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Ab Initio study on nano carrier (*RS*)-2-(1,2,3,4-tetrahydronaphthalen -1-yl)-4,5-dihydro-1*H*-imidazol drug about Substituted effect in energy levels, dipole moment and structural parameters

Shohreh Nikandish*
Department of Chemistry, Faculty of Science, Yazd University, Yazd, I.R. Iran.
*Corresponding Author e-mail Address: Shohrehnikandish@yahoo.com
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Abstract

Tetryzoline(TH) is an adrenergic agent (vasoconstrictors) and derived from imidazoline. This compound is closely related to naphazoline hydrochloride in its pharmacological action. Nanotechnology has been used to provide advanced biomedical research tools in drug delivery. The fullerene family especially C60 derivatives have appealing photo-, electro-chemical and physical properties for biomedical applications. In this report, at the first Tetryzoline drug located on fullerene and halogen derivatives (in carbon position 69) [C60- Tetryzoline – C69-X] (X=F, Cl, Br) were optimized. Then the calculation of natural bond orbital was performed with the NBO technique. All calculations using Hartree- Fock the 6-31G * basis set using Gaussian 98 software and in gas phase has been done. The results showed that the energy levels of molecular orbitals (HOMO & LUMO) in the R-F have the lowest value. C69-F is shortest bond and most Strength. Comparison of the dipole moment of compounds shows this trend: R-F> R-Cl> R-Br.

Keywords: Tetryzoline , nano carrier, fullerene , dipole moments.

1. Introduction

Tetryzoline is a derivative of imidazole, which is found in over – the -counter eye drops and nasal sprays. Other derivatives include Naphazoline, Oxymetazoline, and Xylometazoline. Poisoning can result from an overdose. Tetryzoline is an alpha agonist and its main mechanism of action is the constriction of conjunctival blood vessels. This serves to relieve the redness of the eye caused by minor ocular irritants. An urban legend suggests that Tetryzoline can cause violent diarrhea if administered orally, such as by putting a few drops of Visine in an unsuspecting person's beverage. However, the actual results may be worse, varying from severe nausea and vomiting to seizures or a coma. Diarrhea is not a side effect.

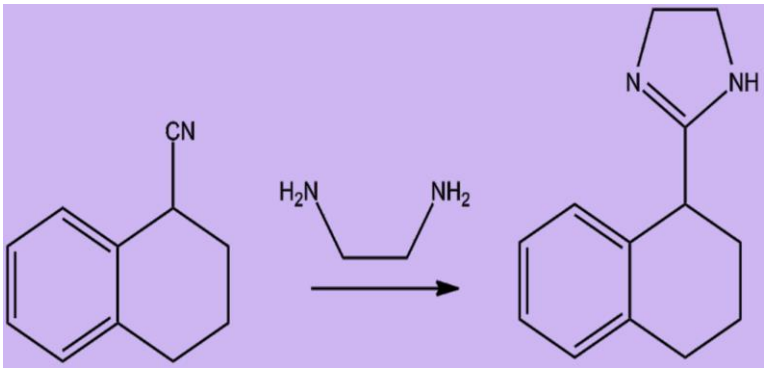

Fig 1. View of Reaction of synthesis of Tetryzoline, 2-(1,2,3,4- tetrahydro-1-naphthalenyl)-2-imidazoline, is synthesized in one step by theheterocyclization of 1- cyanotetraline with ethylenediamine .

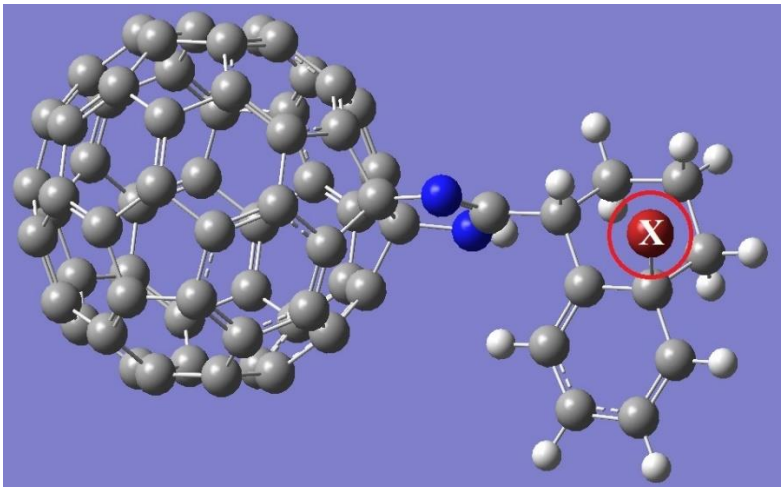

Fig 2. View of Nano-drug Tetryzoline has been obtained from carbon connection of Tetryzoline to Fullerene

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 Tetryzoline 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 Tetryzoline 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.

3. Results

In this study, Tetryzoline drug and its 3 fullerene derivatives investigated. .The results showed that the calculated energy gap is typically much higher of the Tetryzoline than Tetryzoline attached to Fullerene in each three connection is different and the other hand the amount of that in each three Tetryzoline binds to Fullerene to connection forms is different and mostly the same compared with the accuracy

Table 1. **NBO analysis**

LP N61	**→**	**π*C63-N64**	
	F(i,j)	**Ej-Ei**	**Q**
R-H	68.29	0.59	26794.16
R-F	63.75	0.6	22578.13
R-Cl	66.63	0.6	24664.21
R-Br	70.23	0.59	28338.14

LP N64	**→**	**σ*N61-C63**	
	F(i,j)	**Ej-Ei**	**Q**
R-H	15.73	1.23	327.0975
R-F	15.94	1.23	335.8895
R-Cl	15.83	1.23	331.2696
R-Br	15.84	1.23	331.6883

LP N64	**→**	**σ*C31-C55**	
	F(i,j)	**Ej-Ei**	**Q**
R-H	7.39	1.04	100.9839
R-F	7.36	1.04	100.1657
R-Cl	7.38	1.04	100.7108
R-Br	7.44	1.04	102.355

Table2 . Calculated of dipole moment

	Dipole moment (Debye)	
	C60-TETRAHYDROZOLINE	ONLY-TETRAHYDROZOLINE
R-H	32.5555	6.9693
R-F	31.1335	7.8624
R-Cl	30.5429	7.7492
R-Br	29.4681	7.655

Table3 . Calculated of energy (HOMO & LUMO)

	Energy		
	Energy of HOMO	Energy of LUMO	Gap of Energy
R-H	-0.345	-0.153	0.192
R-F	-0.346	-0.177	0.169
R-Cl	-0.346	-0.18	0.166
R-Br	-0.345	-0.179	0.166

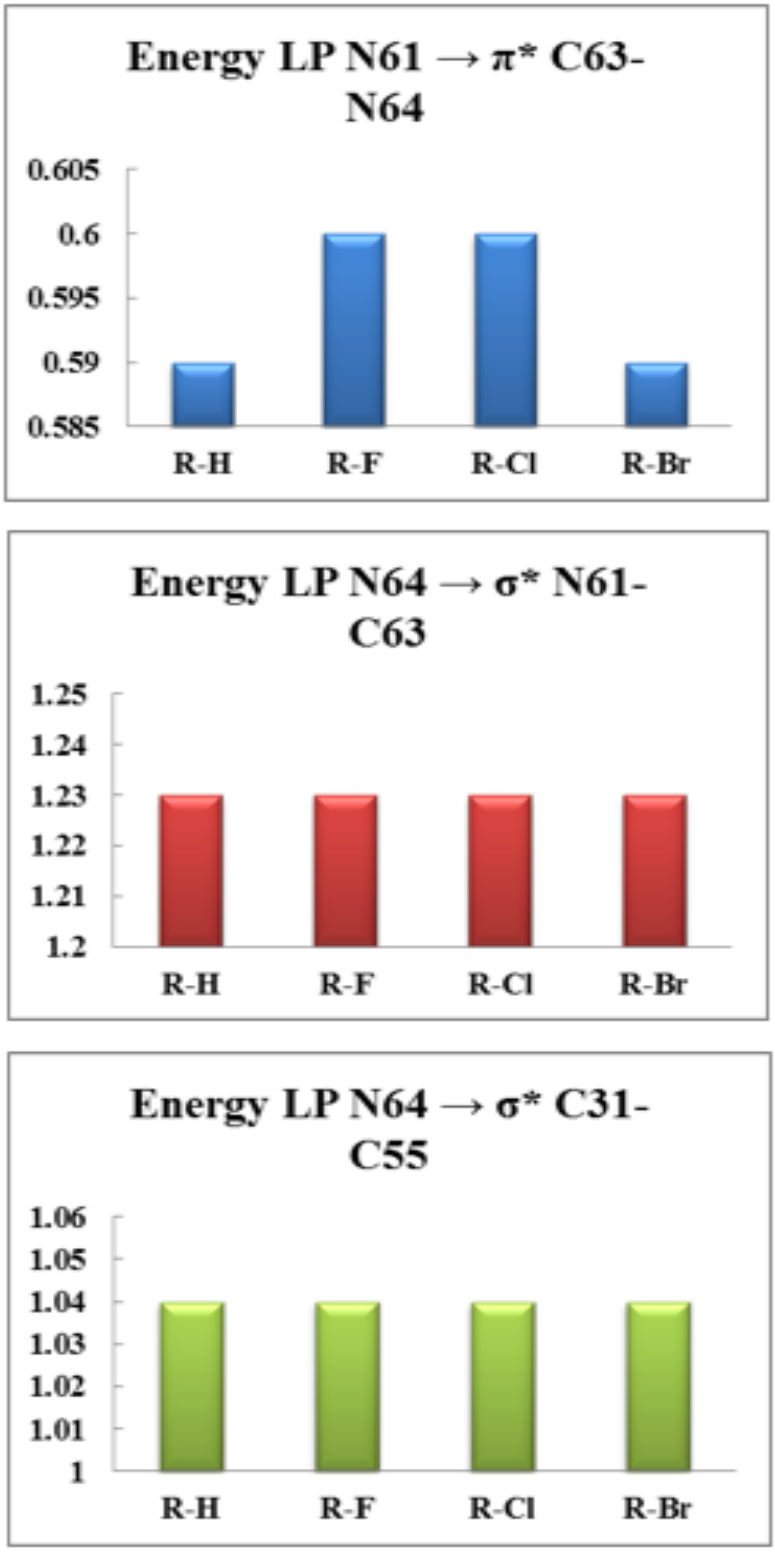

Fig 3. digrams of Values of energies of the frontier molecular orbitals (ε_{HOMO} and ε_{LUMO}, eV), calculated at the B3LYP/6-31G (d) level of theory.

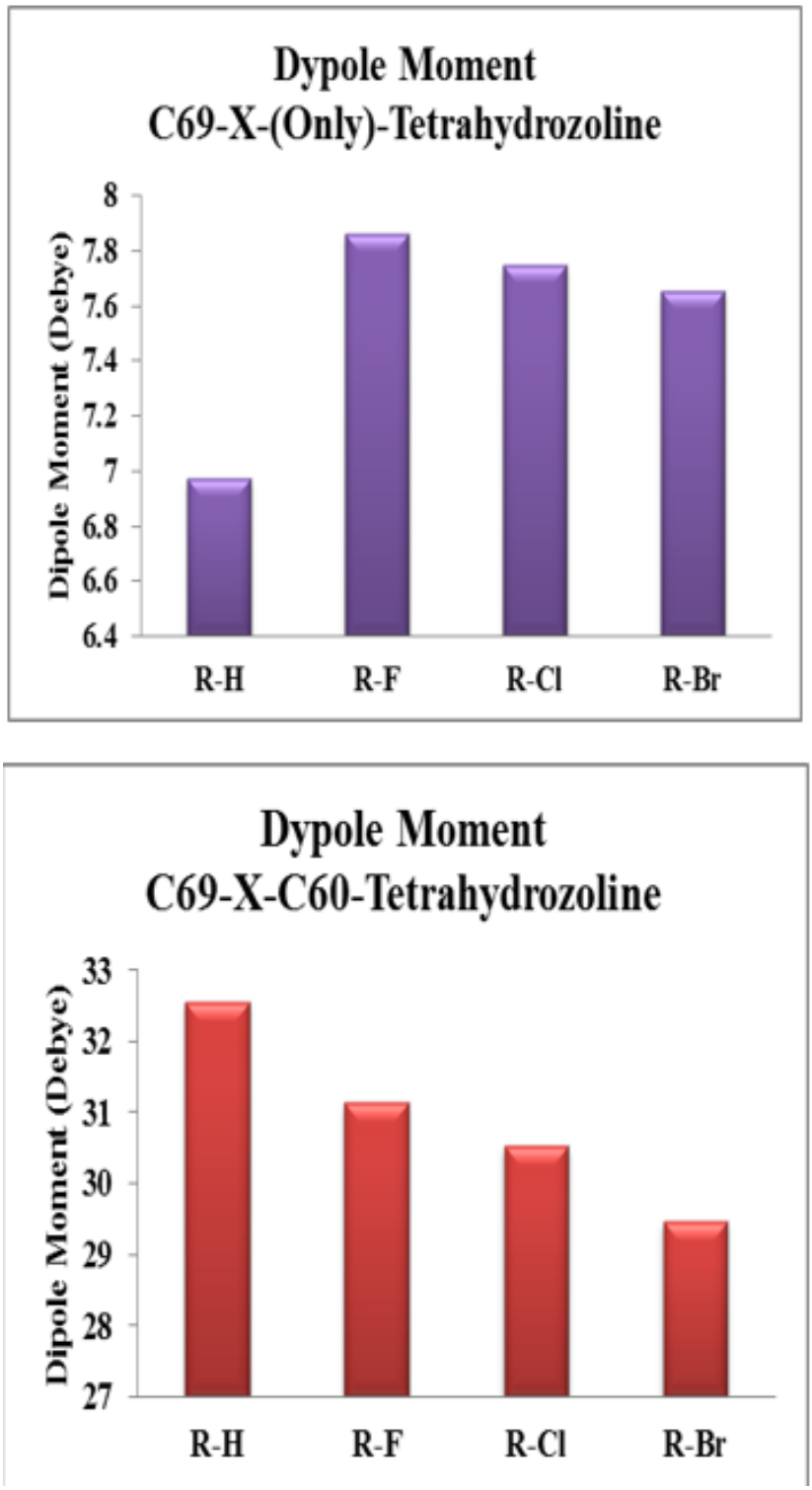

Fig 4. digrams of Values of Dipole moments calculated at the B3LYP/6-31G (d) level of theory

4. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Tetryzoline drug was done separately and only when the structure of Tetryzoline 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 Tetryzoline 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.

Reference

[1] A. Ashnagar, G. Naseri, M. Amini, International Journal of Chem. Tech. Research, 1 (1), 47 (2009).

[2] M. Deodhar, P. Sable, A. Bhosale, K.Juvale, R. Dumbare, P. Sakpal, Turk. J. Chem., 33, 367 (2009).

[3] R. Ahmadi, M. D. Ganji, Int. J. New. Chem., 1, 10 (2014).

[4] H. Usama Ramadhan, Journal of Basrah Researches (Sciences), 38 (4), A (2012).

[5] G.G. Muccioli, J.H. Poupaert, J. Wouters, B. Norberg, W. Poppitz, G. Scriba, Tetrahedron, 59(8), 1301 (2003).

[6] T.S. Jin, T.S. Li, Z.H. Zhang, Synth.Commun., 29, 1601 (1999).

[7] K. Bruns, J. Conrad, A. Steigel,Tetrahedron., 35, 2523 (1979).

[8] E. Bograchov, J. Am. Chem. Soc., 52, 2268 (1950).

[9] C.D. Wang, X.Z. Shi, R.J. Xie, Synth. Commun., 27, 2517 (1997).

[10] H.J. Backer, H.B. Schurink, Rec. Trav. Chim., 50,1066 (1931).

[11] Y.Q. Peng, G.H. Song, X.H. Qian, Synth. Commun., 31, 3735 (2001).

[12] B. Wang, Y. Gu, G. Song, T. Yang, L. Yang, J. Suo, J. Mol. Catal. A: Chem., 233, 121(2005).

[13] Z-H. Zhang, T-S. Li, T-S. Jin, J-T. Li, J. Chem. Res. (S)., 640 (1998).

[14] R. Ghiasi, R. Ahmadi, Int. J. New. Chem., 1, 30 (2014).

[15] D.M. Clode, Chem. Rev., 79, 491 (1979).