International Journal of New Chemistry, 2016, 3 (3), 74-78
Published online January 2016 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Computational study of Chemical properties in fullerene Derivatives of (*RS*)-1-[4-(2-Methoxyethyl)phenoxy]-3-[(propan-2-yl)amino]propan-2-ol or Lopressor

Nooshafarin Aryayinejad*
Department of Chemistry, Shahid Bahonar University of Kerman, P.O. Box 76175-133, Kerman, Iran .
*Corresponding Author e-mail Address: n.aryayinejad@yahoo.com
Received 3 March 2016; Accepted 30 May 2016; Published 1 August 2016

Abstract

In this research at the first (RS)-1-[4-(2-Methoxyethyl)phenoxy]-3-[(propan-2-yl)amino]propan-2-oland 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: Lopressor Fullerenes, Chemical potential, Nano drug carriers.

1. Introduction

Lopressor is a beta-blocker that affects the heart and circulation (blood flow through arteries and veins). Lopressor is used to treat angina (chest pain) and hypertension (high blood pressure). It is also used to treat

or prevent heart attack. Lopressor may also be used for other purposes not listed in this medication guide. Lopressor is used alone or in combination with other medications to treat high blood pressure. It also is used to prevent angina (chest pain) and to improve survival after a heart attack. Extended-release (long-acting) Lopressor also is used in combination with other medications to treat heart failure. Lopressor is in a class of medications called beta blockers. It works by relaxing blood vessels and slowing heart rate to improve blood flow and decrease blood pressure. **Purpose** : Today considerable advances in have been accomplished in applications of nano-particles specifically in medical sciences. Fullerene is one of the other artificial forms of carbon element.Long life cycle of medicines in the human body is a success factor in delivery of medicine to the specific place. Lots of nano-particles are being developed in this field.Considering medical point of view, achieving such goals is vital. The aim of present study was to evaluate the effect of Lopressor Chemical Properties of Antihypertensive Clonidine drug in water by DFT methods. In this study, the drug Lopressor on C_{60} fullerene were the drug and its derivatives were optimized fullerene. NBO and NMR for complex computations required in the HF / 6-31G * and B_3lyp / 6-31G * quantum chemistry method was used. Studies NMR (σ iso) were performed for all conditions and changes in chemical shift (δ) of the desired compound was considered. NBO studies and determine the coefficients of a hybrid of bonds (π, σ) to determine the p orbitals in bonding (π, σ) was. Others were examined in this study, the amount of energy transfer between donor and acceptor of electrons in the atoms of the compound and the chemical potential (μ) and chemical hardness (η) of the compound were studied. This drug is classified as a drug therapy as an adjuvant in the treatment of hypertension and congestive heart failure (CHF) is used.

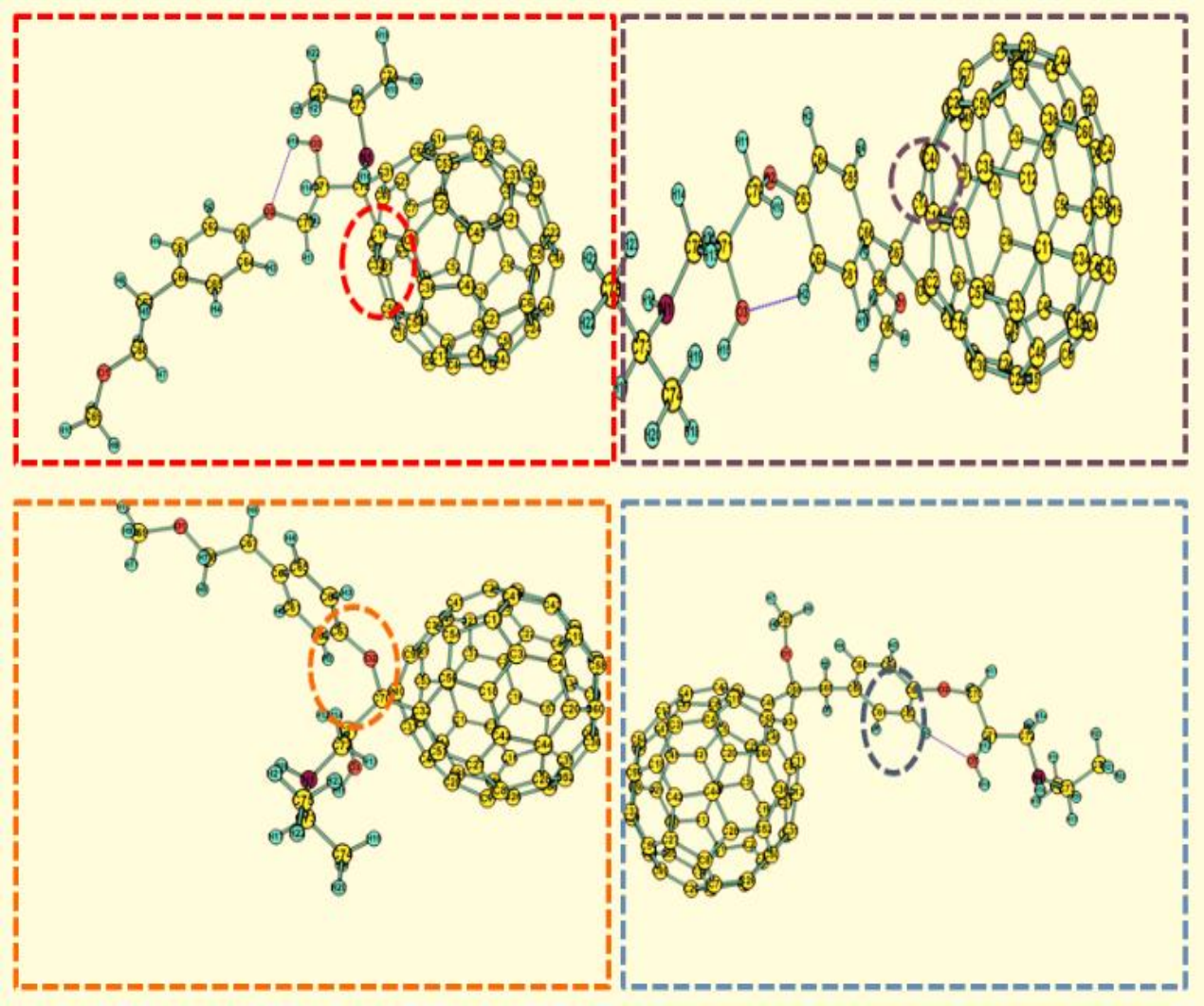

Fig 1. View of Lopressor alone and location of connectable to Fullerene

2. Result and discussion:

In this work Lopressor was linked to the fullerene, Lopressor drug and its 4 fullerene derivatives investigated. Then compare Gap Energy, Hardness, Chemical Potential, Dipole moment parameters between Lopressor alone and nano-fullerene- Lopressor.

3. Materials and methods:

All structure relating to structure of Lopressor and nano Fullerene- Lopressor 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.

4. 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.

5. Conclussion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Lopressor drug was done separately and only when the structure of Lopressor was 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 Lopressor structure to Fullerene 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 FM is the highest and FMT (1)is the lowest. It should be noted that conductivity of FMT (1) is the highest and FM is the lowest.
- Chemical potential of Lopressor is more than FMT (4) and after of them is FMT (2) then FMT (3) and (1).
- Chemical hardness of Lopressor is the highest and the lowest value is related to FMT (1) .
- Dipole moment of FMT (2) is first and FMT (4) is the second.

6. Reference

[1] F.Colak, N.Atar, A.Olgun, *Chem. Eng. J.*,150, 122 (2009).

[2] R. Nadeem, M.H. Nasir, M.S. Hanif, *Chem. Eng. J.*, 150, 40 (2009).

[3] K. Li, X. Wang, *Bioresour. Technol.*, 10,2810 (2009).

[4]Y.S Ho, G. McKay, *Process Biochem.*, 34, 451 (1999).

[5]A. Gucek, S. Sener, S. Bilgen, M. A. Mazmanci, *J. Colloid Interf. Sci.*, 286, 53 (2005).

[6] F. Geiger, M. Stoldt, H. Schweizer, P. Bauerle, E. Umbach, *Adv. Mat.*, 5, 922 (1993).

[7] F. Garnier, G. Horowitz, X. Peng, D. Fichou, *Adv. Mat.*, 2, 592 (1990).

[8] P. bäurele In: K. Müllen and G. Wegner, Editors, Electronic Materials : The oligomer Approach, Wiley-VCH, Weinheim, NY, 105- 197 (1998)

[9] G. Horowitz, M.E. Hajlaoui, *Adv. Mater.*, 12, 1046 (2000); H. Meng, J. Zheng, A.J. Lovinger, B.-C. Wang, P.G. Van Patten, Z. Bao, Chem. Mater., 15, 1778 (2003)

[10] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven, Jr., 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, GAUSSIAN 03, Revision B.04, Gaussian, Inc., Pittsburgh PA, 2003.

[11] M. Mushrush, A. Facchetti, M. Lefenfeld, H.E. Katz, T.J.Marks, J. Am. Chem. Soc., 125, 9414 (2003).

[12] M. Pasini, S. Destri, W. Porzio, C. Botta, U. Giovanella, *J. Mater. Chem.*, 13, 807 (2003);

[13] M. Suzuki, M. Fukuyama, Y. Hori, S.Hotta, *J. Appl. Phys.*, 91, 5706 (2002).

[14] D. Pisignano, M. Anni, G. Gigli, R. Cingolani, M. Zavelani-Rossi, G.Lanzani, G.Barbarella, L. Favaretto, *Appl. Phys. Lett*., 81, 3534 (2002).

[15] L. Torsi, A.J. Lovinger, B. Crone, T. Someya, A. Dodabalapur, H.E. Katz, A.Gelperin, J. Phys. Chem. B., 106, 12563 (2002); J. Roncali, *J. Mater. Chem.*, 9, 1875 (1999).