

Investigation of non-bonded interaction between C₁₀H₈ and B₁₂N₁₂ nano ring: NBO and NMR studies

M. Khaleghian^{1*}; F. Azarakhshi²; Gh. Ghashami³

¹ Department of Chemistry, Islamshahr Branch, Islamic Azad University, Tehran, Iran

² Department of Chemistry, Varamin-Pishva Branch, Islamic Azad University, Varamin, Iran

³ Department of Engineering, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran

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ABSTRACT: To determine the non-bonded interaction energies between Naphthalene and B₁₂N₁₂ Nano ring in different orientations and distances, geometry of molecules with B3LYP method and 6-31g* basis set optimized. Also reactivity and stability of Naphthalene alone and in the presence B₁₂N₁₂ Nano ring checked. Then calculated the NBO, NMR, FREQ, NICS and muliken charge of Naphthalene atoms alone and in the presence B₁₂N₁₂ done. The results of any order to reduce the reactivity and increase stability of Naphthalene in the presence B₁₂N₁₂ Nano ring tells. The Gaussian quantum chemistry package is used for all calculations.

Keywords: *Ab initio; DFT; Nano ring; Naphthalene -B₁₂N₁₂; NBO; NICS; NMR*

INTRODUCTION

Polycyclic Aromatic Hydrocarbons (PAHs) occur naturally in coal, Crude oil and gasoline. PAHs compounds are also products made from fossil fuels, asphalt and pitch. By converting coal to natural gas and the incomplete combustion of fossil fuels and garbage, PAHs compounds are released into the air. Which is much more incomplete combustion process more compounds released. PAHs compounds in the environment, water, soil and air are found and the months and years will remain in these areas.

The amount of these compounds in urban air is 10 times higher than non-urban air. Subject carcinogenic poly nuclear aromatic compounds are still requires

further study. The carcinogenic effects of a number of compounds of this group, in laboratory animals has been proven, but it is not known whether humans as a result of exposure to these compounds is cancer or not. In this study, changes in the properties one of these compounds in the presence of nanostructures reviewed. After the discovery of C₆₀ (Kroto, *et al.*, 1985), carbon nano structures such as fullerene clusters, nanotubes, nano-capsules, cones and cubes have been reported (Kroto, *et al.*, 1985, Iijima, 1991, Oku, *et al.*, 2000, Oku, *et al.*, 2001). Boron nitride Nanostructure has a band gap energy of about 6 eV it is expected that different electronic, optical and magnetic properties reveal (Oku, *et al.*, 2001). Therefore, many studies on BN nanomaterials such as BN nanotubes (Oku, *et al.*,

(*) Corresponding Author - e-mail: mehr_khaleghian@iaau.ac.ir

2001, Mickelson, *et al.*, 2003), BN nanocapsules⁴, BN clusters (Oku, *et al.*, 2000, Oku, *et al.*, 2001) and BN nanoparticles (Oku, *et al.*, 2003, Oku, *et al.*, 2003) 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 (Jensen and Toftlund, 1993, Zandler, *et al.*, 1996, Seifert, *et al.*, 1997, Slanina, *et al.*, 1997, Zhu, *et al.*, 1997, Alexandre, *et al.*, 1999, Fowler, *et al.*, 1999, Pokropivny, *et al.*, 2000, Strout, 2000, Will and Perkins, 2001, Alexandre, *et al.*, 2002) and BN nano-rings (Monajjemi, *et al.*, 2010, Monajjemi, 2011, Monajjemi and Boggs, 2013, Monajjemi and Khaleghian, 2011) have been studied using theoretical methods. Also absorption of benzene and polycyclic hydrocarbons on carbon nanotubes and graphene sheets studied by theoretical methods (Tran-Duc and Thamwattana, 2011, Mishra and Yadav, 2012, Kuc and Heine, 2010). In this study, the Naphthalene aromaticity properties as a known carcinogen combination, in interaction with B12N12 nanoring theoretically studied. The aim of this study, the electronic structure, structural stability or reduction in reactivity of Naphthalene in the presence B12N12 Nano ring by using theoretical methods.

COMPUTATIONAL METHODS

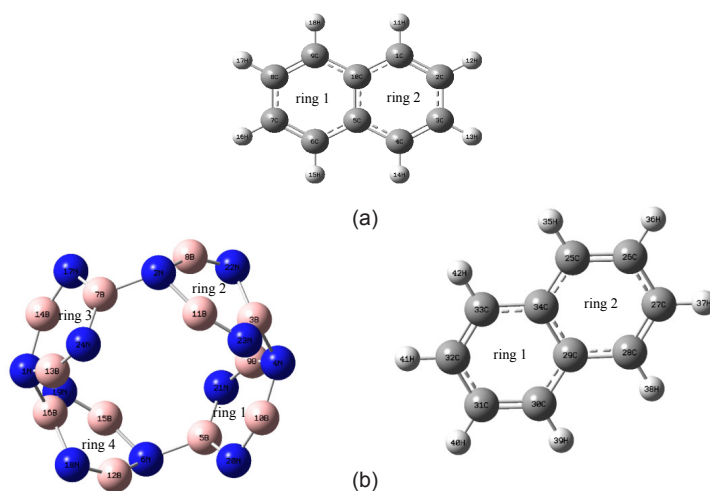
Geometric structure of Naphthalene molecule and B12N12 Nano ring with B3LYP method (Becke, 1993, Lee, *et al.*, 1988) and 6-31g* basis set is optimized by

Table 1: The values of the energy of Naphthalene and B12N12 molecules at different angles

Naphthalene -B12N12	
Angle of rotation	Energy /Hartree
-180	-1341.5632079
-160	-1341.5632372
-140	-1341.5632390
-120	-1341.5632263
-100	-1341.5632556
-80	-1341.5632761
-60	-1341.5632942
-40	-1341.5633148
-20	-1341.5633197
0	-1341.5632904
20	-1341.5633112
40	-1341.5633055
60	-1341.5632782
80	-1341.5632862
100	-1341.5632412
120	-1341.5632466
140	-1341.5632521
160	-1341.5632410
180	-1341.5632079

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



Scheme 1: a) Optimized structure of Naphthalene b) optimized structure of Naphthalene -B12N12 Nano ring.

Table 2: The values of the absorbed energy of Naphthalene and B12N12 molecules at different distances.

Distance /Å	Energy /Hartree			E adsorption /KCal/Mol
	Naphthalene -B12N12	Naphthalene	B12N12	
1.6	-1341.532299			19.22243576
2	-1341.556045			4.321783428
2.4	-1341.562025			0.569464871
2.8	-1341.56326			-0.205823116
2.9	-1341.563347			-0.260165439
3	-1341.563393	-385.8926484	-955.6702839	-0.289281879
3.1	-1341.563411			-0.300263296
3.2	-1341.563406			-0.297000246
3.3	-1341.563382			-0.282316524
3.4	-1341.563347			-0.260416443
3.5	-1341.563304			-0.232994277

Table 3: Relative thermochemical parameters of Naphthalene, B12N12 and Naphthalene - B12N12.

Compounds	ΔG / (Hartree/Particle)	ΔH / (Hartree/Particle)	E (Thermal) /KCal/Mol	S /Cal/Mol-Kelvin
Naphthalene	- 0.116	- 0.155	97.230	82.200
B12N12	- 0.069	- 0.131141	81.700	130.38
Naphthalene -B12N12	- 0.208	- 0.284	146.600	149.343

distance values for the two adsorbed molecules equal to the -20.0° and 3.1 \AA , respectively. Optimized structure shown in Scheme 1 and adsorption energy for optimized structure of Naphthalene -B12N12 equal to $-0.30026 \text{ kcal/mol}$. So other calculations related to NBO, NMR and Freq for optimum structure at the level of B3LYP/6-31g* was used.

RESULT AND DISCUSSION

Thermodynamic Analysis

Thermodynamic quantities such as the gibbs free en-

ergy (ΔG), standard enthalpies (ΔH), entropies (S), thermal energy (T) that is dependent on transfer, vibration and rotation movements of particles and sum of electronic and zero-point Energies (E+ZPE), sum of electronic and thermal Energies (E+T), sum of electronic and thermal Enthalpies (E+H) and sum of electronic and thermal Free Energies (E+G) values of Naphthalene, B12N12 and Naphthalene -B12N12 at B3LYP method with 6-31g* basis set have been calculated.

The energy values are given in Tables 3 and 4. When Naphthalene is in non-bonded interaction with the Nano ring, Gibbs and enthalpy energies values

Table 4: Sum of thermochemical parameters of Naphthalene, B12N12 and Naphthalene - B12N12

Compounds	E+ZPE / (Hartree/Particle)	E+T /Hartree	E+H /Hartree	E+G /Hartree
Naphthalene	-385.744	-385.737	-385.736	-385.775
B12N12	-955.560	-955.543	-955.542	-955.604
Naphthalene -B12N12	-1341.302	-1341.280	-1341.279	-1341.354

decreases. Energy values reflect the reduced reactivity and increase stability of Naphthalene molecule in presence Nano ring field.

NBO Analysis

Density functional theory (DFT) calculations with B3LYP method for studying the effects of B12N12 Nano ring field on aromaticity and stability of the Naphthalene is done. Naphthalene 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 5 and 6. Distribution charge to carbon atoms of Naphthalene in the absence of Nano ring field and in the presence of Nano ring field by NBO method specified. The Mulliken atomic charges given in Table 5. Mulliken charges are obtained theoretically by partitioning of electron density distribution employing the Mulliken approximation (Mulliken, 1955). Table data specifies that the distribution of charge on the (1,4), (2,3), (5,10), (6,9) and (7,8) carbon atoms of Naphthalene is similar in the absence of Nano ring field, But when Naphthalene is in the presence of the Nano ring field, 31, 32 and 33 carbon atoms of Naphthalene that are closer to the nano ring, greater share of charge to allocated in comparison with 7, 8 and 9 carbon atoms. Which represents the electron transfer is from the Nano ring to Naphthalene and this is due to the non-bonded interaction between Naphthalene and nano ring (Atomic label is according to Scheme 1).

Mulliken atomic charge values in Table 5 shows that the total atomic charge of carbon atoms of Naphthalene alone and in the presence of Nano ring equal to -1.031 and -1.048 respectively. And 31, 32 and 33 carbon atoms in the Naphthalene that are closer to the Nano ring receive the additional contribution of atom-

Table 5: Mulliken atomic charges (NBO charges) of Naphthalene and Naphthalene -B12N12.

Mulliken atomic charges/e			
Naphthalene		Naphthalene -B12N12	
1 C	-0.1907	25 C	-0.19051
2 C	-0.13455	26 C	-0.13458
3 C	-0.13455	27 C	-0.13444
4 C	-0.19069	28 C	-0.19094
5 C	0.134754	29 C	0.135392
6 C	-0.19068	30 C	-0.19085
7 C	-0.13456	31 C	-0.13752
8 C	-0.13456	32 C	-0.14505
9 C	-0.19069	33 C	-0.19441
10 C	0.134777	34 C	0.135343
Sum of Mulliken charges		Sum of Mulliken charges	
-1.03146		-1.04756	

ic charges that due to the non-bonded interactions and electron transfer from Nano ring is to Naphthalene.

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 6 can be understood the energy gap for Naphthalene, B12N12 and Naphthalene -B12N12 Nano ring are 4.84 eV, 4.37 eV and 2.59 eV respectively. By comparing these values, we find that the presence of Nano ring with Naphthalene is a factor for Naphthalene is more stable and less reactive. Electron transfer to Naphthalene -B12N12 Nano ring is 2.83 that this represents the flow of electrons from the Nano ring to the Naphthalene, and electron transfer can be seen in the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) Orbitals diagram (Fig. 1). So that

Table 6: Electronic properties of Naphthalene and B12N12- Naphthalene 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)
Naphthalene	-0.945	-5.790	5.790	0.945	4.845	-3.368	2.422	2.341	0.206	1.390
Naphthalene-B12N12	-3.222	-5.809	5.809	3.222	2.587	-4.516	1.294	7.882	0.387	3.491
B12N12	-3.176	-7.547	7.547	3.176	4.371	-5.361	2.185	6.577	0.228	2.453

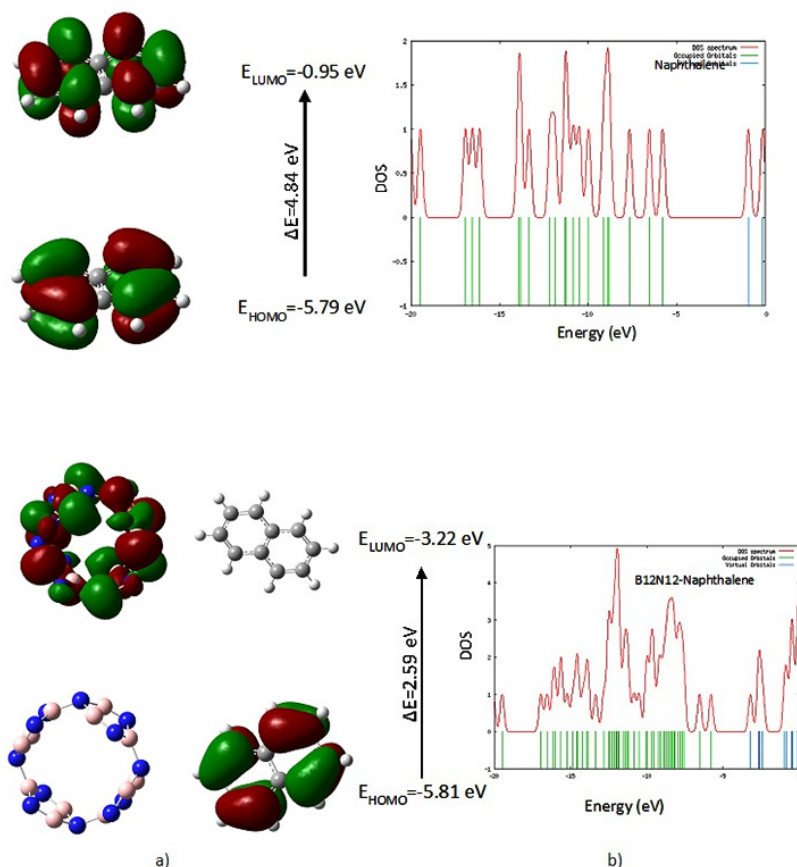


Fig. 1: a) LUMO and HOMO molecular orbitals of Naphthalene and Naphthalene -Nano ring, b) DOS diagrams of Naphthalene and Naphthalene -nano ring.

HOMO orbitals matches the Naphthalene and LUMO orbitals matches the nano ring.

NMR Analysis

Nuclear magnetic resonance (NMR) spectroscopy with the interactions between nuclear and magnetic fields involved. NMR spectroscopy is a powerful technique to study structural and dynamic properties of molecules in different physical states. Theoretical Studies of nuclear magnetic properties is based on advanced methods of quantum mechanics. NMR pa-

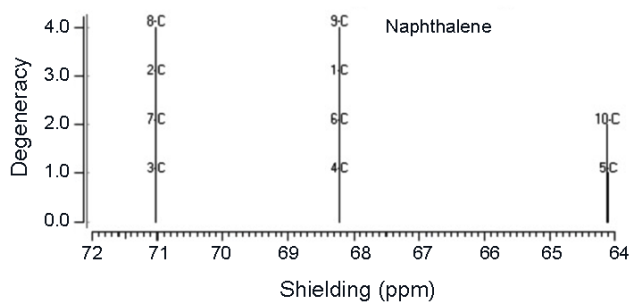


Fig. 2: GIAO magnetic shielding of Naphthalene.

rameters are calculated using the ab initio method, an important role in studying the molecular structure of compounds is applied. There are different methods to determine NMR parameters such as Gauge-Including atomic orbitals (GIAO), Individual gauge for localized orbitals (IGLO), Localized orbitals local origin (LORG) and Continuous set of gauge transformations (CSGT). In this study GIAO method for the measurement NMR parameters of Naphthalene and Naphthalene -B12N12 Nano ring used. The results are report-

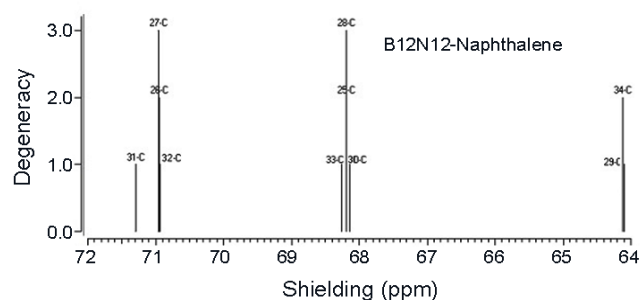


Fig. 3: GIAO magnetic shielding of Naphthalene -B12N12 Nano ring.

Table 7: NMR parameters of Naphthalene and Naphthalene -B12N12 Nano ring at B3LYP/6-31g*.

compounds	NMR parameters/ppm									
Naphthalene-	σ iso	σ aniso	σ_{11}	σ_{22}	σ_{33}	$\Delta\sigma$	δ	η	Ω	κ
1 C	68.207	145.783	-21.584	60.810	165.396	145.783	97.189	0.848	186.980	-0.119
2 C	71.012	161.834	-24.278	58.414	178.902	161.834	107.889	0.766	203.180	-0.186
3 C	71.012	161.835	-24.280	58.414	178.902	161.835	107.890	0.766	203.182	-0.186
4 C	68.204	145.786	-21.590	60.807	165.394	145.786	97.191	0.848	186.985	-0.119
5 C	64.108	199.777	-3.873	-1.096	197.293	199.777	133.185	0.021	201.166	-0.972
6 C	68.205	145.784	-21.588	60.808	165.394	145.784	97.189	0.848	186.982	-0.119
7 C	71.012	161.833	-24.279	58.415	178.901	161.833	107.889	0.766	203.180	-0.186
8 C	71.013	161.832	-24.277	58.414	178.901	161.832	107.888	0.766	203.178	-0.186
9 C	68.208	145.781	-21.582	60.811	165.396	145.781	97.188	0.848	186.978	-0.119
10 C	64.113	199.775	-3.867	-1.092	197.296	199.775	133.183	0.021	201.162	-0.972
Naphthalene-B12N12	σ iso	σ aniso	σ_{11}	σ_{22}	σ_{33}	$\Delta\sigma$	δ	η	Ω	κ
25 C	68.190	145.456	-21.842	61.251	165.160	145.456	96.970	0.857	187.002	-0.111
26 C	70.945	161.628	-24.299	58.437	178.697	161.628	107.752	0.768	202.996	-0.185
27 C	70.957	161.721	-24.029	58.129	178.771	161.721	107.814	0.762	202.800	-0.190
28 C	68.190	145.498	-21.532	60.913	165.189	145.498	96.999	0.850	186.721	-0.117
29 C	64.097	199.449	-4.022	-0.750	197.063	199.449	132.966	0.025	201.085	-0.967
30 C	68.146	145.450	-21.762	61.088	165.113	145.450	96.967	0.854	186.875	-0.113
31 C	71.293	160.676	-24.555	60.024	178.411	160.676	107.117	0.790	202.966	-0.167
32 C	70.932	160.790	-22.081	56.751	178.125	160.790	107.193	0.735	200.206	-0.212
33 C	68.259	145.101	-21.740	61.522	164.993	145.102	96.734	0.861	186.732	-0.108
34 C	64.124	199.368	-4.154	-0.510	197.037	199.369	132.912	0.027	201.190	-0.964

Table 8: Nucleus-Independent Chemical Shifts of Naphthalene and Naphthalene -B12N12

Compounds	Nucleus-Independent Chemical Shifts Values / (ppm)	
	ring 1	ring 2
Naphthalene	-4.1050	-4.1074
Naphthalene-B12N12	-3.3538	-3.8838

ed in Table 7. According to the data of the table it is clear that Naphthalene has three types of carbon that in carbon NMR spectra appears as follows: (5,10) carbon atoms in $\sigma=64.112$ ppm, (1,4) and (6,9) carbon atoms in $\sigma=68.203$ ppm, (2,3) and (7,8) carbon

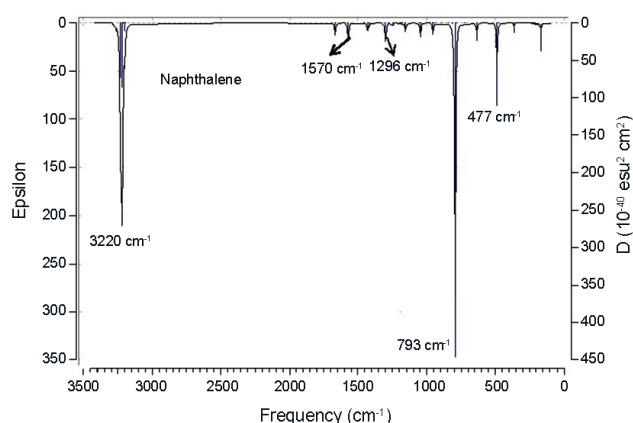


Fig. 4: IR spectrum of Naphthalene.

atoms in $\sigma=71.012$ ppm. 5 and 10 carbon atoms that are common aromatic rings appears in the lowest chemical shift. When Naphthalene is located adjacent to B12N12 Nano ring, 34 and 29 carbon atoms in a similar position to ratio of 5 and 10 carbon atoms of alone Naphthalene appears in the lowest chemical shift, that is $\sigma=64.097$ ppm. When the Naphthalene is located adjacent to B12N12 nano ring, most chemical shift related to 31 carbon atom and appeared at $\sigma=71.293$ ppm that due to being in the center of the magnetic field of Ring 1 of Nano ring. The magnetic field causes deshield and 31 carbon atom of the Naphthalene appear in the higher σ iso than the other carbon atoms of Naphthalene. But 32 carbon atom is located

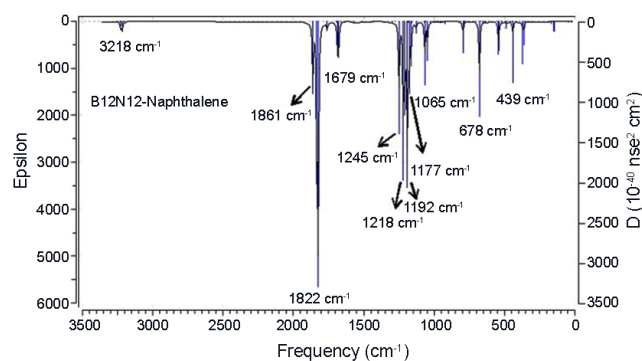


Fig. 5: IR spectrum of Naphthalene -B12N12 Nano ring.

adjacent to the 4 nitrogen atom of Nano ring (with the effect of electron-induced attraction) causes deshieldings 32 carbon atom and appear in $\sigma=70.93$ ppm. 33 carbon atom with the lowest chemical shift and the highest shieldings will appear in the $\sigma=68.258$ ppm. Because 33 carbon atom is located in front of the 3 boron atom that is electropositive atom (Figs. 2, 3).

Nucleus-Independent Chemical Shifts (NICS) calculations is done for Naphthalene and Naphthalene-B12N12. NICS Values are given in Table 8. In the presence of B12N12 Nano ring field, aromaticity of the both of Naphthalene rings reduced and ring 1 that is closer to Nano ring due to greater non bonded interaction with B12N12, shows aromaticity reduction greater than ring 2.

IR Spectroscopy

By observing the IR spectra of Naphthalene (Fig. 4) we find that peak of C-H aromatic bond stretching vibration (C=C-H) at a frequency of $\theta_{C=C-H}=3220$ cm^{-1} and in Naphthalene-Nano ring (Fig. 5) the peak appear in the frequency of $\theta_{C=C-H}=3218$ cm^{-1} . And the peak related to stretching vibration of C=C double bonds of the Naphthalene aromatic rings and Naphthalene-Nano ring appears in $\theta_{C=C-H}=1570$ cm^{-1} and $\theta_{C=C-H}=1679$ cm^{-1} respectively. Also Peak related to bending vibrations of aromatic C-H bonds (C=C-H) of the Naphthalene aromatic rings and Naphthalene-Nano ring appears in $\theta_{C=C-H}=678$ cm^{-1} and $\theta_{C=C-H}=793$ cm^{-1} respectively. For Naphthalene-Nano ring compound peak appeared at a frequency of $\theta_{C=C-H}=1861$ cm^{-1} related to nitrogen atoms top of each loop and sharp peak appeared at a frequency of $\theta_{B=N}=1822$ cm^{-1} related to other boron-nitrogen bonds in Nano ring. Stretching vibration related to Non-bonded interactions of C and N atoms appears at a frequency of $\theta_{C=N}=1218$ cm^{-1} and $\theta_{C=N}=1245$ cm^{-1} which marks the transition of the electron cloud between the Naphthalene aromatic rings and Nano ring. And for the Naphthalene-Nano ring compound C-C stretching vibration peaks appears at $\theta_{C-C}=1177$ cm^{-1} and $\theta_{C-C}=1192$ cm^{-1} .

CONCLUSIONS

Compare Carbon NMR spectra of Naphthalene aro-

matic rings alone and in the presence of Nano ring can be found that the presence of Nano ring on the side aromatic compounds can cause deshield carbon atoms are close to the Nano ring and this leads to a change in chemical shift toward higher values is. Also results of HOMO and LUMO molecular orbitals the justification for the electron transfer of the Nano ring to the Naphthalene aromatic rings. So molecular orbitals diagram related to Naphthalene and Naphthalene-B12N12 shows HOMO orbitals based on Naphthalene aromatic rings and LUMO orbitals based on the Nano ring and as well as the results of the carbon NMR spectra justified. All of calculations shows reduce the reactivity and increase stability of naphthalene in the presence B12N12 Nano ring.

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AUTHOR (S) BIOSKETCHES

Mehrnoosh Khaleghian, Assistant Professor, Department of Chemistry, Islamshahr Branch, Islamic Azad University, Tehran, Iran, *E-mail: mehr_khaleghian@yahoo.com, mehr_khaleghian@iaau.ac.ir*

Fatemeh Azarakhshi, Assistant Professor, Department of Chemistry, Varamin-Pishva Branch, Islamic Azad University, Varamin, Iran

Gholamreza Ghashami, Instructor, Department of Engineering, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran