International Journal of New Chemistry, 2017, 4 (2), 56-60
Published online January 2017 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Computational Computation of the Efferene Structure on the Para phenylene diamine

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Received qJanuary 2017; Accepted 14 February 2017; Published 30 March 2017

Abstract

In this study, the effect of fullerene electron mobility on the composition of paraphenylenediamine and stability was studied. Using quantum chemistry calculations, the first combination of paraffenylenediamine in a single-full-time region connected with fullerene through carbon atoms was reported. Experimental research was simulated and optimized using GIS software. Then the NBO calculations were performed on them. All calculations using the gossip software were performed in the 6-31 G * base series of the Factor Faster Phase. The results showed that when the compound is connected to the fullerene, the energy gap and its chemical hardness are low , Thus increasing its reactivity and bipolarity. Also, the natural gravity of volt-quantum capacities was considered comparing them in similar positions in compound interactions separately and fullerene. All evidence suggests that the electrons are fullerene and the transfer of electrons from paraffenylenediamine to fullerene.

Keywords: paraffenylenediamine, Fullerenes, Chemical potential.

1. Introduction

Paraffenylenediamine, known as PPDA or PPD, is an organic ring and amine compound of aniline derivative that has cosmetic and industrial applications. The chemical compound is used as a common substance in hair dye, the main cause of which is the effect Speed is part of the process of changing the color of the hair. [1]. In recent studies, this combination with fullerene has been identified as an inhibitor of the carbonic anhydrase XII enzyme (including carbonic anhydrase enzymes released in tumor cells in response to oxygen deficiency) [2]. The fullerene consists of a large number of spherical carbon atoms. The structure of the fullerene molecule (C_{60}) is completely stable, and a large number of carbon atom clusters exist in this structure, and the number of carbon atoms in it is paired. Today, the fullerene combination is used as a nanocomposite Because their spherical shape makes it possible to place fullerene molecules in water-soluble enzymes or cells, which makes it interesting to have medicinal properties.The fullerene has interesting biological properties, such as stopping the HIV virus and breaking the DNA by futeri method and acting as an agent for cancer prevention, etc. C60 and C_{70} are among the most stable forms of fullerenes [3]

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [4]. 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 Fluoxetine 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 Fluoxetine 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

All Computations are performed by means of GAUSSIAN 03 packing. 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 Fluoxetine 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 Fluoxetine on Fullerene were investigated. In this study, paraffenylenediamines were first combined in PPD and PPD (C_{60}) compounds and simulated and optimized in empirical studies by Gossive software, and then NBO calculations were performed on them. All calculations with The use of the program of gosin in the 6-31G * series of the Hartree-Factor in the gas phase took place. [5-6] (Fig. 1)

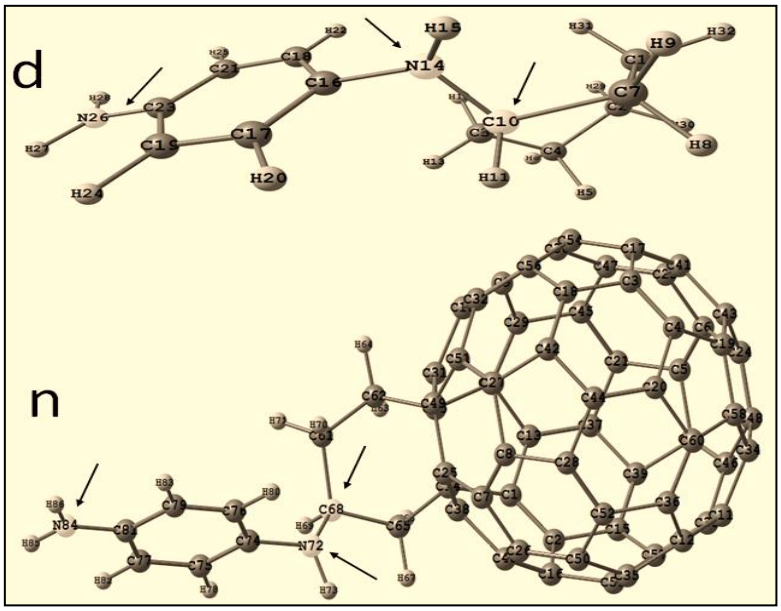


Fig 1. Combination of paraphenylenediamine with fullerenes and similar situations

Table 1-Energy comparison, bipolar hardness parameter in two modes n and d

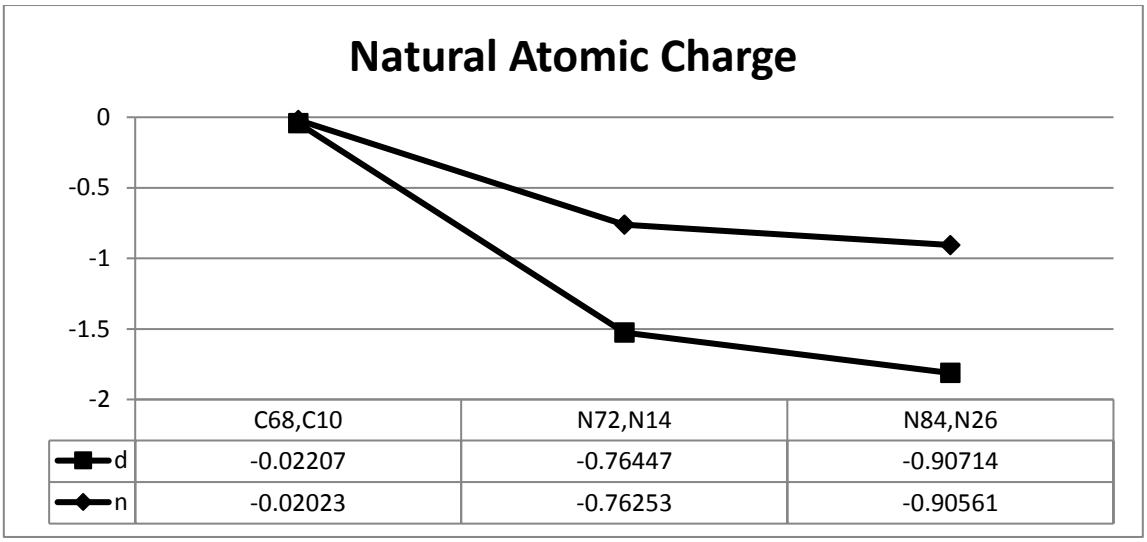
Calculated parameters	n	d
E(RHF) (a.u.)	-2766.47654623	-573.56542048
E(Homo) (a.u.)	-0.25800	-0.27634
E Lumo (a.u.)	-0.02002	0.15131
η	0.11899	0.213825
Gap Energy	0.23798	0.42765
Dipole moment (Debye)	5.6894	1.6950

Formulas for Calculating Hardness and Energy Gap (Gap Energy):

Chemical hardness = (E LUMO-E HOMO)/2 (1)

Energy Gap =(E LUMO-E HOMO) (2)

Fig 2. Comparison of the natural gravity in the n and d modes



By comparing nitrogen and carbon in a similar position to the single-mode, it was found that there is a greater negative charge on nitrogen and carbon atoms than in the case of fullerene.

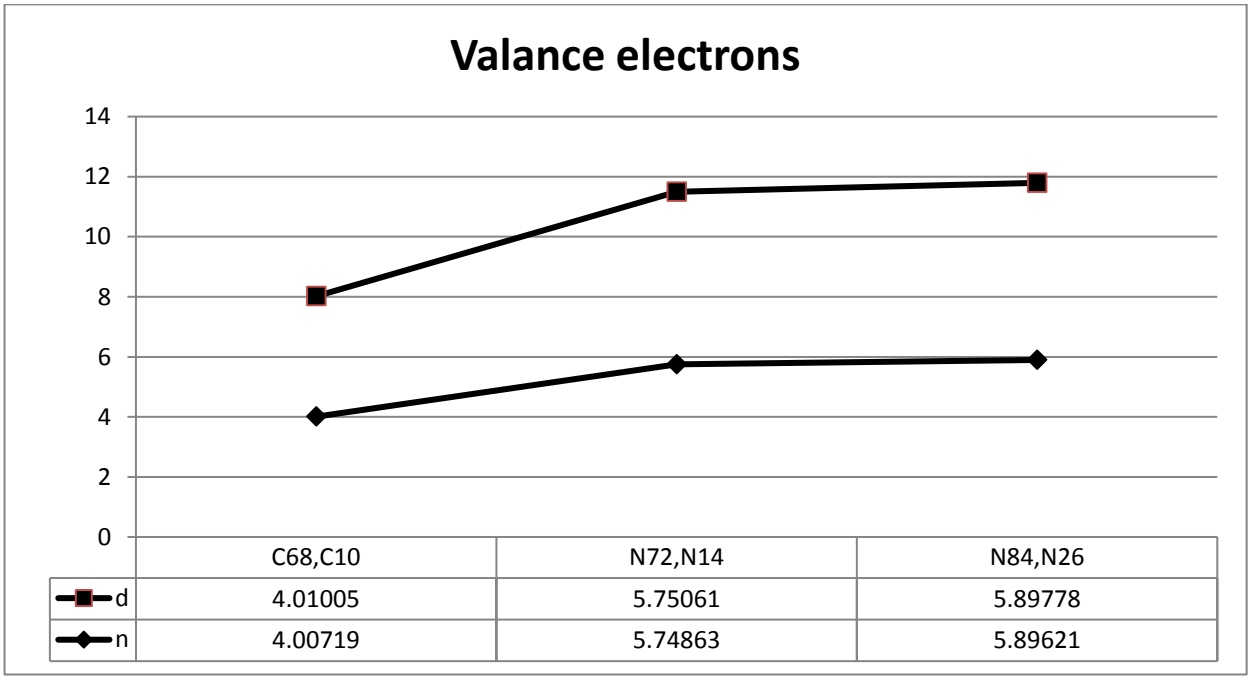


Fig. 3 Comparison of Capacitive Electrons

Comparison of the similar positions of electrons in the paraffinylenediamine interconnected to the fullerene shows that there are more electrons in the composition mode in the form of a single state than the n state

Discussion and conclusion:

By comparing the values of the energy of the hatchery of the Fact between the two compounds of the single compound and connected to the fullerene, it was determined that the composition with the fullerene is more stable. Also, the comparison between the molecular orbital molecular states of Homo and Volumetric energy and the chemical hardness (Table 1) The chemical complexity in the bonded region is less than the reactivity of the compound compared to its detachment state. On the other hand, the comparison of the bipolar momentum of the two compounds suggests an increase in the bipolar momentum in that the compound is connected to the fullerene (Table 1), along with the evidence and the results obtained, Related to the bargraph of atoms Capacitance electrons in the positions of the same situation (see Figs. 2 and 3), it can be observed that the current of electrons from the side of the composition of paraphenylenediamine to fullerene due to its large electron microscopy was created which causes the accumulation of electrons on the fullerene and the occurrence of a bipolar momentum Most of the composition was fullerene

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