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Quantum chemistry studies on reactivity of the 2-Amino-3-(3,4-Dihydroxyphenyl)Propanoic Aciddrug linked to to C_{60}

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Abstract

In this research at the first 2-amino-3-(3,4-dihydroxyphenyl) propanoic aciddrug drug and its fullerene derivative were optimized. NBO calculations and NMR for the complexes were carried out at the B3LYP/6-31G*quantum chemistry level. Different parameters such as energy levels, the amount of Chemical Shift in different atoms, the amount of HOMO/LUMO, chemical potential (μ), chemical hardness (η), Thermodynamic Properties was determined and the coefficients of hybrid bonds (π, σ) and the orbital portion of the bonds p (π, σ) was performed. In another part, the core and the valence electrons of atoms were compared. This drug as a major therapeutic category is antidepressant drug. In this study of fullerenes, we used nano drug carriers. The data in tables and graphs and shapes were compared and discussed.

Keywords: 2-amino-3-(3,4-dihydroxyphenyl)propanoic aciddrug , Fullerenes, Chemical potential, Nano drug carriers.

1. Introduction

Many particular features have made derivatized fullerenes the object of numerous investigations over the last decade [1]. Among them, the chemical, photophysical, and electrochemical properties play amajor role, especially in view of possible applications, ranging from medicine [2] to material science, to artificial photosynthesis. Since macroscopic samples of C60 became available in 1990, many applications have been suggested, particularly in the bio-area. This class of compounds can be active as HIV-protease inhibitors, as antibacterial and neuroprotective agents, and can also induce the photocleavage of DNA. Fullerene is one of the other artificial forms of carbon element which is made by heating graphite. Low solubility of the fullerenes in fluids limits application of these materials as medicinal effective material. But hydrophobic size, three-dimensionality and electron properties cause its use as medicine. Levodopa is a medication used to treat Parkinson's disease. Parkinson's disease is associated with low levels of a chemical called dopamine (doe PA meen) in the brain. Levodopa is turned into dopamine in the body and therefore increases levels of this chemical. Levodopa is used to treat the stiffness, tremors, spasms, and poor muscle control of Parkinson's disease[3]. Levodopa is a chemical building-block that your body converts into dopamine. It replaces the dopamine that is lost in Parkinson’s. Mechanical quantum calculations in theory level of HF/6-31G were performed on structure of levo-dopa and nanofullerene-levo-dopa and some different properties such as σiso and chemical shifts in nano structure of fullerene and levo-dopa drug were studied. [4-5].

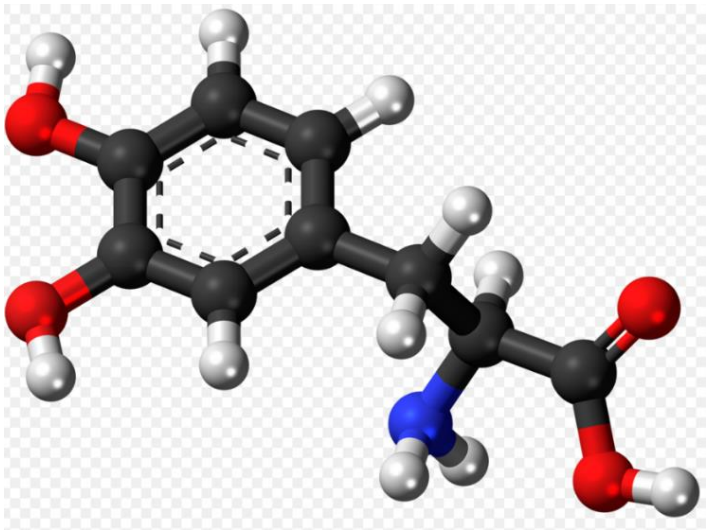

Fig 1. View of 2-amino-3-(3,4-dihydroxyphenyl)propanoic acid

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [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 2-amino-3-(3,4-dihydroxyphenyl)propanoic aciddrug 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 2-amino-3-(3,4-dihydroxyphenyl)propanoic aciddrug 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 report, at the first levo-dopa drug located on fullerene and its derivatives with c_{60} were optimized. then NICS calculations have done in 6-31G* basis set in HF methods and in gas phase. The gauge-included atomic orbital (GIAO) approach was used in the chemical shielding tensor calculations and chemical shielding isotropy (σ_{iso}) and chemical shift (δ) were obtained by $\sigma_{iso} = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3$ and $\delta = \sigma_{11} - \sigma_{iso}$

in this report was used of computer for calculating the values of chemical shielding isotropy and chemical shift.total calculations were done with use of pentium 3,with processor intel®,core i4, with memory of 4 gigabytes and inside of operating system of windows xp. All calculations were done in Hartree- Fock and in the 6-31G * basis set using Gaussian 98 software and in gas phase.the figure of levo-dopa(R) and its nano carrier with c_{60}(R-C_{60}) carrier of F,is shown in figure 1.

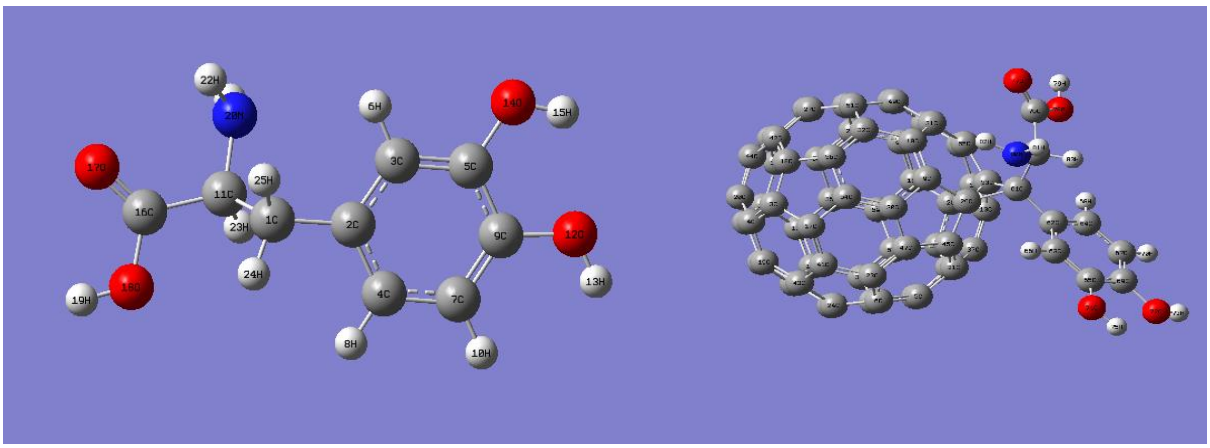

figure.1. levo-dopa and its nano carrier with C_{60}(R-C_{60})

3. Result and discussion:

Table.1.values of σiso and δ in (R-C60), and (R)

	R-C60			R		
	H66	**H68**	**H70**	**H6**	**H8**	**H10**
σiso	24.6168	25.3174	26.5701	25.2617	26.3944	26.8601
δ	7.9808	7.2802	6.0275	7.3359	6.2032	5.7375

Table.2.values of gap energy ,chemical hardness,Dipole moment,chemical potential in ($R-C_{60}$), and (R)

	gap energy	chemical hardness	Dipole moment	chemical potential
R	0.14380	0.224515	4.2838	-0.080715
$R-C_{60}$	0.26548	0.13274	5.5242	-0.14669

The results showed that the values of gap energy and chemical hardness were decreased in nano carrier, whereas dipole moment and chemical potential had higher value. in addition, considering NICS(0) parameter inside benzene ring, the comparison between drug and nano carrier showed that the value of this parameter in nano is more than the one in drug ,also the hydrogens inside benzene ring more have been deshielded.

4. Conclusion:

The result showed by connecting of fullerene to drug, reactivity will be more. in the other hand , the value of dipole moment indicated that solubility of drug will increase in polar solvent in body, such as aqua. Hydrogen deshielding in benzene ring of fullerene Nano carrier of drug, and decreasing of chemical shielding isotropy can be indicated the capacity of these hydrogens in participating in electrophilic substitution reactions.

Reference

[1] R. Ahmadi, E. Farajpour, Ce. N., 37, 6 (2015).

[2] S. Sokolova, A. Luchow, J. B. Anderson,Chem. Phys. Lett., 323, 229 (2000).

[3] H. Prinzbach, A. Weiler, P. Landenberger,F. Wahl, J. Worth, L. T. Scott, M. D. Gelmont,D. Olevano, B. V. Issendorff, Nature, 60, 407(2000).

[4] D. Zeng, H. Wang, B. Wang, J. G. Hou,Appl. Phys. Lett., 77, 3595 (2000).

[5] J. Taylor, H. Guo, J. Wang, Phys. Rev. B, 63,121104 (2001).

[6] R. Gutierrez, G. Fagas, G. Cuniberti, F.Grossmann, R. Schmidt, K. Richter, Phys. Rev. B, 65, 113410 (2002).

[7] C. Zhanga, W. Sun, Z. Caob, The Journal of Chemical Physics, 126, 144306 (2007).

[8] M. J. Frisch, G. W. Trucks, H. B. Schlegel,G. E. Scuseria, M. A. Robb, J. R. Cheeseman,J. A. Montgomery, Jr., T. Vreven, K. N. Kudin,J. C. Burant, J. M. Millam, S. S. Iyengar, J.Tomasi, V. Barone, B. Mennucci, M. Cossi,G. Scalmani, N. Rega, G. A. Petersson, H.Nakatsuji, M. Hada, M. Ehara, K. Toyota, R.Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,Y. Honda, O. Kitao, H. Nakai, M. Klene, X.Li, J. E. Knox,

H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E.Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K.Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich,A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B.Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu,A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong,C. Gonzalez, J. A. Pople, Revision B.03 ed.,Gaussian, Inc., Pittsburgh PA,, 2003.