 10. Effect of nitrogen binding of N4 on the liquid phase of image (a) before optimization and image (b) after optimization.

The rate of change of angles in the drug molecule after binding to the nanotube surface in gas and aqueous phase has been calculated. When the molecule is attached to the nanotube via N1 nitrogen, in the gas phase, angles 1, 2 and 3 changes by approximately 34 ° and angle 3 by 24 ° relative to the initial state, indicating the

transfer of non-bonded electrons of nitrogen to the nanotube. Also, other pairs of unbounded electrons can interact with n-πstacking with π orbitals in nanotube rings.

The presence of a double bond between the carbon atoms and N4 provides the possibility of π-π stacking interaction. In the presence of an aqueous solvent, the bond changes within the drug molecule are approximately equal for all four bonds, in which case the solubilization of the molecule by water and the involvement of non-bonded electrons in the aqueous reaction are due to this When bonding is done through the N2 atom, in the gas phase, the rate of change of angles 1, 2 and 4 is less than the previous state, but angle 3 shows more change than the bond state through N1, but with the addition of water solvent. The rate of change of angle 4 increases with the environment. When the drug molecule is attached to the surface through nitrogen N3, in the gas phase, the rate of change of angles is almost equal, but in the aqueous phase, angle 1 shows a large change, which is a sign of more nitrogen coverage of N1 nitrogen. By binding the drug through nitrogen N4 in the aqueous and gas phases, little change has been achieved in angles 2, 3 and 4, but in the presence of water, angle 1 has shown a greater change, in which case nitrogen N1 coating is also involved. By binding nitrogen N1, the greatest changes are obtained during the bonds 1 and 2, but in the aqueous phase, the entire length of the bonds has changed to the same extent, which in this case is also due to the solubility of the molecule. When connected via N2, the bond length changes in the gas phase are equal, but in the presence of the solvent this equality is lost and bonds 1 and 2 show the most change compared to the other two bonds, similar to the gas phase of N1 bond when connected via nitrogen N3. In the gas phase, bonds 1 and 4 show the most changes, but in the presence of solvent, the most change is seen in bond 1. When the drug molecule is attached to the nanotube via N4 nitrogen, in the gas and aqueous phases, all four bonds change to the same extent.

4. CONCLUSION

In this study, by examining the adsorption of pimagedine on nanotubes and carbon nanotubes and calculating different parameters, we concluded that the highest adsorption was on the surface of nanotubes related to nanotubes (8,0) with a length of 8 angstroms and nanocone with an angle of 180 ° and a length of 8 Angstrom can use these nanotubes and Nano cells in pharmacy to deliver medicine to diabetic patients.

REFERENCES

[1] M. Kautt, S. Walsh, K. Bittner, Global distribution of micro–nano technology and fabrication centers: A portfolio analysis approach, J. Technological Forecasting and Social Change.74 (2007)1697–1717.

[2] X. Zhang, X. Xu, N. Bertrand, E. Pridgen, A. Swami, O. Farokhzad, Interactions of nanomaterials and biological systems: Implications to personalized nanomedicine, J. Advanced Drug Delivery Reviews.64 (2012) 1363–1384.

[3] Kumari, S. Kumar Yadav, S. Yadav, Biodegradable polymeric nanoparticles based drug delivery systems Colloids and Surfaces, J. Biointerfaces. 75 (2010) 1–180.

[4] V. Popov, Carbon nanotubes: properties and application, J. Science and Engineering R: Reports. 43 (2004) 61–102.

[5] J. Delmotte, A. Rubio, Mechanical properties of carbon nanotubes: a fiber digest for beginners,Carbon.40(2002) 1729–1734.

[6] Philip G. Whitten, Geoffrey M. Spinks, Gordon G. Wallace, Mechanical properties of carbon nanotube paper in ionic liquid and aqueous electrolytes, J. Carbon. 43 (2005) 1891–1896.
[7] M. Paradise, T. Goswami, Carbon nanotubes – Production and industrial applications, J. Materials & Design. 28 (2007) 1477–1489.
[8] N. Braidy, M. Khakani. G. Botton, Effect of laser intensity on yield and physical characteristics of single wall carbon nanotubes produced by the Nd: YAG laser vaporization method, J. Carbon. 40 (2002) 2835–2842.
[9] J. Kim, H. Chang, B. Kim, J. Park, Enhancement of electron emission and long-term stability of tip-type carbon nanotube field emitters via lithium coating, J. Thin Solid Films. 528 (2013) 242–246.
[10] S. Demoustier, E. Minoux, M. Le Baillif, M. Charles, A. Ziaei, Review of two microwave applications of carbon nanotubes: nano-antennas and nano-switches Revue d'applications des nanotubes de carbone aux micro-ondes: nano-antennes et nano-commutateurs, J. Comptes Rendus Physique. 9 (2008) 53–66.
[11] F. Guo, N. Ma, Y. Horibe, S. Kawanishi, M. Murata, Y. Hiraku, Nitrative DNA damage induced by multi-walled carbon nanotube via endocytosis in human lung epithelial cells, J. Toxicology and Applied Pharmacology. 260 (2012) 183–192.
[12] J. Zhong, L. Song, Z. Wu, S. Xie, M. Abbas, K. Ibrahim, H. Qian, X-ray adsorption near-edge structure and photoelectron spectroscopy of single-walled carbon nanotubes modified by a HBr solution, J. Carbon. 44 (2006) 866–872.
[13] R. Monllau, M. Esplandiu, J. Bartrolí, M. Baeza, F. Céspedes, Strategies for the optimization of carbon nanotube/polymer ratio in composite materials: Applications as voltammetric sensors, Sensors and Actuators J. Chemical. 46 (2010) 353–360.
[14] S. Prakash, M. Malhotra, W. Shao, C. Duchesneau, S. Abbasi, Polymeric nanohybrids and functionalized carbon nanotubes as drug delivery carriers for cancer therapy, J. Advanced Drug Delivery Reviews. 63 (2011) 1340–1351.
[15] F. Karchemski, D. Zucker, Y. Barenholz, O. Regev, Carbon nanotubes-liposomes conjugate as a platform for drug delivery into cells, J. of Controlled Rel. 160 (2012) 339–345.
[16] Z. Ji, G. Lin, Q. Lu, L. Meng, X. Shen, L. Dong, C. Fu, X. Zhang, Targeted therapy of SMMC-7721 liver cancer invitro and invivo with carbon nanotubes based drug delivery system, J. Science. 365 (2012) 143–149.
[17] M. Chen, A. Stott, S. Li, D. Dixon, Construction of a robust, large-scale, collaborative database for raw data in computational chemistry: The Collaborative Chemistry Database Tool (CCDBT), J. of Molecular Graphics and Modelling. 34 (2012) 67–75.
[18] H. Marques, K. Brown, A molecular mechanics force field for the cobalt corrinoids, J. Molecular Structure: THEOCHEM. 340 (1995) 97–124.
[19] P. Ordejón, Order-N tight-binding methods for electronic-structure and molecular dynamics, Computational Materials, J. Science.12 (1998) 157–191.
[20] Chaudhari, S. Lee, Computational study of glycine–(water) 3 complex by density functional method, J.

Chemical Physics. 305 (2005) 281–285.

[21] Ramraj, I. Hillier, M. Vincent, Assessment of approximate quantum chemical methods for calculating theinteraction energy of nucleic acid bases with graphene and carbon nanotubes, J. Chemical Physics Letters. 484 (2010) 295-298.

[22] P. K. Shukla, P. C. Mishra, Effects of diameter, length, chirality and defects on the scavenging action ofsingle-walled carbon nanotubes for OH radicals: A quantum computational study, J. Chemical Physics.

[23] 369 (2010) 101-107. Salimi Beni, A. Najafi Chermahini, H. Sharghi, MP2 DFT and ab initio calculations on thioxanthone, J. Spectrochimica Acta. 82 (2011) 49-55.

[24] J. Talla, Ab initio simulations of doped single-walled carbon nanotube sensors, J. Chemical Physics. 392 (2012) 71-77.

[25] J. Whitney, S. Sarkar, J. Zhang, T. Young, Single Walled Carbon Nanohorns as Photothermal Cancer Agents, J. Lasers in Surgery and Medicine. 53 (2011) 43-51.