

Quantum mechanical study of electronic and structural properties of methyl benzoate in interaction with boron nitride (BN) nanotube

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ABSTRACT: To determine the non-bonded interaction between methyl benzoate and boron nitride nanotube, we focused on an armchair single-wall boron nitride nanotube (9,9) With length 5 angstroms. The geometry of molecules was optimized using B3LYP method with 6-31g* basis set. Also reactivity and stability of methyl benzoate and boron nitride nanotube (9,9) was checked. Then NBO, FREQ, adsorption energy of methyl benzoate alone and in the presence of BNNT Field were derived to estimate methyl benzoate structural stability. The results of any order was found reduce of reactivity and increase of stability for methyl benzoate in the presence BNNT field.

Keywords: BNNTs; DFT; FREQ; Methyl benzoate; NBO; Quantum mechanical study

INTRODUCTION

The main reason for choosing boron nitride nanotubes is their interesting properties compared to carbon nanotubes. Depending on the diameter of nanotube and chirality, carbon nanotubes can act as a conductive or semi-conductive material, but all boron nitride nanotubes are semi-conductive and have higher thermal and chemical stability. Another property of boron nitride nanotubes is that unlike chirality of carbon nanotubes, the type of chirality has no significant impact on their properties. Therefore, during the synthesis of this com-

pound in the lab with different chirality, its comparison with theoretical work becomes easier. In the present research, methyl benzoate which is an ester compound is nano-encapsulated by boron nitride nanotube (9, 9) with length of 5 angstrom. Esters are often volatile and sometimes with a bitter taste as well as they are used as reactive, solvent and emollient in the pharmaceutical industry. For example, acetaminophen and aspirin contain ester; therefore, through nano- encapsulating ester compounds, they can be used more targeted and effective in the body. In other words, there is this opportu-

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nity in the process of nano-encapsulating that useful nutrient or drug is directly entered the bloodstream and absorbed into the body without being destroyed during the process of making, cooking or by enzymes in the mouth and stomach. Another function of nano-encapsulating is that useful nutrients with unpleasant flavors can be added to the main food through these capsules without feeling unpleasant taste. After the discovery of C60 (Kroto, *et al.*, 1985), carbon nano structures such as fullerene clusters, nanotubes, nanocapsules, cones and cubes have been reported (Kroto, *et al.*, 1985, Iijima, S., 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.*, 2001, Mickelson, *et al.*, 2003), BN Nano capsules (Oku, *et al.*, 2001), BN clusters (Oku, *et al.*, 2000, Oku, *et al.*, 2001) and BN nanoparticles (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 was studied by theoretical methods (Tran-Duc and Thamwattana, 2011, Mishra and Yadav, 2012, Kuc and Heine, 2010). Fullerene compounds as nano-structures that have special properties considered Late Twentieth Century. Boron nitride Fullerenes is also one of the most stable fullerene structures that in recent years due to their inherent capabilities and special properties compared to similar carbon compounds in the fields of scientific and theoretical research have done. Carbon Fullerenes bonds are non-polar, while boron nitride fullerenes due to electronegativity difference between the atoms are polar bonds and can have an effective interaction. In the present research, non-binding nature of inter-

action of methyl benzoate is investigated through boron nitride nanotube (armchair type) using quantum mechanical methods of density functional theory and Hybrid DFT. Furthermore, to better understand the nature of inter-molecular interactions and electronic structure of the methyl benzoate in the presence of nanotube, natural bond orbital analysis (NBO) is conducted. Electron and structural changes, electrical conductivity and energy absorbed are investigated in the process of absorption of methyl benzoate in the field of boron nitride nanotube. Also, the interaction effect on physical characteristics such as chemical potential and chemical hardness and electrical conductivity will be studied in nanotube interaction with methyl benzoate. After optimizing structures, base thermodynamic functions, vibrational frequencies, electron occupancies, energy of orbitals involved, absorption energy, HOMO–LUMO Energy bond gaps and electron density of states (DOS) are studied.

COMPUTATIONAL DETAIL

To determine the electromagnetic interactions of methyl benzoate and B45N45H36 nanotube, their geometric structure was optimized using B3LYP method (Becke, 1993, Lee, *et al.*, 1988) and 6-31g* basis set. The main purpose of this study was to evaluate changes of reactivity and stability of compound in BNNT field. Thus the adsorption energy of two molecules was calculated. In a more stable configuration, the adsorption energy is much more. The results were listed in Table 1. & Fig. 1 that shows optimized structure of methyl benzoate and BNNT and methyl benzoate - BNNT. Adsorption energy of methyl benzoate - BNNT in gas phase equal to -10.342 kcal/mol. The adsorption energy (E_{ad}) according to eq. (1):

$$E_{\text{adsorption}} = E_{\text{methyl benzoate-BNNT}} - (E_{\text{methyl benzoate}} - E_{\text{BNNT}}) \quad (1)$$

Where $E_{\text{methyl benzoate-BNNT}}$ the total energy of the BNNT in is interacting with the methyl benzoate, $E_{\text{methyl benzoate}}$ is total energy of the methyl benzoate alone and E_{BNNT} is the total energy of BNNT alone. So other calculations related to NBO and Frequency were performed for optimized structures at the level of B3LYP/6-31g*.

Table 1. Adsorption energy in gas phase for methyl benzoate –BNNT.

SCF done energy (kcal/mol)		Adsorption Energy (kcal/mol)	
Methyl benzoate – B45N45H36	Methyl benzoate	B45N45H36	$E_{\text{adsorption}}$
-2553236.941	-288735.153	-2264491.445	-10.342

Table 2. Adsorption energy in solution phase for methyl benzoate –BNNT.

Compounds	Electronic Energies in various solvents at B3LYP/6-31g* in (kcal/mol)				
	Water	Ethanol	Dichloromethane	chloroform	Heptane
	$\epsilon = 78.39$	$\epsilon = 24.55$	$\epsilon = 8.93$	$\epsilon = 4.9$	$\epsilon = 1.99$
Methyl benzoate/ a0 = 4.43 Å	-460.129	-460.129	-460.129	-460.128	-460.129
BNNT/ a0 = 7.87 Å	-3608.696	-3608.696	-3608.696	-3608.696	-3608.696
Methyl benzoate-BNNT/ a0 = 8.32 Å	-4068.843	-4068.843	-4068.842	-4068.842	-4068.842
Adsorption energy	-10.7461	-10.758	-10.779	-10.805	-10.767

The electron energy values obtained from calculations in the solution phase at the theoretical level of B3LYP/6-31g* are calculated for all three methyl benzoate compounds and boron nitride nanotubes, as well as methyl benzoate - boron nitride nanotube mixture (Table 2). Chloroform solvent is chosen as the most suitable solvent with the lowest electron energy (E_{el}) for the reaction. And By calculating the frequency, the thermodynamic functions and the amount of enthalpy of the solvation are calculated.

RESULTS AND DISCUSSION

Thermodynamic Analysis

Thermodynamic quantities such as the Gibbs free en-

ergy (ΔG), standard enthalpies (ΔH), entropies (S), thermal energy (E_{thermal}), that is dependent on transfer; vibration and rotation movements of particles, and sum of electronic and zero-point Energies ($E_{\text{el}}+ZPE$), sum of electronic and thermal Energies ($E_{\text{el}}+E_{\text{thermal}}$), sum of electronic and thermal Enthalpies ($E_{\text{el}}+H$) and sum of electronic and thermal Free Energies ($E_{\text{el}}+G$) values of methyl benzoate, BNNT and methyl benzoate-BNNT at B3LYP method with 6-31g* basis set have been calculated. The energy values in gas phase were given in Tables 3 and 4 and in solution phase were given in Tables 5 and 6.

NBO analysis

In analysis of NBO, the functions of electronic wave are interpreted in terms of a class of occupied Lewis or-

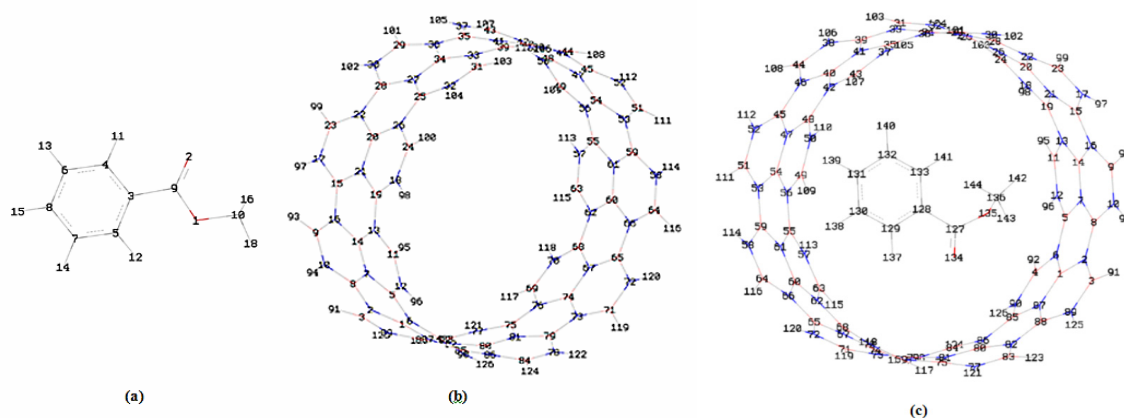


Fig. 1. a) Optimized structures of a) methyl benzoate b) BNNT nanotube c) methyl benzoate - BNNT.

Table 3. The thermodynamic parameters in the gas phase for methyl benzoate, BNNT and methyl benzoate-BNNT.

Compounds	Thermodynamic functions/ B3LYP/6-31G*					Cal/mol.K
	Hartree					
	G+E _{el}	H+E _{el}	E _{thermal} +E _{el}	E ₀ = ZPE+E _{el}	E _{el}	
Methyl benzoate	-460.019	-459.974	-459.975	-459.984	-460.128	92.85
BNNT	-3607.907	-3607.752	-3607.753	-3607.817	-3608.696	325.0
Methyl benzoate –BNNT	-4067.927	-4067.744	-4067.745	-4067.819	-4068.841	385.09

Table 4. Difference of thermodynamic functions in the gas phase for methyl benzoate, BNNT and methyl benzoate - BNNT.

Compounds	Difference of thermodynamic functions/B3LYP/6-31G*				
	Hartree				
	ΔG	ΔH	ΔE _{thermal}	ΔE ₀	ΔS
Methyl benzoate –BNNT	-0.00127	-0.01684	-0.01589	-0.01782	-32.759

bitals and a class of Lewis non-occupied independent orbitals. Due to transition of electron between Lewis occupied orbitals (donor) and Lewis unoccupied orbitals (acceptor) ne molecular orbitals are highly more stable than pure Lewis orbitals which comes with stabilizing the functions of electronic waves (Soltania, *et al.*, 2012, Ishigami, *et al.*, 2003). Since the effect of lack of non-covalence establishment on superposition between orbitals donor-acceptor are accumulated, it is natural that for explaining them as donor –acceptor the charge transition is presented with type of general-

ized Lewis acid-Lewis base.

NBO analysis of superposition (bonding-antibonding–antibonding), based on calculations at theoretic level of B3LYP/6-31G* shows that for mixture of methyl benzoate-BN nanotube, the greatest resonance energy is related to $\pi^*(B45-N46) \rightarrow \sigma^*C131-H139$ with $E_2=0.4$ kCal/mol and the smallest resonance energy is related to $\pi^*(N78-B79) \rightarrow \sigma^*C129-H137$ with $E_2=0.05$ kcal/mol deriving from lack of electronic establishment from BN nanotube to methyl benzoate (Table 7). Similarly, based on results from NBO anal-

Table 5. The thermodynamic parameters in the solution phase for methyl benzoate, BNNT and methyl benzoate-BNNT.

Compounds	Thermodynamic functions/ B3LYP/6-31G*					Cal/mol.K
	Hartree					
	G+E _{el}	H+E _{el}	E _{thermal} +E _{el}	E ₀ = ZPE+E _{el}	E _{el}	
Methyl benzoate	-460.019	-459.975	-459.976	-459.985	-460.129	92.874
BNNT	-3607.907	-3607.753	-3607.754	-3607.817	-3608.697	325.017
Methyl benzoate –BNNT	-4067.928	-4067.745	-4067.746	-4067.820	-4068.843	385.247

Table 6. Difference of thermodynamic functions in the solution phase for methyl benzoate, BNNT and methyl benzoate-BNNT.

Compounds	Changes the thermodynamic functions/B3LYP/6-31G*				
	Hartree				
	ΔG	ΔH	ΔE _{thermal}	ΔE ₀	ΔS
Methyl benzoate –BNNT	-0.00119	-0.01670	-0.01576	-0.01768	-32.644

Table 7. Resonance energies (E(2) / kcal/mol), energy difference of orbitals ($\Delta E = E(j)-E(i)$, a.u.), off-diagonal elements (Fij, a.u.), from boron nitride nanotube to methyl benzoate using DFT calculations at the level of theory B3LYP/6-31G*.

Second Order Perturbation Theory Analysis of Fock Matrix in NBO analysis				
from unit 1(BNNT) to unit 2(Methyl benzoate)				
Donor NBO (i)	Acceptor NBO (j)	E(2)/ kcal/mol	E(j)-E(i)/ a.u.	F(i,j)/ a.u.
BD*(2) B 45 - N 46	BD*(1) C 131 - H 139	0.4	0.42	0.031
LP*(1) B 14	BD*(1) C 136 - H 142	0.36	0.45	0.025
BD*(2) N 53 - B 59	BD*(1) C 130 - H 138	0.32	0.42	0.027
BD*(2) B 15 - N 17	BD*(1) C 136 - H 142	0.23	0.39	0.023
BD*(2) N 33 - B 39	BD*(1) C 132 - H 140	0.16	0.41	0.019
BD*(2) N 58 - B 64	BD*(1) C 130 - H 138	0.11	0.43	0.022
BD*(2) B 60 - N 61	BD*(1) C 130 - H 138	0.11	0.42	0.017
BD*(2) B 51 - N 52	BD*(1) C 131 - H 139	0.08	0.43	0.019
BD*(2) N 73 - B 74	BD*(1) C 129 - H 137	0.08	0.42	0.014
BD (2) N 47 - B 48	BD*(1) C 131 - H 139	0.06	0.75	0.006
BD*(2) N 78 - B 79	BD*(1) C 129 - H 137	0.05	0.4	0.011
Sum of E2		1.96		

ysis for mixture of methyl benzoate –BN nanotube, the greatest resonance energy is related to LP1(0134) $\rightarrow \pi^*B85-N90$ with $E2=0.85$ kcal/mol and least resonance energy is related to LP1(0134) $\rightarrow \sigma^* B84-N86$

with $E2=0.05$ kcal/mol that derives from lack of electronic establishment from methyl benzoate to BN nanotube (Table 8).

Other resonance energies derive from lack of elec-

Table 8. Resonance energies (E (2)/ kcal/mol), energy difference of orbitals ($\Delta E = E(j)-E(i)$, au), off-diagonal elements (Fij, a.u.), from methyl benzoate to boron nitride nanotube Using DFT calculations at the theoretical level B3LYP/6-31G*.

Second Order Perturbation Theory Analysis of Fock Matrix in NBO analysis				
from unit 2(Methyl benzoate) to unit 1(BNNT)				
Donor NBO (i)	Acceptor NBO (j)	E(2)/ kcal/mol	E(j)-E(i)/ a.u.	F(i,j)/ a.u.
LP (1) O 134	BD*(2) B 85 - N 90	0.85	0.77	0.024
LP (2) O 134	BD*(2) B 85 - N 90	0.74	0.34	0.015
BD*(2) C 127 - O 134	BD*(2) B 80 - N 81	0.38	0.03	0.006
LP (1) O 135	BD*(2) B 1 - N 87	0.28	0.6	0.012
LP (1) O 135	BD*(2) B 5 - N 7	0.19	0.59	0.01
LP (1) O 134	BD*(2) B 80 - N 81	0.15	0.76	0.01
LP (1) O 134	BD*(2) B 84 - N 86	0.14	0.75	0.01
BD (2) C 127 - O 134	BD*(2) B 80 - N 81	0.08	0.5	0.006
BD*(2) C 127 - O 134	BD*(2) N 78 - B 79	0.08	0.03	0.003
LP (1) O 134	BD*(1) B 85 - N 86	0.07	1.19	0.008
LP (2) O 134	BD*(1) B 85 - N 87	0.07	0.77	0.007
BD*(2) C 127 - O 134	BD*(2) B 85 - N 90	0.07	0.04	0.003
LP*(1) C 131	BD*(2) B 45 - N 46	0.06	0.18	0.004
LP (1) O 134	BD*(1) B 84 - N 86	0.05	1.17	0.007
Sum of E2		3.21		

tronic establishment from methyl benzoate to BN nanotube and vice versa presented in Tables 7 and 8. Sum of resonance energies from BN nanotube to methyl benzoate and vice versa are Sum of $E_2=1.96$ and Sum of $E_2=3.21$ kcal/mol, respectively.

Then one can say that when E_2 in transitions from nanotube to methyl benzoate is less than E_2 in transition from methyl benzoate to nanotube, this shows that nanotube serves as acceptor alongside methyl benzoate. For methyl benzoate solely the greatest resonance energy is related to $LP(2)O1 \rightarrow \pi^*O2-C9$ with $E_2=48$

kcal/mol and the smallest resonance energy is related to $\sigma(C3-C9) \rightarrow \sigma^*O2-C9$ with $E_2=0.95$ kcal/mol. For methyl benzoate in mixture of methyl benzoate-BN nanotube, the greatest resonance energy is related to $LP(2)C134 \rightarrow \sigma^*C127-O135$ with $E_2=33.08$ kcal/mol and the least resonance energy is related to $\sigma C127-C128 \rightarrow \sigma^*O135-C136$ with $E_2=0.53$ kcal/mol. Other resonance energies derive from lack of electronic establishment presented in Table 9.

Given the Table 9, it is obvious that when methyl benzoate and nanotube are under influence of mag-

Table 9. Resonance energies ($E(2)$ / kcal/mol), energy differences of orbital ($\Delta E = E(j)-E(i)$, a.u.), off-diagonal elements (F_{ij} , a.u.), methyl benzoate Alone and methyl benzoate in the presence of boron nitride nanotube.

Second Order Perturbation Theory Analysis of Fock Matrix in NBO analysis / B3LYP/6-31G*									
Within (Methyl benzoate)					Within (Methyl benzoate) in BNNT- Methyl benzoate				
Donor NBO (i)	Acceptor NBO (j)	$E(2)$	$E(j)-E(i)$	$F(i,j)$	Donor NBO (i)	Acceptor NBO (j)	$E(2)$	$E(j)-E(i)$	$F(i,j)$
LP (2) O 1	BD*(2) O 2 - C 9	48	0.33	0.114	LP (2) O 135	BD*(2) C 127 - O 134	17.79	0.41	0.077
LP (2) O 2	BD*(1) O 1 - C 9	33.91	0.63	0.132	LP (2) O 134	BD*(1) C 127 - O 135	33.08	0.61	0.128
BD (2) C 3 - C 5	BD*(2) O 2 - C 9	22.3	0.26	0.070	BD (1) C 128 - C 133	BD*(1) C 127 - O 134	1.78	1.27	0.043
LP (1) O 1	BD*(1) O 2 - C 9	7.68	1.17	0.085	LP (1) O 135	BD*(1) C 127 - O 134	1.76	1.08	0.039
BD (1) C 3 - C 5	BD*(1) C 3 - C 4	3.97	1.27	0.063	BD (1) C 128 - C 133	BD*(1) C 128 - C 129	3.90	1.27	0.063
BD (1) C 3 - C 4	BD*(1) C 3 - C 5	3.93	1.26	0.063	BD (1) C 128 - C 129	BD*(1) C 128 - C 133	3.94	1.26	0.063
BD (1) C 3 - C 9	BD*(1) O 1 - C 10	3.44	0.93	0.051	BD (1) C 127 - C 128	BD*(1) O 135 - C 136	0.53	0.94	0.02
BD (1) C 5 - C 7	BD*(1) C 3 - C 9	3.43	1.13	0.056	BD (1) C 132 - C 133	BD*(1) C 127 - C 128	3.25	1.12	0.055
BD (1) C 4 - C 6	BD*(1) C 3 - C 9	2.91	1.13	0.052	BD (1) C 129 - C 130	BD*(1) C 127 - C 128	2.96	1.12	0.052
BD (1) C 5 - C 7	BD*(1) C 3 - C 5	2.91	1.27	0.054	BD (1) C 132 - C 133	BD*(1) C 128 - C 133	3.03	1.26	0.055
BD (1) C 4 - C 6	BD*(1) C 3 - C 4	2.83	1.27	0.053	BD (1) C 129 - C 130	BD*(1) C 128 - C 129	2.84	1.26	0.053
LP (1) O 2	BD*(1) C 3 - C 9	2.78	1.12	0.05	LP (1) O 134	BD*(1) C 127 - C 128	2.35	1.10	0.046
BD (1) C 7 - C 8	BD*(1) C 5 - C 7	2.51	1.28	0.051	BD (1) C 131 - C 132	BD*(1) C 132 - C 133	2.54	1.27	0.051
BD (1) C 6 - C 8	BD*(1) C 4 - C 6	2.51	1.28	0.051	BD (1) C 130 - C 131	BD*(1) C 129 - C 130	2.47	1.28	0.05
BD (1) C 4 - C 6	BD*(1) C 6 - C 8	2.47	1.27	0.05	BD (1) C 129 - C 130	BD*(1) C 130 - C 131	2.42	1.27	0.049
BD (1) C 5 - C 7	BD*(1) C 7 - C 8	2.47	1.27	0.05	BD (1) C 132 - C 133	BD*(1) C 131 - C 132	2.45	1.27	0.05
BD (1) C 3 - C 5	BD*(1) C 5 - C 7	2.41	1.28	0.05	BD (1) C 128 - C 133	BD*(1) C 132 - C 133	2.50	1.28	0.051
BD (1) C 3 - C 9	BD*(1) C 4 - C 6	2.41	1.25	0.049	BD (1) C 127 - C 128	BD*(1) C 129 - C 130	2.36	1.25	0.049
BD (1) C 7 - C 8	BD*(1) C 6 - C 8	2.39	1.27	0.049	BD (1) C 131 - C 132	BD*(1) C 130 - C 131	2.35	1.27	0.049
BD (1) C 6 - C 8	BD*(1) C 7 - C 8	2.39	1.27	0.049	BD (1) C 130 - C 131	BD*(1) C 131 - C 132	2.36	1.27	0.049
BD (1) C 3 - C 4	BD*(1) C 4 - C 6	2.34	1.28	0.049	BD (1) C 128 - C 129	BD*(1) C 129 - C 130	2.35	1.28	0.049
BD (1) C 3 - C 9	BD*(1) C 3 - C 5	2.10	1.24	0.046	BD (1) C 127 - C 128	BD*(1) C 128 - C 133	1.86	1.23	0.043
BD (1) C 3 - C 4	BD*(1) O 1 - C 9	2.03	1.06	0.042	BD (1) C 128 - C 129	BD*(1) C 127 - O 135	1.98	1.05	0.042
BD (1) C 3 - C 9	BD*(1) C 5 - C 7	1.94	1.25	0.044	BD (1) C 127 - C 128	BD*(1) C 132 - C 133	2.17	1.25	0.046
BD (1) C 3 - C 4	BD*(1) C 3 - C 9	1.65	1.12	0.039	BD (1) C 128 - C 129	BD*(1) C 127 - C 128	1.62	1.11	0.038
BD (1) O 2 - C 9	BD*(1) C 3 - C 9	1.57	1.51	0.044	BD (1) C 127 - O 134	BD*(1) C 127 - C 128	1.01	1.46	0.035
BD (1) O 1 - C 9	BD*(1) C 3 - C 4	1.57	1.48	0.043	BD (1) C 127 - O 135	BD*(1) C 128 - C 129	1.08	1.46	0.036
BD (1) C 3 - C 9	BD*(1) C 3 - C 4	1.56	1.24	0.039	BD (1) C 127 - C 128	BD*(1) C 128 - C 129	1.67	1.24	0.041
BD (1) C 3 - C 5	BD*(1) C 3 - C 9	1.55	1.13	0.038	BD (1) C 128 - C 133	BD*(1) C 127 - C 128	1.49	1.12	0.037
LP (1) O 2	BD*(1) O 1 - C 9	1.27	1.05	0.033	LP (1) O 134	BD*(1) C 127 - O 135	1.21	1.04	0.032
BD (1) O 2 - C 9	BD*(1) C 3 - C 5	1.09	1.65	0.038	BD (1) C 127 - O 134	BD*(1) C 128 - C 133	1.24	1.60	0.04
BD (1) C 3 - C 9	BD*(1) O 2 - C 9	0.95	1.27	0.031	BD (1) C 127 - C 128	BD*(1) C 127 - O 134	0.71	1.24	0.027

netic field of each other, the energy of a series of electronic transitions in molecular orbitals in methyl benzoate solely in comparison with the mixture has considerable changes (increase and decrease) which suggests these molecular orbitals react more in mixture when compared with pure model of methyl benzoate. As it can be seen in table 9, the greatest ex-

tent of resonance energy for methyl benzoate solely is $LP(2)01 \rightarrow \pi^*02-C9$ with $E_2=48$ kcal/mol and $\Delta E = E(j)-E(i) = 0.33$ a.u and $F(i,j)=0.114$ a.u that resonance energy E_i-E_j , $F(i,j)$ of the same orbital from methyl benzoate in mixture methyl benzoate-BN nanotube is $LP(2)0135 \rightarrow \pi^*0134-C127$, $E_2=17.79$ kcal/mol a.u and $\Delta E = E(j)-E(i) = 0.41$ a.u and $F(i,j)=0.077$ a.u. With

Table 10. Molecular orbitals energies and Orbital occupancy of Methyl Benzoate alone and Methyl Benzoate - boron nitride nanotube.

Natural Bond Orbitals / B3LYP/6-31G*					
Within (Methyl benzoate)			Within (Methyl benzoate) in BNNT - Methyl benzoate		
Bond orbital	Occupancy	Energy	Bond orbital	Occupancy	Energy
BD (1)O 2 - C 9	1.99685	-1.07346	BD (1)C 127 - O 134	1.996	-1.0403
BD (1)O 1 - C 9	1.99283	-0.91066	BD (1)C 127 - O 135	1.99266	-0.89902
BD (1)O 1 - C 10	1.99157	-0.80998	BD (1)O 135 - C 136	1.98227	-0.81074
BD (2)O 2 - C 9	1.98289	-0.37208	BD (2)C 127 - O 134	1.97993	-0.42564
BD (1)C 6 - C 8	1.98146	-0.69269	BD (1)C 130 - C 131	1.98114	-0.69809
BD (1)C 7 - C 8	1.98146	-0.69339	BD (1)C 131 - C 132	1.9812	-0.70004
BD (1)C 4 - C 6	1.98025	-0.69399	BD (1)C 129 - C 130	1.98017	-0.70099
BD (1)C 5 - C 7	1.98013	-0.6942	BD (1)C 132 - C 133	1.97989	-0.70348
LP (1)O 2	1.97699	-0.67959	LP (1)O 134	1.9735	-0.68403
BD (1)C 3 - C 5	1.97628	-0.69338	BD (1)C 128 - C 133	1.97428	-0.70434
BD (1)C 3 - C 9	1.97462	-0.6649	BD (1)C 127 - C 128	1.98111	-0.67373
BD (1)C 3 - C 4	1.97386	-0.68831	BD (1)C 128 - C 129	1.97273	-0.69861
LP (1)O 1	1.96422	-0.56347	LP (1)O 135	1.95086	-0.51473
LP (2)O 2	1.84654	-0.25186	LP (2)O 134	1.8466	-0.25752
LP (2)O 1	1.79484	-0.31787	LP (2)O 135	1.83949	-0.36054
BD (2)C 4 - C 6	1.65077	-0.24726	LP (1)C 130	0.99144	-0.11412
BD (2)C 7 - C 8	1.6478	-0.24866	LP (1)C 132	0.99535	-0.11599
BD (2)C 3 - C 5	1.63908	-0.24785	LP (1)C 128	1.0479	-0.1198
BD*(2)C 3 - C 5	0.36958	0.03325	LP*(1)C 133	0.98067	-0.11971
BD*(2)C 7 - C 8	0.32529	0.03173	LP*(1)C 131	0.96974	-0.11521
BD*(2)C 4 - C 6	0.29756	0.03646	LP*(1)C 129	0.95404	-0.112
BD*(2)O 2 - C 9	0.25984	0.01412	BD*(2)C 127 - O 134	0.19042	0.0488
BD*(1)O 1 - C 9	0.10241	0.3732	BD*(1)C 127 - O 135	0.10384	0.35329
BD*(1)C 3 - C 9	0.06487	0.43633	BD*(1)C 127 - C 128	0.07176	0.41537
BD*(1)C 3 - C 5	0.02255	0.57312	BD*(1)C 128 - C 133	0.02353	0.55727
BD*(1)C 3 - C 4	0.02093	0.57295	BD*(1)C 128 - C 129	0.02198	0.56264
BD*(1)O 2 - C 9	0.01781	0.60278	BD*(1)C 127 - O 134	0.03664	0.56865
BD*(1)C 6 - C 8	0.01592	0.57499	BD*(1)C 130 - C 131	0.01586	0.56871
BD*(1)C 7 - C 8	0.01581	0.57522	BD*(1)C 131 - C 132	0.01564	0.56915
BD*(1)C 5 - C 7	0.01524	0.58383	BD*(1)C 132 - C 133	0.01535	0.57217
BD*(1)O 1 - C 10	0.01465	0.26751	BD*(1)O 135 - C 136	0.01328	0.26283
BD*(1)C 4 - C 6	0.01463	0.58721	BD*(1)C 129 - C 130	0.01476	0.57913

comparing the numerical value of $F_{i,j}$ (orbital overlap) obtained for electronic transitions (Table 9) one can note that decrease of orbital overlap justifies effectively the decrease of resonance energies derived from electronic non-establishment (Darvish Ganji, *et al.*, 2015, Becke, 1993). Electron population and energy of bonding and antibonding and antibonding orbital in the mixture of methyl benzoate-BN nanotube are studied in BN-nanotube and methyl benzoate (Table 10). Level of energy of antibonding orbital of methyl benzoate LP(2)01 has decreased (-0.31787 a.u.) with regard to the same orbital from methyl benzoate in mixture of methyl benzoate-BN nanotube LP(2)0135 (-0.36054 a.u.), and energy level of antibonding orbital π^*02-C9 has increased (0.01412 a.u.) with regard to the same orbital from the methyl benzoate in the mixture of methyl benzoate-nitride nanotube $\pi^*0134-C127$ (0.0488 a.u.). According to Boltzmann distribution law, more the difference of population between donor and acceptor molecular orbitals is, better the electron transition takes place, if the difference of population is small or equal, it is saturation mode and electron transitions fail to take place effectively. For example, difference of population in methyl benzoate is high between donor molecular orbitals (LP (2) O1, OCC=1.79484) and acceptor (π^*O2-C9 , OCC=0.25984 and in methyl benzoate at the presence of nanotube it is high between acceptor orbitals (LP (2) O135, OCC=1.83949) and acceptor ($\pi^* C127-$

O134, OCC=0.19042) and according to Boltzmann law the transition takes place effectively (Table 10).

Boltzmann law with the assumption of equality of multiplicity of energies:

$$\frac{N_j}{N_i} = e^{\frac{-(\epsilon_j - \epsilon_i)}{kT}}, \epsilon_j > \epsilon_i$$

N_j : population of acceptor orbital

N_i : population of donor orbital

Molecular electrostatic potential

One of useful features for studying the reactivity is determining the molecular electrostatic potential. Molecular electrostatic potential (MEP) shows that a region with most negative charge is red and a suitable place for attack of electrophile molecule. Similarly a region with most positive charge is blue and a good place for attack of nucleophile molecule. MEP is of high importance because it is used for showing size of molecule, shape of molecule as centers with positive and negative electrostatic potential as a colorful range. Generally, nucleophile and electrophile sites are specified in a molecule by (MEP) and one can predict the active sites for participating in a reaction (Lesarri, *et al.*, 2011, Reed, *et al.*, 1988). In the mixture of methyl benzoate-BN nanotube the density of positive charge on nitrogen atoms is more dominant than BN nanotube and the density of negative charge on oxygen atom of methyl benzoate is dominant thus the reactivity centers can be specified in this complex. In the Fig. 2 the transversal lines show that in the nano-capsulation of methyl benzoate, which part of methyl benzoate and BN nanotube is of interaction and electron resonance.

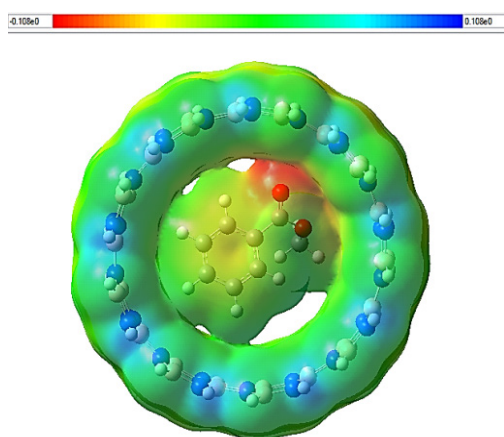


Fig. 2. The Electro-static Molecular Potential (MEP) calculated by the self-consistent field theory (SCF) of a methyl benzoate - boron nitride nanotube complex, a system with 114 atom and 648 electrons, in neutral form and in base state.

Molecule reactivity indices

DFT approach is useful for studying the features of chemical structures based on molecule reactivity indices. For a n -electron system with total energy (E) and external chemical potential $v(r)$, chemical hardness (η), electrophilicity (w) electro-negativity (χ), chemical softness (S), electronic chemical potential (μ) and maximum amount of electronic charge index (ΔN_{max}) at balance in the temperature (T) can be calculated based on following equations (Masnabadi, *et al.*, 2013, Masnabadi, *et al.*, 2012):

$$\chi = -\left(\frac{\partial E}{\partial N}\right)_{v(r),T} = -\mu \quad (1) \quad EI = -E_{\text{HOMO}} \quad (9)$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{v(r),T} = \frac{1}{2}\left(\frac{\partial \mu}{\partial N}\right)_{v(r),T} \quad (2) \quad EA = -E_{\text{LUMO}} \quad (10)$$

$$S = \left(\frac{\partial N}{\partial \mu}\right)_{v(r),T} \quad (3)$$

According to the theory of Pauling, the concept of electro-negativity (χ) is stated as the ability of an atom in molecule for absorption of electron and electrophilicity (w) as a scale of electrophile power of molecule. Chemical potential (μ) of molecule is calculated by Koopmans theory. Equations 4,5 and 6 are obtained from equations 1,2 and 3, respectively (Tasi, *et al.*, 1993, (Petrucci, *et al.*, 2007, Sundaraganesan, *et al.*, 2009, Muthu, *et al.*, 2011).

$$\mu = \frac{(E_{\text{HOMO}} + E_{\text{LUMO}})}{2} = -\chi \quad (4)$$

$$\eta = \frac{(E_{\text{LUMO}} + E_{\text{HOMO}})}{2} \quad (5)$$

$$S = \frac{1}{2\eta} \quad (6)$$

$$w = \left(\frac{\mu^2}{2\eta}\right) \quad (7)$$

$$\Delta N_{\text{max}} = \frac{-\mu}{\eta} \quad (8)$$

Amount of bipolar torque (in terms of Debye), electronic chemical potential (μ), chemical hardness (η), electrophilicity (w), electro-negativity (x) and chemical softness (s), amount of electron charge transition (ΔN_{max}), molecular orbitals energy gap ($E_{\text{HOMO}}-E_{\text{LUMO}}$ energy gaps), electron affinity (EA) and ionization energy (EI) are calculated in terms of electron volt by DFT/B3LYP method at B3LYP/6-31g* and the results are presented in table 11. Similarly (ΔN) quantity shows the amount of charge transition in the system. If ($\Delta N > 0$) and positive, it suggests the electron transition from nanotube (B) to intended molecule (A) and if ($\Delta N < 0$) and negative it suggests the electron transition from molecule (A) to nanotube (B). The amount of quantity (ΔN) (charge transition) in the system of mixture of methyl benzoate-boron nitride nanotube is 1.562 suggesting that electron flow is from BN nanotube to methyl benzoate.

Results from the calculations of B3LYP/6-31G* shows that energy gap in mixture of methyl benzoate –BN nanotube is decreased with regard to methyl benzoate. From one side, reactivity of a molecule is related to its energy gap (Sen and Jorgensen, 1987,

Table 11. Reaction indicators for Methyl Benzoate, Boron Nitride Nanotube and Methyl Benzoate - Boron Nitride Nanotube.

Property / B3LYP/6-31g*	Compounds				
	Methyl benzoate	BNNT	Methyl benzoate- BNNT	BQ- BNNT	Methyl benzoate- BQ
E_{HOMO} / (eV)	-1.18	-0.14	-1.38	-6.37	-6.97
E_{LUMO} / (eV)	-6.99	-6.38	-6.27	-0.15	-1.26
Energy gap (Eg) / (eV)	5.82	6.24	4.89	6.22	5.71
Ionization potential (EI) / (eV)	7.0	6.38	6.27	6.37	6.97
Electron affinity (EA) / (eV)	1.18	0.14	1.38	0.15	1.26
Electronegativity (χ) / (eV)	4.09	3.26	3.82	3.26	4.11
Global hardness (η) / (eV)	2.91	3.12	2.44	3.11	2.86
Chemical potential (μ) / (eV)	-4.09	-3.26	-3.82	-3.26	-4.11
Global electrophilicity (w) / (eV)	2.87	1.70	2.99	1.71	2.96
Chemical softness (S) / (eV ⁻¹)	0.17	0.16	0.20	0.16	0.17
Dipole Moment / (Debye)	1.86	0.02	3.83	0.32	4.29
ΔN_{max}	-	-	1.56	-	-

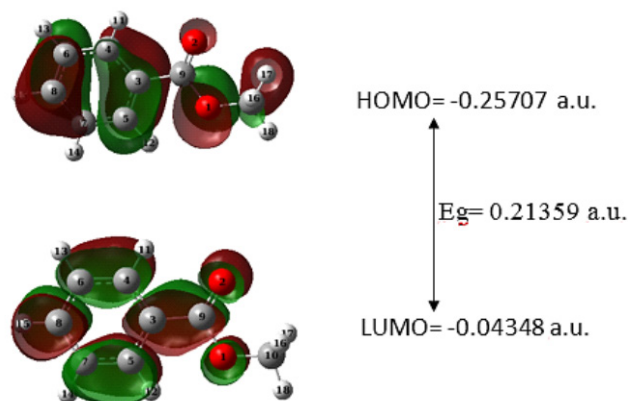


Fig. 3. Molecular orbital diagram of methyl benzoate

Gomez and Martinez-Magadan, 2005) (Figs. 3, 4). Similarly, in the mixture of methyl benzoate–BN nanotube as energy gap (EG) decreases the amount of hardness parameter decreases, softness increases and electrophilicity decreases. ELUMO-EHOMO Orbitals energy gap and chemical hardness shows that a soft molecule has a small energy gap and a hard molecule has great energy gap. Stabilizer orbital interactions increase by decrease of energy level of electron acceptor orbital and increase of energy level of electron donor orbital. In addition to electron non-stabilization is confirmed by change of population of donor and ac-

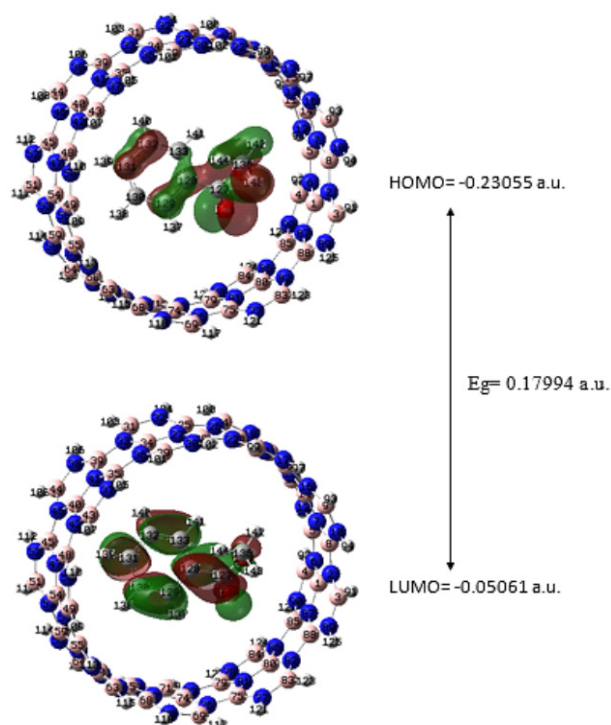


Fig. 4. Molecular orbital diagram of methyl benzoate - boron nitride nanotube

ceptor of electron.

Figs. 3 and 4 show the amount of energy gap of molecular orbitals HOMO and LUMO as well as DOS diagram. When examining the shape of molecular orbitals of methyl benzoate, one can see that HOMO orbitals are expanded on the entire structure of methyl benzoate yet LUMO orbitals are expanded on entire structure of methyl benzoate except methyl part. It is predicted that reaction is possible with electrophile types in the part with more HOMO orbitals distribution and possibility of reaction with nucleophile types exists in the part with more LUMO orbitals distribution (Chattaraj and Poddar, 1999, Pearson, *et al.*, 1999). At examining the shape of molecular orbitals of mixture of methyl benzoate-BN nanotube, it can be seen that the expansion of HOMO orbitals and LUMO orbitals on the methyl benzoate hasn't any great change.

CONCLUSIONS

In this research, boron nitride nanotube (9.9) with a length of 5 angstroms, which consists of 27 hexagonal loops, is chosen because the presence of BN polar bonds compared to non-polar C-C bonds makes this compound suitable for studying the absorption of other suitable compounds makes it. The results of quantum mechanical calculations at the B3LYP/6-31G* level of theory and NBO analysis, show structural, energetic, transcriptional and stereoelectronic interactions and the reactivity of methyl benzoate in the presence of a single wall B45N45H36 boron nitride. The results of the NBO calculations at the B3LYP/6-31G * level indicate that in the methyl benzoate mixture the energy is $E_g = 5.82$ eV and in the boron nitride nanotube equal to $E_g = 6.24$ eV and in the methyl benzoate-nanotube mixture of energy boron nitride $E_g = 4.89$ eV. The energy gap in the methyl benzoate-boron nitride nanotube compound in comparison to methyl benzoate has decreased in the absence of the nanotubes and the semiconducting property of the mixture has been strengthened in comparison with methyl benzoate and nanotube. Also, in the methyl benzoate-nanoparticle mixture of nitride, the boron decreases with decreasing E_g energy, the hardness parameter decreases, the softness parameter increases, and the electrophysicity

increases.

Abbreviations and notations

DFT, Density Functional Theory

HOMO, Highest Occupied Molecular Orbital

LUMO, Lowest Unoccupied Molecular Orbital

NBO, Natural Bond Orbital

BNNT, Boron Nitride Nanotube

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