Islamic Azad University

Journal of

Optoelectronical Nanostructures

Winter 2019 / Vol. 4, No. 1

Computational Investigation on Structural Properties of Carbon Nanotube Binding to Nucleotides According to the QM Methods

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(Received 16 Dec. 2018; Revised 26 Jan. 2019; Accepted 25 Feb. 2019; Published 15 Mar. 2019)

Abstract: The interaction between nucleotides and carbon nanotubes (CNTs) is a subject of many investigations for treating diseases but there are many questions in this field that remain unanswered. Because of experimental methods involve assumptions and interpretation besides limitations, there are many problems that the best study for them is using theoretical study. Consequently, theoretical methods have become a competitive alternative to experiments for biochemical investigations. In order to search about the response of SWCNTs in binding to DNA, the interaction between 3 different sequences of B-form single-strand DNA (ssDNA) and outer surface of single-walled carbon nanotubes (SWCNTs) is considered. So we studied the interaction between (5`-ATC-3`,5`-TCA-3`,5`-TCG-3`) and SWCNT by using Molecular Mechanic(MM) ,Hartree-Fock(HF) and Density Functional Theory(DFT,B3LYP) methods in gas phase. The basis sets used were STO-3G, 6–31G.In current interest, energy, dipole moment, total atomic charges and NMR parameters calculated to obtain information about the molecular structures and stability of these combinations. Our results revealed the effect of DNA base and the sequence of nucleotides on the interaction of DNA/SWCNTs systems. So, we can predict that diseases with special mutation are the better aim for Gene therapy. Therefore, the outcome reported in this paper indicates that theoretical data can give us essential insights into the nature of molecular structures interacted to nanotubes.

Keywords: Single Walled Carbon Nanotube (SWCNT), Density Functional Theory (DFT), Hartree-Fock (HF)

1. INTRODUCTION

A study of nanoparticles is a novel scientific technology especially because of its wonderful properties and unique applications .Nowadays scientists have been paid attention to the materials in the nanometer scale size range of different chemical composition to produce nanoparticles, nanowires or notubes. [1-3]Carbon nanotube (CNT) is a relatively new man-made material with fascinating atomic and electronic structures. Nanotubes are only described by the pair of integers (n, m) which is related to the chiral vector. The values of n and m determine the chirality of the nanotubes and affect the optical, mechanical and electronic properties. [4] So CNT has potential for many technological, mechanical, electrical and sensing applications. [5-10] Nano materials have been widely studied in the past decades [11]. SWCNTs has been considered as the leading candidate for nanodevice applications because of their one-dimensional electronic band structure, molecular size, biocompatibility and controllable property of electrical conductivity and reversible response to biochemical reagents. [12, 13]

The combination of CNTs with biological structures, such as DNA, is particularly intriguing since it opens the door to novel biotechnology and nanotechnology applications [14].Many unique properties of biological material with SWCNTs lead to exploring nanobiological research. Therefore, the interaction of bimolecules with SWCNTs has generated a great deal of interest over the past few years [15, 16]. SWCNTs and ssDNA could be interacting with different mechanism because they have complementary structural features, which make it possible to assemble them into a single [17].Recently literatures have shown that ssDNA binds to SWCNTs with covalent and non-covalent conjugations [18-20] but the details and the effect of these interactions have yet many questions [21]. ssDNA can be interact with outer surface of SWCNT, inserted into a SWCNT or interacted to open ends of SWCNTs [22–24].Molecular modeling by Zheng et al. suggested that DNA molecules hybridize with SWCNTs by wrapping around them, with the interaction strength being provided by Π-stacking (non-covalently binding), with the plane of the aromatic nucleotide bases oriented parallel to the surface of the SWCNTs. It has been indicated that DNA can be interact covalently with oxidizing open-ends of SWCNTs. [25,26] It remains to be seen that the strong interaction between DNA and CNT is depend on the base of DNA .

In this article, the interaction between different sequences of codons and the outer surface of the SWCNTs have been investigated. Energy, dipole moment and total atomic charge of this interaction have been reported .Since Nuclear magnetic

resonance can be used as a tool for structural analysis and it`s parameters are very sensitive to small changes in molecular geometry and chemical environment. So nuclear magnetic resonance as a major and a remarkable tool for investigating the variations of systems has been applied to obtain more information about these structures.

This study has been carried out using quantum mechanics (QM) method to increase the practical application of ssDNA/SWCNT system. We believe that this research could be used in nanotechnology as well as Gene therapy.

2. COMPUTATIONAL METHOD

In the present study, different sequences of B-form ssDNA include three nucleotides were linked to the outer surface of SWCNT .This combination has been modeled with Chem. Office and Hyper Chem.7 package.The quantum chemical calculations have been performed by using Gaussian 03 computational package [26] and based on the geometries optimization by the UFF method . Then Hartree-Fock (HF) theory and density functional theory methods (DFT) have been used [27-30].

DFT is based on a theorem due to Hohenberg and Kohn, which states that all ground state properties are functions of the total electronic charge density $\rho(r)$ [31-36]. There are several different DFT functional available differing primarily in the choice of the basis functions, in which, the electronic wave functions are expanded and the scheme of integration.

The Becke's three parameter exact exchange functional (B3) combined with gradient corrected correlation functional of Lee–Yang–Parr (LYP) have been employed to calculate energy, dipole moment, charge distribution and NMR parameters by implementing the 6-31G,STO-3G basis sets. All the NMR shielding parameters were calculated supposing gauge-included atomic orbital (GIAO) method.

NMR spectroscopy is a research technique that exploits the magnetic properties of certain atomic nuclei to determine physical and chemical properties of atoms or the molecules in which they are contained. It relies on the phenomenon of nuclear magnetic resonance and can provide detailed information about the structure, dynamics, reaction state, and chemical environment of molecules. Ab initio calculation of nuclear magnetic shielding has become an indispensable aid

in the analysis of molecular structure and accurate assignment of NMR spectra of compounds.

NMR is based on the quantum mechanical property of nuclei. The chemical shielding refers to the phenomenon, which is associated with the secondary magnetic field created by the induced motions of the electrons that surrounding the nuclei when in the presence of an applied magnetic field. The energy, in a magnetic field, B, is as follow:

$$E = -\mu \cdot (1 - \sigma)\, B \tag{1}$$

Where the shielding σ is the differential resonance shift due to the induced motion of the electrons. [30] In general, the electron distribution around a nucleus in a molecule is more spherically symmetric. Therefore, the size of electron current around the field, and hence the size of the shielding, will depend on the orientation of the molecule within the applied field B_0.

For chemical shielding (CS) tensor, which describes how the size of shielding varies with molecular orientation, the following convention can be used for the three principle components, if:

$$|\sigma 11 - \sigma iso| \leq |\sigma 33 - \sigma iso| \tag{2}$$

The three values of the shielding tensor are frequently expressed as the isotropic value (σ_{iso}), the anisotropic value (σ_{aniso}), and the asymmetry parameter (η) .There quantities are defined as follows:

The isotropic value σ_{iso}:

$$\sigma iso = \frac{(\sigma 11 + \sigma 22 + \sigma 33)}{3} \tag{3}$$

The chemical shielding (Δσ):

$$\Delta\sigma = \sigma 33 - \frac{(\sigma 11 + \sigma 22)}{2} \tag{4}$$

The asymmetry parameter (η):

$$\eta = \frac{|\sigma 22 - \sigma 11|}{|\sigma 33 - \sigma iso|} \tag{5}$$

And if the following relation exists between the three principle parameters:

$$|\sigma 11 - \sigma iso| \geq |\sigma 33 - \sigma iso| \quad (6)$$

We have chemical shielding ($\Delta\sigma$) and the asymmetry parameter (η) as follows:

$$\Delta\sigma = \sigma 11 - \frac{(\sigma 33 + \sigma 22)}{2} \quad (7)$$

And

$$\eta = \frac{|\sigma 22 - \sigma 33|}{|\sigma 11 - \sigma iso|} \quad (8)$$

And the other NMR parameter δ is obtained by equation 9 and 10 sequentially for the first and second conditions that are mentioned above:

$$\delta = \sigma 33 - \sigma iso \quad (9)$$

$$\delta = \sigma 11 - \sigma iso \quad (10)$$

Calculations of nucleus-dependent and -independent chemical shifts were carried out using the gauge-invariant atomic orbital (GIAO) approach. [37, 38]
Moreover, the calculations were performed at two levels of theory to obtain the more accurate equilibrium geometrical parameters and data of energy, dipole moment and atomic charge for each of the determined structure.

3. RESULTS AND DISCUSSION:

Many investigations have been carried out on ssDNA interaction with SWCNTs whereas interaction quality for practical area is important. In this article, different sequences of B-form ssDNA include three nucleotides were linked to outer surface of SWCNT to develop practical application of ssDNA interaction with SWCNTs. We modeled 5'….ATC…3', 5'…TCA…3' and 5'…TCG…3' of DNA and coupled them with SWCNTs. These coupling have been performed between NH2 groups of nucleotide A in ATC sequence of DNA, nucleotide T in TCA sequence of DNA, nucleotide T in TCG sequence of DNA and C atom in CNT. In figure 1 the interactions between the sequences of ssDNA atoms (ATC, TCG and TCA) with outer surface of SWCNT have been displayed.

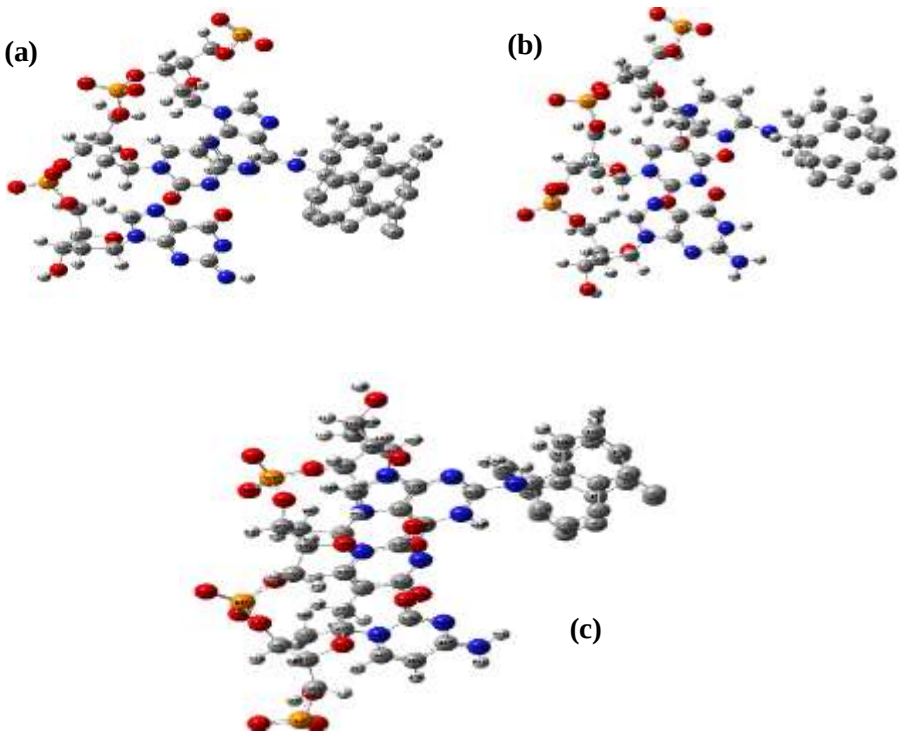


Fig1. Optimized structure of **a)** ATC **b)** TCA **c)** TCG linking to SWCNTs. Grey for carbon, blue for nitrogen, red for oxygen, white for hydrogen and orange for phosphorus.

To demonstrate the characteristics of these interactions, the calculated physical properties have been investigated in gas phase which are important in molecular properties. Energy and dipole moment of these structures which were performed at the HF, B3LYP levels with the STO-3G, 6-31G basis sets are reported in table1. According to Table 1, the smallest value of energy is related to the coupling of ATC/SWCNT and the largest value is connected to TCA/SWCNT combination. So ATC/SWCNT is the most stable combination and has the most dipole moment. There aren`t different values of energy in each combination with changing methods.

Table1.Theoretically values of total E (kcal) and dipole moment (Debye) caused by interaction of ATC, TCA and TCG with outer surface of SWCNT in gas phase.

Method	**HF**		**B3LYP**	
Basis	**STO-3G**		**STO-3G**	
set	**6-31G**		**6-31G**	
Atom	**E**	**μ**	**E**	**μ**
ATC	-3132365	50.8545	-3172342	20.6370
	-3163681	60.6242	-3124579	32.0136
TCA	-3057663	42.0945	-3097021	11.6462
	-3038062	51.1643	-3075803	25.2766
TCG	-3013640	30.0943	-3083086	10.9478
	-3010519	27.5470	-3052696	21.4806

The total atomic charges (a. u.) of various atoms from different regions of codons binding to SWCNTs calculated with HF and B3LYP methods using STO-3G and 6-31G basis sets in gas phase. Among all the atoms of ATC in the equilibrium binding to SWCNT 19 atoms of different types has been selected from different regions of ATC/SWCNT. The number of selected random atoms in TCA in binding to SWCNT was 19 and about the TCG binding to SWCNT was 18 atoms. In the first system (ATC in the binding to SWCNT) P_{58} and P_{77} show the maximum charge changes between all selected atoms from different regions of ATC/SWCNT and atoms specified by N_{49}, N_{54}, O_{59}, N_{71}, O_{83},O_{98}, N_{128} showed the negative charges because they have high electron affinity. In addition to these atoms, C_{19} compare to the other C atoms in this system show relatively more negative charge. It should be noted that C_{19} is in interaction place between codon and SWCNT. (FIG.2a)

In figure (2b) the same situation has been seen about TCA binding to SWCNT. It means that P_{88} show the maximum charge changes among the selected atoms and O_{31}, O_{33}, N_{42}, N_{49}, N_{69} show more negative charges .Also Interacted atoms of SWCNT show a little different charge distribution. The Carbon atom (C_1, C_2, C_3,

C_4, C_{12}, C_{13}) in the TCA /SWCNT system have different charge distribution in comparable with C atoms in the other part of the system (C_{43}, C_{48}).

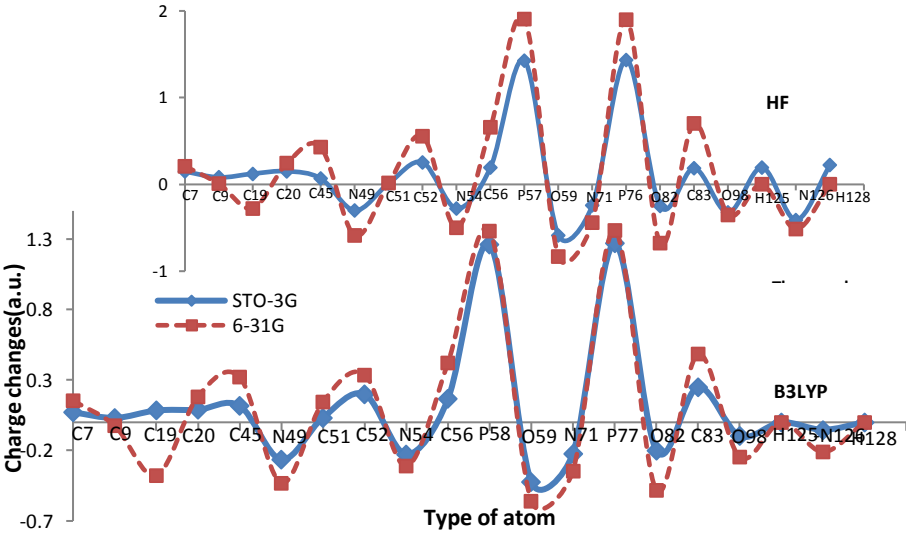
The results of TCG binding to SWCNT are in agreement with the conclusion of the last two considered systems. According to figure (2c) P_{32} and P_{60} in TCG binding to SWCNT show maximum charge changes and O_{32}, O_{39}, O_{62}, O_{83}, N_{85}, O_{110}, N_{111}, N_{121} show more negative charges too. It is interesting to point out that interacted atoms of TCG/SWCNT (C_5,C_{10}) exhibited particularly different charge distribution in contrast to carbon in the other parts of TCG/SWCNT (C_{68}, C_{80}, C_{109}, C_{112}).

The results of the total charge for these systems are accord with the electronegativity of the atoms; although the NMR parameters can help to search about the effect of the other atoms in the systems on the charge of atoms. Attention to figures2 (a, b, c) indicate that HF and B3LYP in STO-3G and 6-31G follow the same results and agree with each other.

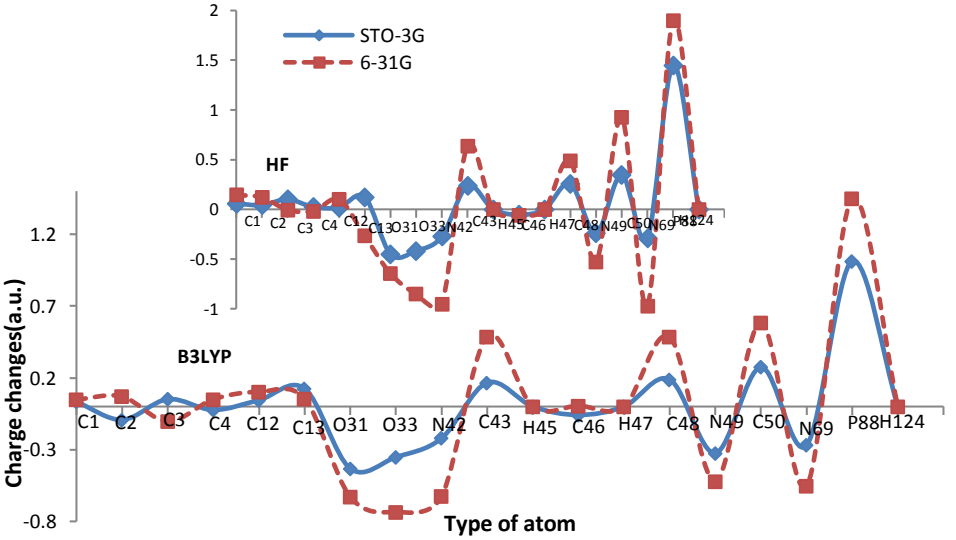
The calculated data of NMR shifts with the magnetic field perturbation method of GIAO (gauge in dependent atomic orbital) was the isotropic chemical shielding (σ_{iso}), asymmetry parameter (η), chemical shielding ($\Delta\ \sigma$) and δ for selected atoms of different regions of the structures ATC ,TCA and TCG binding to SWCNTs that are sequentially summarized in Table 2, 3 and 4. The maximum value of all calculated magnetic shielding included σ_{aniso} for selected atoms of ATC with SWCNT was investigated by O_{59}. (fig.3a). The largest value of σ_{aniso} of mentioned atoms of TCA/SWCNT combination was observed for O_{31}.(fig.3b) In another sequences of nucleotide TCG in binding to SWCNT, the maximum value of similar parameters belongs to N_{85}. (fig.3c).

Now the results of this study show that different atoms in each structure (O_{59} in ATC/SWCNT, O_{33} in TCA/SWCNT, and N_{85} in TCG/SWCNT combinations) have maximum value in all calculated NMR parameters. It's obvious that the sequence of nucleotides effect on the properties of the DNA/SWCNT combination.

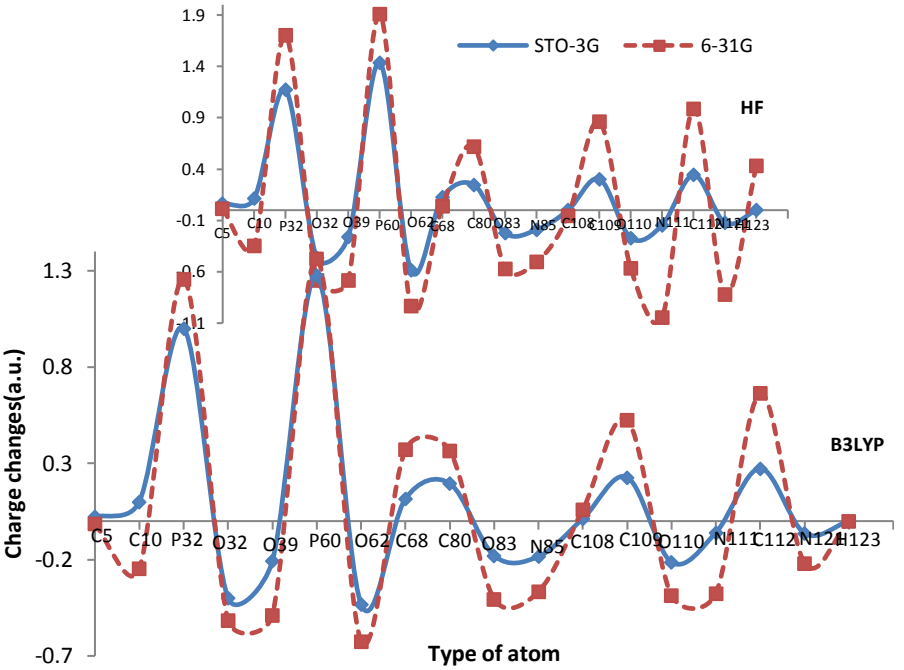
It should be noted that the results of calculation with HF and B3LYP in STO-3G and 6-31G follow the same process and indicate the consistency between these calculation methods.


HF
B3LYP
STO-3G
6-31G
Charge changes(a.u.)
Type of atom

(a)


HF
B3LYP
STO-3G
6-31G
Charge changes(a.u.)
Type of atom

(b)



(c)

Fig 2c. Total atomic charges (a .u.)diagram of propose atoms of a) ATC ,b) TCA ,c)TCG binding to SWCNTs calculated by HF and B3LYP method using 6-31G and STO-3G basis sets in gas phase.

Table 2. NMR parameters of ATC/SWCNT in gas phases at HF and B3LYP level with the STO-3G and 6-31G basis sets in GIAO methods.

Method	**B3LYP**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**$\Delta\sigma$**	**δ**	**η**
C4	128.837	-196.886	-131.257	0.561813
	-20.002	-393.258	-262.172	0.420848
C6	125.462	-122.994	-81.9961	0.647884
	57.1847	136.920	91.2802	0.671804
C18	183.685	-39.7888	-26.5253	0.505022
	147.318	-73.7091	-49.1394	0.975742
C19	146.693	-115.803	-77.2021	0.488676
	108.119	-142.689	-95.1262	0.659509
C45	168.887	-28.6097	-19.0725	0.810107
	119.566	-22.3274	-14.8846	1.802916
N49	81.9486	-341.858	-227.906	0.894921
	15.5818	342.961	228.647	0.740052
C51	132.718	98.2489	65.4998	0.325993
	75.8573	98.0072	65.3389	0.951354
C52	112.782	-104.217	-69.4787	0.863645
	46.3534	-123.665	-82.4435	0.703866
N54	55.1953	416.514	277.671	0.078127
	-32.620	439.504	293.002	0.487468
C56	112.411	104.782	69.8543	0.722939
	48.4923	133.989	89.3264	0.305620
P58	494.330	-86.3671	-57.5781	0.854181
	391.966	343.967	229.312	0.220252
O59	995.740	5487.43	3658.23	0.966643
	-1530.5	-5214.34	-3476.1	0.976094
	391.811	429.844	286.564	0.417355

N71	-29.115	-1161.59	-774.396	0.964365
P77	489.287	-49.6504	-62.0471	0.090436
	398.714	350.319	233.542	0.309987
O82	282.996	-111.215	-74.1434	0.758428
	207.078	-173.720	-115.812	0.701739
C83	152.386	-54.7024	-36.4685	0.45172`
	108.979	-74.0223	-49.3485	0.44761
O98	318.166	81.9417	54.6271	0.294022
	259.745	-93.3739	-62.2492	0.512225
H120	33.7187	18.50452	12.3363	0.309892
	32.9045	16.47065	10.9804	0.605554
N122	273.991	250.252	166.831	0.555311
	202.527	358.744	239.162	0.690392
H128	31.1339	-21.8076	-14.534	0.089533
	28.7655	-18.4165	-12.276	0.788234

Method	**HF**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**Δσ**	**δ**	**η**
C4	75.9231	-132.704	-101.842	0.705566
	11.6430	-238.718	-259.172	0.242009
C6	88.6495	179.085	139.857	0.296250
	-10.210	-275.257	-228.982	0.547984
C18	103.017	52.0172	28.7248	0.524021
	126.057	29.6480	19.7787	0.895332
C19	125.181	-176.955	-93.967	0.554527
	90.2769	-128.445	-100.67	0.535044
C45	121.021	-52.7474	-21.8316	0.800962
	142.491	74.5599	46.7066	0.864630
N49	77.0912	297.052	244.701	0.835772

	36.3907	288.693	149.128	0.769049
C51	119.503	153.621	50.4142	0.119175
	68.0865	126.134	78.0893	0.301495
C52	117.526	-84.531	-66.3541	0.851410
	44.2493	-173.73	-110.492	0.691434
N54	99.9283	363.560	257.707	0.367887
	-29.115	448.957	299.305	0.549275
C56	198.205	135.083	90.0555	0.795844
	146.196	175.010	116.734	0.547869
P58	2766.63	1697.01	4822.61	0.083853
	109.629	237.463	171.702	0.220352
O59	-7689.3	-39568.0	-25612.6	0.982422
	241.068	-829.583	-468.599	0.902650
N71	-5.7632	-351.412	-367.621	0.346093
	-72.446	-566.719	-377.812	0.704842
P77	151.325	-139.576	-93.0508	0.662895
	102.462	248.798	165.865	0.232890
O82	334.074	-106.198	-70.7919	0.333150
	204.007	-154.797	-103.191	0.209504
C83	125.703	-53.5478	-35.6986	0.861364
	48.4923	-52.6846	-35.1231	0.758693
O98	327.849	61.8966	41.2644	0.317941
	287.485	99.0946	66.0641	0.286973
H120	35.4372	19.5795	13.0531	0.272895
	33.0803	19.4168	12.9445	0.306647
N122	321.551	279.085	186.056	0.089338
	139.826	256.370	170.913	0.254200
H127	33.123	-24.1338	-16.0892	0.566553
	33.9357	-24.2761	-16.1841	0.296989

Table 3. NMR parameters of TCA/SWCNT in gas phases at HF and B3LYP levels with the STO-3G and 6-31G basis sets in GIAO methods.

Method	**B3LYP**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**Δσ**	**δ**	**η**
	237.157	293.017	205.624	1.547530
C1	230.981	136.104	221.547	1.135420
	181.753	-257.726	-247.609	1094939
C2	240.321	142.659	321.647	1.68356
	125.433	-235.091	-146.350	0.903645
C3	149.687	147.463	123.157	0 794106
	35.658	-130.678	-137.125	1.974180
C4	83.709	141.647	14.8461	1.095109
	24.610	-317.346	-231.390	0.531876
C12	87.942	135.125	160.637	0753273
	32.649	-123.903	-238.180	1.690474
C13	47.394	108.275	235.127	1.903787
	708.34	109.543	1772.15	0.850791
O31	457.92	208.905	1099.27	0.549823
	315.131	120.016	126.895	0.950405
O33	219.763	131.570	153.043	0.439806
	632.571	209.840	146.747	0.539605
N42	490.725	137.560	123.270	0.795463
	326.531	230.277	145.439	0.476908
C43	237.578	257.426	234.612	0.874304
	71.9476	-19.162	56.1270	1.639093
H45	78.7508	29.371	30.6129	1.548953
	230.176	-128.34	-65.122	0.909126
C46	148.942	567.136	17.4857	0.548652
H47	517.307	14.3791	109.645	0.743062

	256.136	19.3611	34.1297	0.549827
	163.173	-189.942	-169.21	1.097561
C48	183.942	106.435	129.322	1.892189
	133.953	215.317	136.890	0.908110
N49	169.194	245.038	204.575	0.860148
	901.849	-164.241	-166.504	0.649737
C50	748.153	143.570	205.208	0.857393
	32.0172	-235.094	-129.857	1.83125
N69	81.4314	128.845	145.063	1.84309
	128.577	-248.125	-20.973	0.23580
P88	72.5893	542.812	136.201	0.65678
	129.346	-104.1953	-90.413	1.51004
H124	147.420	18.7021	35.0649	1.48174

Method	**HF**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**$\Delta\sigma$**	**δ**	**η**
	-388.163	-247.751	-15.812	1.871593
C1	-34.5345	361.529	23.601	1.983872
	-26.7031	784.909	54.036	2.984525
C2	86.4563	-54.694	-19.094	2.348552
	325.015	34.0862	53.785	0.896452
C3	27.6308	91.1071	871.464	0.235665
	265.046	37.2081	35.895	1.213436
C4	98.3842	-98.963	-53.057	1.432788
	184.436	83.108	195.492	0.876405
C12	98.3944	-320.81	-231.241	0.208371

	163.067	93.516	92.954	2.652105
C13	951.065	126.067	18.571	2.409131
	-96.8049	-274.98	-241.260	0.430178
O31	137.207	-235.16	-353.675	1.954019
	189.134	-271.30	76.9027	1.185016
O33	304.065	-246.41	190.918	0.439617
	38.4827	-64.781	-43.087	1.905239
N42	119.507	96.382	74.468	0.438690
	39.8907	72.039	625.12	0.598012
C43	50.9474	98.320	84.903	0.380945
	10.6131	-86.135	-163.98	0.904831
H45	74.0994	-102.42	-37.942	0.241796
	720.573	-95.305	-275.78	0.734954
C46	65.1502	-78.174	-285.46	0.053239
	138.431	38.460	342.657	1.953012
H47	187.252	15.547	6 5.041	1.953027
	35.2575	94.832	97.0546	2.184502
C48	176.154	38.265	46.8353	2.094304
	234.081	57.5961	190.942	0.976302
N49	132.280	27.8299	73.8527	0.390225
	236.865	-98.701	-234.845	1.984023
C50	382.343	-13.646	-193.159	1.840528
	162.606	-54.932	-436.041	0.160427
N69	137.098	-19.948	-461.379	1.690434
	198.290	237.92	1099.68	0.579745
P88	279.587	97.213	191.469	0.082999
	157.1094	181.347	74.2561	0.406745
H124	180.1749	-102.90	-8.63415	1.299037

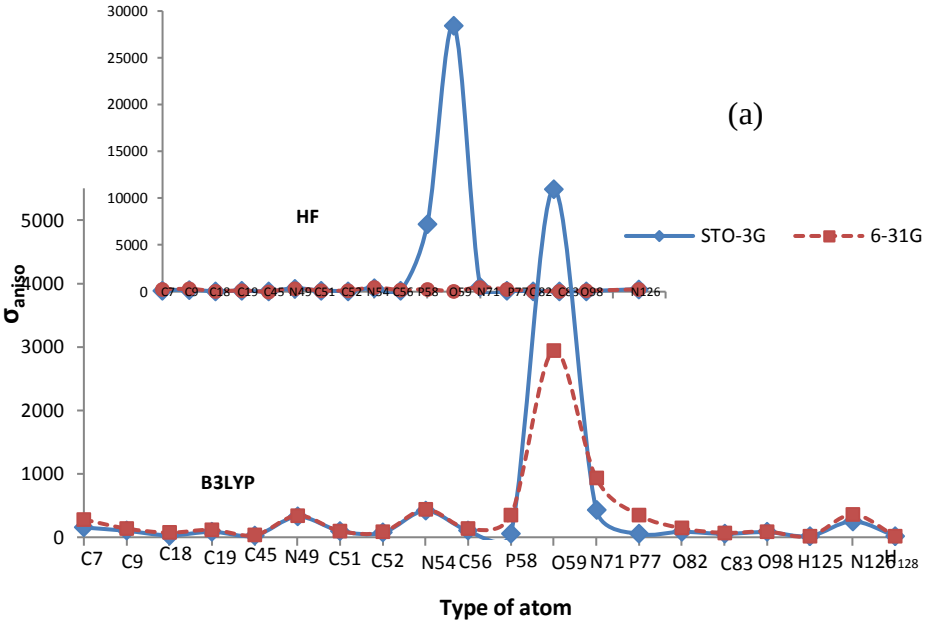
Table 4. NMR parameters of TCG/SWCNT in gas phases at HF and B3LYP levels with the STO-3G and 6-31G basis sets in GIAO methods.

Method	**HF**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**Δσ**	**δ**	**η**
	-98.5732	48.0657	-1367.77	-0.23784
C5	-287.626	431.521	-1324.19	0.19062
	503.753	168.065	-21.105	-0.0346
C10	153.209	214.203	-983.04	0.4382
	-875.98	312.817	-4389.06	-0.59091
P32	142.645	-759.901	-623.602	0.45186
	-187.105	-267.116	-2634.23	0.34794
O32	-258.443	-549.613	-248.575	0.79412
	437.507	163.784	34.0245	0.90416
O39	154.967	-253.790	-248.605	0.95040
	92.7435	318.540	-315.911	-0.59318
P60	25.0927	-412.104	-901.458	0.78041
	168.190	431.812	2314.50	-0.31613
O62	322.569	130.215	234.850	0.29071
	267.376	325.573	24.5238	0.28041
C68	142.022	94.0429	42.7303	0.78907
	-146.034	218.461	-3205.15	-0.65461
C80	-19.5273	150.942	217.701	0.90644
O83	-190.31	875.051	-3624.0	-0.04980
	-32.293	-124.503	-537.13	0.95841
	15250.5	2165.41	38759.2	1.39607
N85	-932.310	3102.50	23954.3	1.45341
C108	61.4326	216.540	-284.079	-0.94863

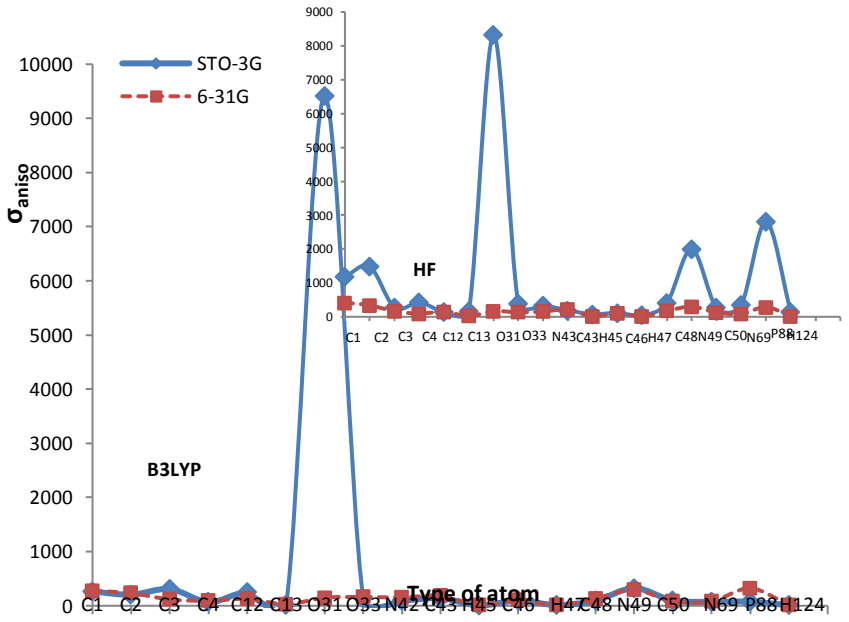
	40.8940	312.847	84.9578	0.98045
	153.838	188.289	-2064.16	-0.6452
C109	151.903	-238.987	-274.698	0.24583
	-661.930	490.85	3176.94	-0.35723
O110	-52.7696	389.42	695.285	0.64307
	165.079	152.749	-2845.47	-0.29647
N111	216.510	268.05	-151.230	0.45981
	-897.319	804.943	-2043.92	-0.57904
C112	49.6929	602.368	-235.671	0.46987
	197.281	542.093	950.482	0.48934
N121	101.833	482.098	351.642	0.93052
	34.3942	94.5904	34.5293	-0.64721
H123	76.8213	59.1986	96.5309	0.97246

Method	**B3LYP**			
Basis set	**STO-3G**			
	6-31G			
Atoms	**σ_{iso}**	**Δσ**	**δ**	**η**
	83.6867	-105.328	214.146	0.54675
C5	58.5916	-379.016	-329.756	0.32689
	170.331	-164.981	-52.3467	0.62088
C10	190.265	38.0164	77.2951	0.68571
	324.816	292.601	211.043	0.53118
P32	341.124	-142.132	-124.753	0.15878
	-162.52	152.214	247.501	0.85430
O32	-214.54	204.574	353.721	0.25775
	345.647	-232.193	-241.342	0.26447
O39	236.770	-153.742	211.153	0.90510

	275.411	-125.123	-54.632	0.36721
P60	321.756	421.568	132.421	0.54827
	12.0355	259.97	250.314	0.38965
O62	-1496.8	-573.06	-129.609	0.42812
	205.153	93.530	69.0977	0.37243
C68	232.985	-64.899	-95.7124	0.53166
	35.0894	-294.012	-87.8718	0.75401
C80	-79.184	-235.946	-153.810	0.76353
	-678.28	-310.84	-1379.17	0.47617
O83	-84.361	-125.17	-856.902	0.45293
	1187.54	-1789.86	1763.21	1.39604
N85	6361.2	-2304.60	13495.0	1.41031
	138.830	90.7985	78.6701	0.25383
C108	39.8532	-174.232	-98.2148	0.43108
	251.874	-236.651	107.356	0.74297
C109	36.6928	-207.095	-150.523	0.32594
	-197.64	-329.293	-639.675	0.43812
O110	-326.85	-216.74	-659.964	0.24643
	145.573	-75.6487	-79.9068	0.43801
N111	125.262	-205.437	-85.2381	0.32604
	237.573	-93.4395	-67.5698	0.45903
C112	95.8514	-258.143	-246.706	0.47936
	149.103	-239.253	-79.5436	0.35891
N121	89.0952	131.467	210.697	0.30483
	99.0563	-78.0643	-83.3462	0.45782
H123	78.4046	78.9025	25.1510	0.49208


(a)
HF
B3LYP
STO-3G
6-31G
σaniso
Type of atom
C7 C9 C18 C19 C45 N49 C51 C52 N54 C56 P58 O59 N71 P77 O82 C83 O98 H125 N126 H128

(b)


STO-3G
6-31G
HF
B3LYP
σaniso
Type of atom
C1 C2 C3 C4 C12 C13 O31 O33 N43 C43 H45 C46 H47 C48 N49 C50 N69 P88 H124

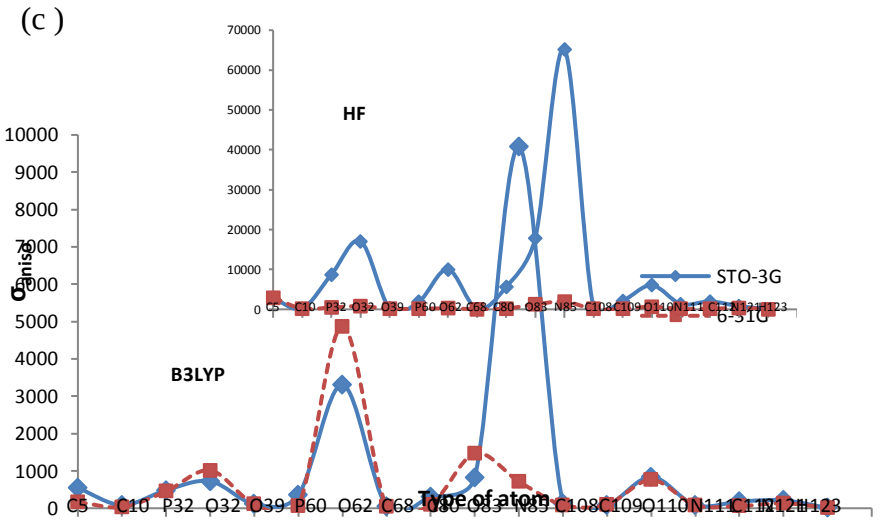


Fig. 3. The graphs of anisotropic shielding values(σ_{aniso}) of propose atoms of a)ATC binding to SWCNTs, b)TCA binding to SWCNTs, c)TCG binding to SWCNTs in gas phases at the HF,B3LYP levels with the STO-3G,6-31G basis sets in GIAO method.

4. CONCLUSION

The results reported in this article indicate that it is possible to estimate the stability of different relevant molecular structures of DNA binding to SWCNTs according to obtained relative energy values and thermodynamic properties. The system of ATC/SWCNT is more stable than TCA/SWCNT and TCA is more stable than TCG/SWCNT.

The largest values of NMR data that is shown with σ_{iso},σ_{aniso},$\Delta\sigma$,δ,η for mentioned atoms of ATC/SWCNT observed for O_{59} , Whereas the largest one in TCA and TCG coupled with SWCNT sequentially belong to O_{31} and N_{85} .So, The calculated parameters of nuclear magnetic resonance (NMR) provides information about the local environment of selected atoms and their nearest neighbors and show these atoms as an active sites.

In addition, we have shown that theoretical calculations can be used to successfully explain charge distributions in these biological systems. Among the

different atoms of ATC linking to SWCNT, only the atomic charge of P_{58} and P_{77} have maximum changes. Our investigations show that maximum values of total atomic charge specified by P_{88} for TCA and $P_{32,}$ P_{60} for TCG in binding with SWCNTs. Also the total atomic charges of the other atoms are in accord with the conceptions of electron affinity and the influence of the environmental factors.
It is noticeable that our obtained theoretical results indicate the consistency between used calculation methods and basis sets.
Finally this investigation confirms that the theoretical calculation is quite useful for predicting the stability of indicated structures and show active sites of the system and molecular structures of these compounds.

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