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ORIGINAL ARTICLE

Electronic properties studies of Benzene under Boron Nitride nano ring field

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Abstract

In this study, B12N12 Nano ring has been selected because it consist of four 6-side rings and polar bonds B-N which in comparison with non-polar bonds C-C, is more suitable for the study of the absorption of other compounds. So reactivity and stability of Benzene alone and in the presence B12N12 nano ring field checked. To determine the non-bonded interaction energies between Benzene and B12N12 nano ring in different orientations and distances, geometry of molecules with density functional theory B3LYP method and 6-31g *basis set optimized. Then calculated the natural bond orbital (NBO), nuclear independent chemical shift (NICS) and muliken charge of Benzene atoms alone and in the presence B12N12 done. The results of any order explains reduce the reactivity and increase stability of Benzene in the presence B12N12 nano ring and electron transfer from the nano ring to Benzene. The gaussian quantum chemistry package is used for all calculations.

Keywords: *Ab initio; DFT; NBO; NICS; NMR.*

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INTRODUCTION

After the discovery of C60 [1], carbon nano structures such as fullerene clusters, nanotubes, nano-capsules, cones and cubes have been reported[1-4]. Boron nitride Nanostructure has a band gap energy of about 6 eV it is expected that different electronic, optical and magnetic properties reveal [4]. Therefore, many studies on BN nanomaterials such as BN nanotubes[4,5], BN nanocapsules [4], BN clusters [3, 4] and BN nanoparticles [6, 7] have been reported, it is expected that these compounds to be useful for the electronics, semiconductor with high thermal stability and nanowires. The number of BN clusters [8-18] and BN nano-rings [19-22] have been studied using theoretical methods. Also, absorption of Benzene and polycyclic hydrocarbons on carbon nanotubes and graphene sheets has studied by theoretical methods [23-25]. In this study, the Benzene aromaticity properties as a known carcinogen combination, in interaction with B12N12 nano ring theoretically studied. Because prolonged contact to Benzene, causes detrimental effects on manufacturer tissue of blood cells. The aim of this research is study of the electronic structure, structural stability or reduction in reactivity of Benzene in the presence B12N12 nano ring by using theoretical methods.

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EXPERIMENTAL

Geometric structure of Benzene molecule and B12N12 Nano ring with B3LYP method [26, 27] and 6-31g* basis set is optimized by using ab initio gaussian quantum chemical package. The main purpose of this study was to evaluate changes of reactivity of aromatic compound in nano ring field. Thus the energy of interaction between two molecules in different orientations and distances are calculated. The energy values are given in Tables 1 and 2. The Table data shows that the best angle and distance values for the two adsorbed molecules equal to the -140.0 ° and 3.1

Å, respectively. Optimized structure shown in Fig. 1 and adsorption energy for optimized structure of Benzene-B12N12 equal to -0.3061 kcal/mol. So other calculations related to NBO, NMR, Freq and NICS for optimum structure at the level of B3LYP/ 6-31g * was used.

RESULTS AND DISCUSSION

Density functional theory (DFT) calculations with B3LYP method for studying the effects of B12N12 Nano ring field on aromaticity and stability of the Benzene is done. Benzene and B12N12 structures by B3LYP/6-31g* can be optimized, and calculations NBO analysis done for these compounds. NBO analysis results are reported in Table 3 and 4. Distribution charge to carbon atoms of Benzene in the absence of nano ring field and in the presence of nano ring field by NBO method specified. The Mulliken atomic charges have given in Table 3. Mulliken charges are obtained theoretically by partitioning of electron density distribution employing the Mulliken approximation [28]. Table data specifies that the distribution of charge on the carbon atoms of Benzene in the absence of nano ring field is similar, but when Benzene is in the presence of the Nano ring field, 25, 26 and 27 atoms of Benzene that are closer to the nano ring, greater share of charge allocated. Which represents the electron transfer from the nano ring to Benzene and this is due to the non-bonded interaction between Benzene and nano ring. (Atomic label is according to Fig. 1.)

Electronic properties such as Ionization energy (I), Electron affinity (A), energy gap (Eg), electronic chemical potential (μ), chemical hardness (η), electro philicity index (ω), global hardness (s) and electron transfer (Δn) can be obtained using NBO analysis. According to the data of Table 4 can be understood the energy gap for Benzene, B12N12 and Benzene-B12N12 nano ring are 6.82 eV, 4.37 eV and 3.51 eV respectively. By comparing these values, we find that the presence of nano ring with

Table. 1: The values of the energy of Benzene - B12N12 molecule at different angles

Benzene-B12N12	
angle of rotation	Energy (Hartree)
-180	-1187.916680
-160	-1187.916691
-140	-1187.916701
-120	-1187.916664
-100	-1187.916619
-80	-1187.916602
-60	-1187.91663
-40	-1187.916668
-20	-1187.916682
0	-1187.916683
20	-1187.916688
40	-1187.916685
60	-1187.916629
80	-1187.916566
100	-1187.916545
120	-1187.916587
140	-1187.916646
160	-1187.916674
180	-1187.916681

Benzene is a factor for Benzene is more stable and less reactive.

Electron transfer for Benzene-B12N12 nano ring is 2.83 eV, that represents the flow of electrons from the nano ring to the Benzene, and electron transfer can be seen in the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) Orbitals diagram (Fig. 2a and b).

Table. 2: The values of the absorbed energy of Benzene - B12N12 molecule at different distances.

Distance (Å)	Energy(/Hartree)			E adsorption (KCal/Mol)
	Benzene-B12N12	Benzene	B12N12	
1	-1187.714752	-232.2483901	-955.6702839	127.9629923
1.4	-1187.859371			37.21294487
1.8	-1187.903613			9.450857829
2.2	-1187.915844			1.775977387
2.6	-1187.918645			0.018386028
2.9	-1187.919102			-0.268574066
3	-1187.919146			-0.296372737
3.1	-1187.919162			-0.306099134
3.2	-1187.919155			-0.301706568
3.3	-1187.91913			-0.286144332
3.4	-1187.919094			-0.263616741
3.8	-1187.918893			-0.137487332
4	-1187.918802			-0.080195714

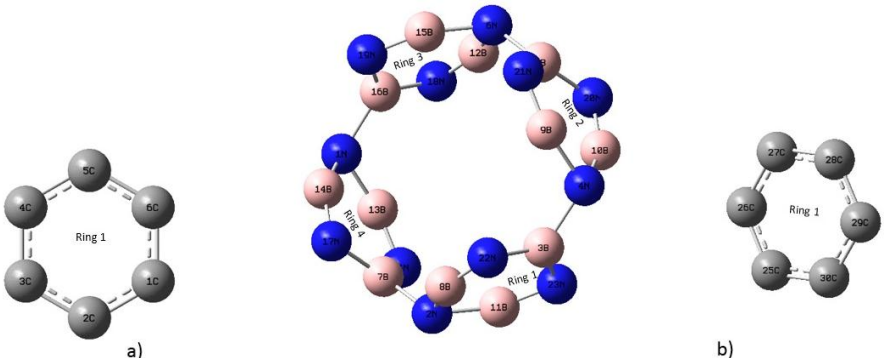

Fig. 1: a) Optimized structure of Benzene b) optimized structure of Benzene-B12N12 Nano ring

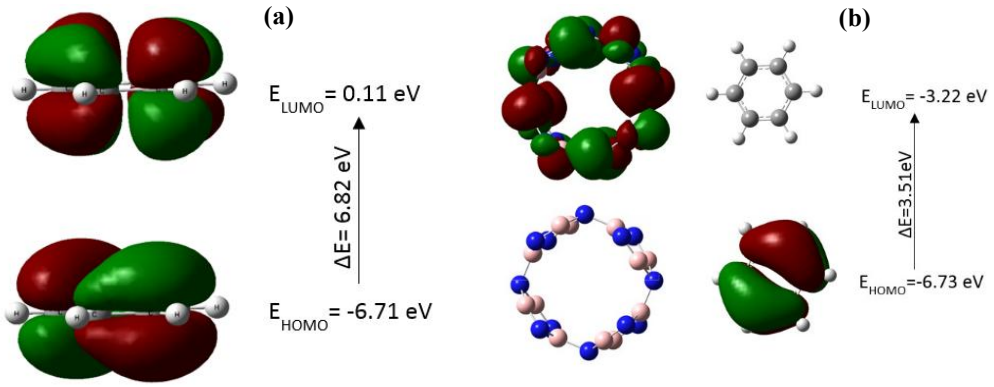

Fig. 2: a) LUMO and HOMO molecular orbitals of Benzene. b) LUMO and HOMO molecular orbitals of Benzene-Nano ring

Table. 3: Mulliken atomic charges (NBO charges) of Benzene and Benzene - B12N12

Mulliken atomic charges(e)			
Benzene		Benzene-B12N12	
1 C	-0.128157	25 C	-0.130063
2 C	-0.128271	26 C	-0.138806
3 C	-0.128306	27 C	-0.130055
4 C	-0.128153	28 C	-0.128063
5 C	-0.128278	29 C	-0.127663
6 C	-0.128302	30 C	-0.128059
Sum of Mulliken charges	-0.76947	Sum of Mulliken charges	-0.78271

Table. 4: Electronic properties of Benzene and B12N12-Benzene at B3LYP / 6-31g *

Compounds	NBO data at B3LYP / 6-31g *									
	LUMO(ev)	HOMO(ev)	I(ev)	A(ev)	Eg (ev)	μ (ev)	η(ev)	ω(ev)	$s(ev^{-1})$	Δn(ev)
Benzene	0.110	-6.704	6.704	-0.110	6.814	-3.296	3.407	1.594	0.146	0.967
B12N12-Benzene	-3.215	-6.728	6.728	3.215	3.512	-4.971	1.756	7.038	0.284	2.831
B12N12	-3.176	-7.547	7.547	3.176	4.371	-5.361	2.185	6.577	0.228	2.453

So that HOMO orbitals matches the Benzene and LUMO orbitals matches the nano ring.

CONCLUSIONS

Compare results of HOMO and LUMO molecular orbitals the justification for the electron transfer of the nano ring to the Benzene. So that the shape related to molecular orbitals, HOMO orbitals based on aromatic compound and LUMO orbitals based on the nano ring as well as the results of the carbon NMR spectrum is justified. Mulliken atomic charge values in Table 3 shows that the total atomic charge carbon atoms of Benzene alone and in the presence of nano ring equal to -0.769 and -0.783 respectively. And 25, 26 and 27 carbon atoms in the Benzene that are closer to the Nano ring receive the additional contribution of atomic charges that due to the non-bonded interactions and electron transfer from nano ring is to Benzene.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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