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A DFT study on the NMR and NQR chemical shifts of molecules confined in boron nitride nanotubes

Ashraf Sadat Ghasemi[1, *], Alireza Soltani[1], Mobin Molla[2]

[1]Dept. Chemistry, Payame Noor University, P.O. Box, 19395-3697, Tehran, Iran
[2]Department of Petroleum Engineering, Research, Sciences, Islamic Azad University, Tehran, Iran

Email address
Ashraf.Ghasemi@gmail.com (A. S. Ghasemi)

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Abstract
We performed a computational study to calculate the quadrupole coupling constants(C_Q) and isotropic and anisotropic chemical shielding (CS_I and CS_A) parameters in the aluminum doped (Al-doped) single-walled boron nitride nanotube (BNNT) based on the density functional theory (DFT) calculations. The adsorption behavior of the SCN and NCS adsorbed on the external surface of H-capped (6,0) zigzag (Al-doped, BNNT) as a functional group, calculated for the optimized structures, was also studied by using DFT calculations. Geometry optimizations were carried out at the B3LYP/6-31G* level. Comparison with the available data on the pristine Al-BNNT reveals the influence of (Al-BNNT) on the C_Q, CS_I and CS_A parameters of 11-B, 14-N and 15-N atoms in the Al-BNNT structures. For most lattice sites, the magnitude of influence on the C_Q, CS_I and CS_A parameters of the Al-NCS is larger than that of the Al-SCN adsorbed on the external surface of H-capped (6,0) zigzag (Al-doped, BNNT). Similar values of the C_Q, CS_I and CS_A parameters of 27-Al atoms are obtained for zigzag Al-BNNT when the same element is replaced with Al, but the C_Q, CS_I and CS_A parameters are larger for Al when it forms a B-Al-NCS bond than when it forms a B-Al-SCN bond.

1. Introduction

Single-walled carbon nanotubes (SWCNTs), synthesized by Ijima in 1991 [1,2], carbon nanotubes (CNTs) have attracted great interest owing to their extraordinary structural, mechanical, chemical, physical, and electronic properties [3,4,5,6]. In 1981, Ishii et al. Reported on a discovery of one-dimensional BN nano structures, which possess bamboo-like structure. These were named BN whiskers [7]. However, the nano scaled BN with a perfect tubular structure was firstly theoretically predicted only in 1994 [8, 9] and then experimentally synthesized by arc-discharge in 1995 [10]. Moreover, these studies have The determination of the electronic and structural properties of NCS and SCN / (Al-doped, BNNT). This complex is also important for understanding its bonding and reactivity in catalysis and other surface phenomena, nuclear magnetic resonance (NMR) including CS_I and CS_A parameters [11,12] and nuclear quadrupole resonance (NQR) including CQ [13]. Spectroscopy is the best techniques to study the electronic structure properties of materials by quantum calculations [14,15,16,17], could be well reproduced by density functional theory (DFT) calculations [18, 19]. At first, the NCS and SCN structures have been allowed to relax by all atomic geometrical optimization. Subsequently, the isotropic and anisotropic chemical shielding (CS_I and CS_A) parameters have been calculated for the 11-B, 15-N,

and NQR calculations at the sites of 11-B, 14-N atoms structures. However, the influence of the NCS and SCN on the electronic structure of the (6, 0) zigzag (Al-doped, BNNT) has rarely been studied. By performing density functional theory (DFT) calculations, this computational work has investigated the properties of the electronic structure of the NCS and SCN / (Al-doped, BNNT), including bond lengths, bond angles, dipole moments (μ), energies, band gaps, NMR and NQR parameters which have been listed in Tables 1–3. To this end, both representative models of (6, 0) zigzag (Al-doped, BNNT) (Figs. 1and 2) have been investigated.

C_Q parameters of the 27-Al atom and the magnitudes of calculating values of C_Q (27-Al) in the same positions in the zigzag model is almost the same. When 11-B is doped by 27-Al, the C_Q value of 27-Al is about 26MHz whereas when14-N is doped with Al, this value is increased to 43MHz. The magnitudes of these values for the C_Q of 27-Al in the two situations of Al-doping reveal that the strength of SCN-Al–B bond is more than that of NCS-Al–B bond in the (6, 0) zigzag BNNT (Al-doped), SCN-Al-BNNT, NCS-Al-BNNT. This trend is proven by referring to the difference of electro negativities between S/Al/B and N/Al/B in which the magnitude of this difference is larger for S/Al/B; therefore, stronger SCN-Al–B bond rather than NCS-Al–B bond is expected [20].

2. Computational Aspects

All DFT calculations are performed using the Gaussian98 package [18]. In the present work, the electronic structure, properties and adsorption behavior of NCS and SCN on the (6, 0) Zigzag single walled (Al-doped, BNNT) with a length of 7.1 A ° and 4.7 diameter was used. Due to the absence of periodic boundary conditions in molecular calculations, The SCN-Al- BNNT (6,0) zigzag model (Fig. a) and The NCS -Al- BNNT (6,0) zigzag model (Fig. b) consisted of 24 B and 23 N atoms in (Al-doped, BNNT that the two the ends of the nanotube is saturated by 12 hydrogen atoms. The geometries of the considered (Al-doped, BNNT) was optimized at the B3LYP/6- 31G* level of theory. Subsequently, the 11-B, 14-N, 27-Al and 15-N C_Q, CS_I and CS_A tensors have been calculated for the optimized structures at the same level of the theory based on the gauge included atomic orbital (GIAO) approach [19]. The NMR parameters of 11-B and 15-N nuclei for the investigated model of the (6,0) zigzag single-walled SCN -Al- BNNT and NCS-Al- BNNT are summarized in Table 1,2. Since quantum chemical calculations yield the CS tensors in the principal axes system (PAS) ($\sigma_{33}>\sigma_{22}>\sigma_{11}$) they have been converted to CS_I, CS_A uses Eqs. 1 and 2, respectively.

$$CS_I\,(ppm) = \frac{1}{3}(\sigma_{11}+\sigma_{22}+\sigma_{33})$$

$$CS_A\,(ppm) = \sigma_{33} - \frac{1}{2}(\sigma_{11}+\sigma_{22})$$

The NQR parameters of 11-B nuclei for the investigated models of the (6,0) zigzag single-walled SCN -Al- BNNT and NCS-Al- BNNT are summarized in Table 3. C_Q is the interaction energy of the nuclear electric quadrupole moment (eQ) with EFG tensors at the sites of quadrupole nuclei, but the asymmetry parameter (η_Q) is a quantity of the EFG tensors that describes the deviation from tubular symmetry at the sites of quadrupole nuclei. Nuclei with $I > \frac{1}{2}$ (where I is the nuclear spin angular momentum) are active in NQR spectroscopy [21].

$$C_Q\,(MHz) = e^2 Q q_{zz} h^{-1}$$

$$\eta_Q = \left|\left(q_{xx} - q_{yy}\right)/q_{zz}\right|$$

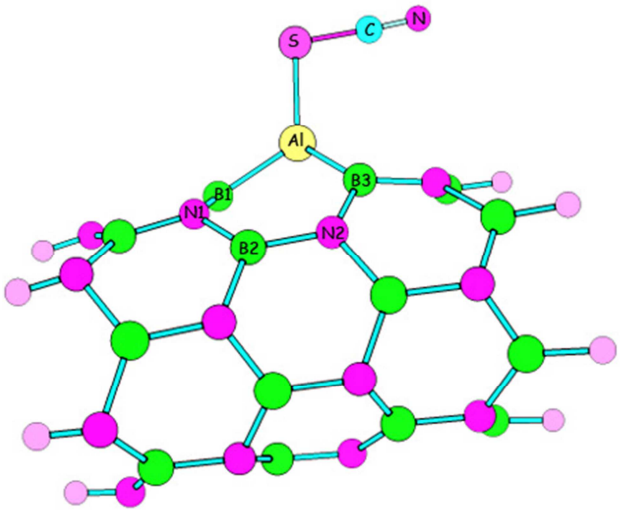
$$0 < \eta_Q < 1$$

3. Results and Discussion

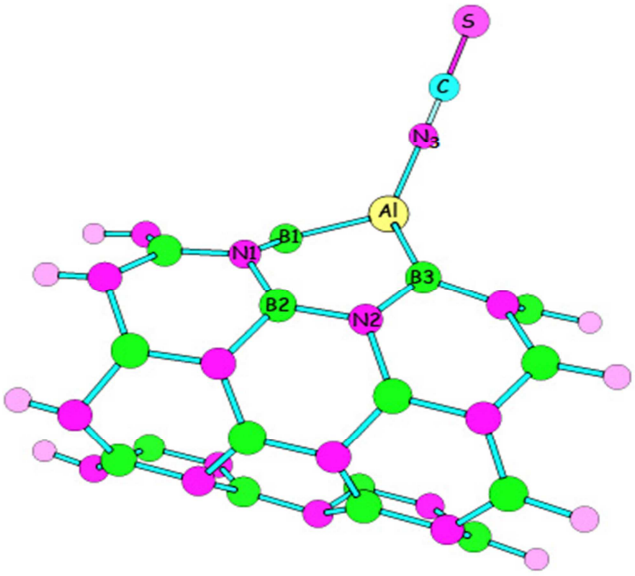
3.1. Structures of the Al-BNNT

The structural properties, consisting of the Al-B, B–N bond lengths, bond angles, dipole moments (μ), energies, and energy gaps for the investigated models of the (6, 0) zigzag Al-BNNT, are summarized in Table 1. There are two forms of SCN-Al- BNNT and NCS-Al- BNNT for the (6,0) zigzag model, namely with the SCN molecules adsorbs at an AL-B–N bond site (Fig.1 a) and the NCS molecules adsorb at a Al-B–N bond site (Fig.1 b). There is B–N bonds in the SCN -Al- BNNT and NCS-Al- BNNT complexes. In Fig. 1 c, the atoms of the Al-BNNT are numbered in order to describe the relevant structural parameters. The calculated Results showed that the average B–N bond lengths are almost the same in the investigated (6, 0) zigzag SCN-Al- BNNT and NCS -Al-BNNT complexes, respectively. In Fig. 1. a and b, the S–Al-B and N3–Al-B, bond lengths are the largest among the investigated (6, 0) zigzag Al-BNNT model. Compared with the pristine model, the Al atom relaxes out of the nanotube surface in Fig.1. a and b. The distances between the 27-Al atom and the S, N3 and B atoms in Fig. 1. a and b are 1.780 and 2.330 Å, respectively (Table 1). The S–Al–B_1 and S–Al–B_3 bond angles in Fig. 1.a are 126.88 and 125.01˚, and the N3–Al-B_1 and N3–Al-B_3 bond angles in Fig.1.b are 126.14 and 126.76˚, respectively, indicating some structural deformation. Furthermore, in the pristine model, it should be noted that B, N atoms relax in, yielding different diameters (6, 0) zigzag SCN-Al- BNNT mouth 4.76 Å and for NCS-Al-BNNT mouth 5.02 Å systems, respectively. For the SCN -Al-BNNT complex (Fig.1. a) the diameter values are decreased, whereas in the NCS-Al- BNNT complex (Fig.1. b) the changes of the diameters were negligible. We studied the influence of Al-doping on the electronic properties of the Al-BNNT and the SCN molecules adsorb at an Al-B–N bond site (Fig.1. a) and the NCS molecule adsorbs at an Al-B–N bond site (Fig.1. b) on the electronic properties. The total

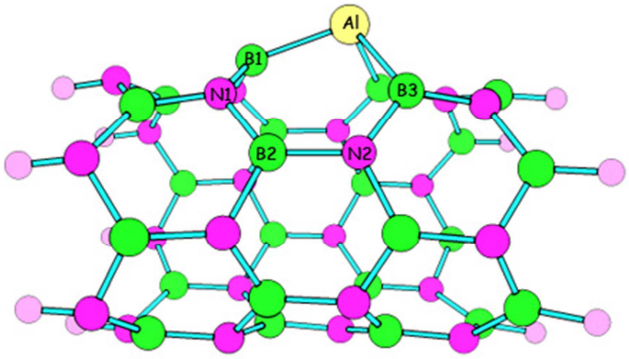
density of states (DOS) of this tube is shown in Fig. 2.



1a



1b



1c

Fig. 1. *a b. Two-dimensional views of the Al-doped (6,0) zigzag BNNT in the SCN -Al- BNNT and NCS-Al- BNNT and Fig.1 c view of the pristine (6,0) zigzag Al-BNNT model.*

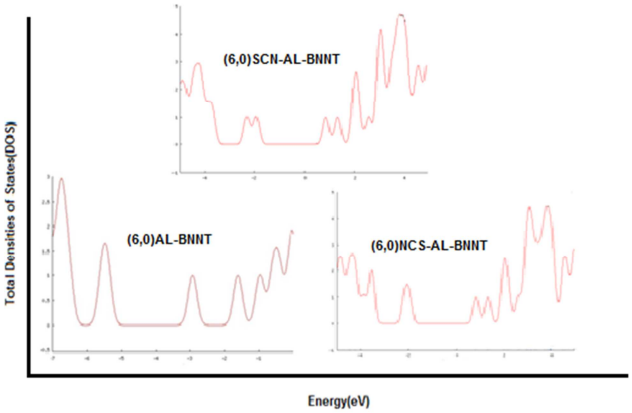


Fig. 2. *c, b and a Total density of states (DOS) for AL- BNNT, SCN-AL-BNNT and NCS -AL- BNNT models, respectively.*

As is evident from Fig. 2, the calculated energy gap (E_{LUMO} - E_{HOMO}) of the perfect (6, 0) zigzag single-walled Al-BNNT is 1.30 eV [22], whereas the calculated energy gaps of the SCN-Al- BNNT complex (Fig. 2. a) and the NCS-Al-BNNT complex (Fig. 2. b) for molecular orbitals are 1.40, 0.70, respectively. The total density of states (TDOS) of these tubes shows significant changes due to Al-doping in the gap regions of the TDOS plots. Also, the energy gaps showed differences between the two forms (Fig. 2. a, 2. b). In comparison with the pristine complex, the band gaps of the complex shown in Fig. 2. b was reduced while their electrical conductance was increased, and 2.a electrical conductance was decreased with the adsorbed in the NCS -Al- BNNT complex having a stronger effect than the adsorbed in the SCN -Al- BNNT complex on the band gap of the Al-BNNT (Table 2). The dipole moments (μ) of the Al-doped BNNT structures (Fig. 1. a, 1. b ,1. c) showed slight changes due to the SCN-Al- BNNT complex and NCS -AL- BNNT complex with respect to the Al-doped BNNT pristine model. Also, the dipole moment (μ) value of this model is presented in Fig. 1. b that is somewhat different from that of the model is shown in Fig. 1. a.

4. NMR Parameters of the (6, 0) Zigzag Al-BNNT

The NMR parameters for the investigated (6, 0) zigzag Al-BNNT model is summarized in Table 2. In the model of the pristine (6, 0) zigzag Al-BNNT, there are Al-doping, 24 B and 23 N atoms and the NMR parameters are separated into attached to an Al ring (Table 2, Fig. 1. a, b, c) [22]. In the model, the values of the NMR parameters of each complex were the same; however, the results in Table 2 show that the calculated NMR parameters were not similar for different bond, meaning that the C_S parameters for the atoms of the Al-B_1 and the Al- B_3 bond have equivalent chemical environment and electrostatic properties. The atoms of B_1 to B_3 and N_1 to N_2, which are located at near the 27-Al atom is doped by the B_1 to B_3 atoms that is the smallest values of the

CS_I parameters but the largest values of the CS_A parameters among the 11-B and 15-N atoms in the model of the pristine (6,0) zigzag Al-BNNT. The atoms of B_1 to B_3 and N_1 to N_2, which are located at the surface of the (6, 0) zigzag Al-BNNT that is the largest values of the CS_I parameters. In Fig. 1.a, i.e., the (6, 0) zigzag Al-BNNT model, Al atom is doped by the B_1 to B_3 atoms, which results in an Al–B_1 and Al–B_3 bonds. The calculated results in Table 1 show that, among the B atoms of the model is shown in Fig. c, Al-B, for the B_1 to B_3 atoms are located at the surface of the (6,0) zigzag Al-BNNT (Al-doped), the changes of the CS_I and CS_A values of the 11-B and 15-N atoms are negligible. For the B_1 to B_3 atoms, which are located at near near the SCN-Al, the CS_I and CS_A values of the B_1 and B_3 atoms show some significant changes due to the Al-doping; the CS_I values of the atoms are increased, whereas the CS_A values of the atoms are decreased. However, other 11-B atoms of this group show no significant change due to the Al-doping of the (6, 0) zigzag BNNT. The values of the NMR parameters (CS_I and CS_A) of the 27-Al atom in the Al-doped (6, 0) zigzag BNNT is summarized in Table 2. The results in Table 2 show that the values of the CS_I parameters of the 27-Al atom, the Al-B_1 model, is larger than in Fig. 1. C, the Al-B_3 model, whereas the values of the CS_A parameters of Fig.1. C, the Al-B model, are larger than in Fig. 1. C., the Al-B model of the (6, 0) zigzag BNNT. However, no table changes in the CS_I parameters are observed for all of the B atoms due to the direct and indirect effect of the Al-B doped ring. The doping of B_1 and B_3 atoms by the Al atom and the doping of B_1 and B_3 atoms by the 15-N atoms take place in the form(1. b) of the Al-doped zigzag BNNT (Fig. 1. b) which yield Al-B and B–N bonds. Among the 11-B atoms, the most significant changes in both NMR parameters (CS_I and CS_A) are observed for B_1 and B_3 atoms which are directly bonded to the Al atom. The CS_A parameter of B_1 also detects some changes due to indirect effect of the Al-B-doped ring. The most significant changes in the NMR parameters of the 15-N atoms of the form (1. b), in comparison to the pristine model, are observed for N_1 and N_2 atoms for which both of the CS_I and the CS_A parameters detect significant changes. The change values of the CS parameters for N_1 and N_2 atoms are summarized in the (table. 2). This trend is in agreement with the change in the band gap of the form (2. b) in comparison to the pristine model of the zigzag Al- BNNT.

Table (1). *Structural properties of representative (6, 0) zigzag BNNT (Al-doped), SCN-Al-BNNT, NCS-Al-BNNT model.*

Property, Figs (c, a, b)[a]			
The bond length (°A)		***The bond angles (deg)***	
Al-S	(-, 2.33, -)	Al- B21-N22	(116.67, 122.93, 122.72)
Al-N_3	(-, -, 1.78)	Al-B59- N_{19}	(116.87, 120.78, 121.29)
Al-B_1	(2.09, 2.13, 2.14)	B21-N22- B20	(125.79, 123.44, 123.55)
Al-B_3	(2.03, 2.05, 2.05)	N22-B20- N19	(126.78, 126.28, 126.66)
B_1-N_1	(1.47, 1.49, 1.4)	B_{20}-N19- B_{59}	(119.85, 119.14, 118.30)
N_1-B_2	(1.49, 1.48, 1.48)	S- Al-B21	(-, 126.88, -)
B_2-N_2	(1.47, 1.46, 1.46)	S-Al-B59	(-, 125.01, -)
N_2-B_3	(1.46, 1.49, 1.50)	N63- Al-B21	(-, - , 126.14)
N_3-Al-B_3	(- , - , 126.76)		
Energy (keV)	(-57.35, -70.72, -)		
Band gaps (eV)	(1.30, 0. 71, 1.40)		
μ (Debye)	(8.2906, 37.5823, 36.6002)		

[a]See Figs. 1.a, b and c for details. The first number is for the pristine fig (1. c) which BNNT is doped with Al, the second one is for the fig (1. a) which SCN-Al-BNNT and the third one is for the fig (1. b) which SCN-Al-BNNT.

Table (2). *NMR parameters (ppm) of the (6,0) zigzag BNNT (Al-doped), SCN-Al-BNNT, NCS-Al-BNNT.*

Nucleus	**Fig. 1. a SCN**		**Fig. 1. b NCS**		**Fig. 1. c**	
	CSI	**CSA**	**CSI**	**CSA**	**CSI**	**CSA**
S	770.61	-102.81	759.27	-46.90	-	-
C	51.85	-89.20	82.82	-27.80	-	-
N3	-	-	6.01	-63.90	-	-
N4	131.12	-92.73	-	-	-	-
Al	512.67	16.22	483.32	24.57	-52.39	621.76
B1	37.83	83.32	38.34	83.99	54.33	67.49
B2	80.85	15.36	80.70	14.97	82.57	16.45
B3	38.56	-88.33	36.72	-89.04	62.64	30.88
N1	104.31	113.33	105.09	113.10	117.34	156.10
N2	100.03	-49.75	100.22	-47.46	109.64	74.28

Data for the pristine model are from Ref. [19]

Table (3). *NQR parameters of the (6, 0) zigzag BNNT (Al-doped), SCN-Al-BNNT, NCS-Al-BNNT [20].*

Sait	11- B atoms	CQ/MHz η_Q	14 –N atoms		CQ/MHz η_Q	
Al-BNNT	B_1	3.46	0.29	N_1	0.88	0.70
	B_2	2.77	0.04	N_2	2.91	0.70
	B_3	4.26	0.26	-	-	-
	Average	3.49	0.19	-	1.89	0.70
SCN-Al-BNNT	B_1	3.63	0.49	N_1	0.48	0.59
	B_2	2.77	0.16	N_2	1.23	0.82
	B_3	4.41	0.54	N_3	2.96	0.32
	Average	3.60	0.39		1.55	0.57
NCS-Al-BNNT	B_1	3.63	0.47	N_1	0.47	0.60
	B_2	2.77	0.16	N_2	1.27	0.77
	B_3	4.43	0.53	N_4	0.07	0.01
	Average	3.61	0.38		0.60	0.46

Data for the pristine model are from Ref. [19]

5. 11-B, 14-N Electric Field Gradient Tensors of the (6, 0) Zigzag BNNT (Al-Doped)

The NQR parameters at the sites of various 11-B and 14-N nuclei in the investigated (6, 0) zigzag BNNT model doped by an aluminum atom (27-Al) is summarized in Table 3. There are 24-B and 23-N atoms in the considered (6, 0) zigzag model. As shown in Fig. 1. a, b, c boron-Nitrogen (Al-doped) atom (11-B, 14-N) of the zigzag model doped by a 27-Al, which results in the SCN–Al-B_1 and SCN–Al-B_3 complex. In our recent study [23], it was shown that due to the similarity of electronic properties, the atoms of the pristine Al-BNNT could be divided based on the equivalent calculated NQR parameters. However, doping of the Al-BNNT by other molecules (SCN and NCN) corrupts this characteristic feature of the pristine Al-BNNT. Comparing the calculated NQR parameters of 11-B atoms in this form of the SCN–Al-B_1, SCN–Al-B_3, NCS–Al-B_1, NCS–Al-B_3 complex and the Al-doped model (Table 3) with those of the pristine model that were obtained previously [23], reveals that the EFG tensors at the sites of 14-N atoms do not undergo significant changes because they are not directly correlated to the Al-doped atom. The largest magnitudes of changes belong to B_1 and B_3 in which the values of their C_Q are reduced by a magnitude of about 0.2 MHz in the Al-doped model. The changes belonging to the NQR parameters of 11-B atoms are more significant. Three 11-B atoms, B_1, B_2, and B_3, are directly connected to the Al atom. Comparison of the results of SCN–Al-B-N and NCS–Al-B-N with those of Table 3 indicates that the values of C_Q (14-N) for N_1 and N_2, which belong to the Al-membered ring, undergo significant changes. The C_Q value of N_2, placed at the surface of nanotube, is reduced by a magnitude of 1.23 and 1.27MHz, Respectively, in comparison to that of the pristine model. However, the C_Q value of N_2 is increased by a magnitude of 2.91MHz. C_Q of B_1 and B_3 undergoes the most significant change among other 11-B atoms in this form of the Al-doped zigzag nanotube, which is increased by a magnitude of 0.23 and 0.15 MHz, Respectively, from pristine to the Al-doped model. The changes of other C_Q (14-N and 11-B) values are almost negligible. As shown in Fig.1. a, SCN a sulfur atom (S) of the zigzag model of SCN-Al-BNNT is doped by a 27-Al atom, resulting in S–Al-B_1 and S–Al-B_3. In this form, two 11-B atoms, B_1 and B_3, are directly connected to the 27-Al atom and as shown in Fig. b, NCS a nitrogen atom (N3) of the zigzag model of BNNT is doped by an Al atom, resulting in N_3–Al-B_1 and N_3–Al-B_3. In this form, two 11-B atoms, B_1 and B_3, are directly connected to the 27-Al atom. The most significant change of the value of C_Q(11-B) belongs to B_1, which is increased by a magnitude of 0.21MHz from pristine to the Al-doped model; furthermore, those of B_3 is also increased by a magnitude of 0.15MHz. The next degree of changes is for B_2 in which its C_Q is not changed by a magnitude of 2.77MHz.Comparing situations 11-B and 14-N, where both atoms are located at the surface of the nanotube, it is revealed that the C_Q value of 11-B is increased where as that of 14-N is reduced. It is known that the valence shells of these two atoms are different, where 14-N has an excess of two unpaired electrons where as 11-B has lack of electrons. These differences may cause different behaviors of these atoms in similar situations. Changes of C_Q values for other 11-B and 14-N atoms are not in the table.

6. Comparison of NQR and NMR Parameters

Comparison of the results of this work and those of an earlier NMR and NQR study [17] indicates that the values of two studies mostly support each other. The NMR parameter can measure only changes in those atoms directly connected to the 27-Al impurity, while the C_Q parameter can measure the effects of the 27-Al impurity on several atoms. This trend indicates that the C_Q parameters are more sensitive to the electronic sites of atoms than the NMR parameters and it can detect any employed perturbations on these sites. Hence, the calculations of C_Q parameters can be a complementary tool for studying the electronic and structural properties of nanotubes. Unfortunately, the C_Q and NMR parameters could not be

calculated for all atoms because the dipolar atoms are active in NMR where as quadrupolar atoms are active in NQR. In some cases, the atoms are active in both techniques, e.g., 14-N, 11-B and 27-Al, but some atoms are active only in a technique, e.g. 15-N, which is active only in the NMR technique. This trend is also mainly dependent on the natural abundance of different isotopes of atoms. We have performed a DFT study to calculate the C_Q parameters for 11-B, 14-N, and 27-Al in the structures of Al-doped zigzag BNNT and in the SCN–Al-BNNT and NCS–Al- BNNT complexes. Due to the different elements of Al-BNNT and B band. The results reveal that the C_Q parameters of the B atoms directly bonded to Al-doping atom are more influenced rather than those of the N atoms in the same situation of binding. Furthermore, comparison with the pristine model indicates that the changes in the values of C_Q parameters are more in the NCS–Al- BNNT model. The Al–NCS bond is stronger than the Al–SCN bond; therefore, the value of C_Q of Al atom, which is connected to the Al–N bond, is larger than that of the Al–S bond.

7. Conclusions

We studied the electronic structure, properties including bond lengths, bond angles, tip diameters, dipole moments (μ), energies, band gaps, and NMR and NQR parameters of pristine and SCN–and NCS doped Al-BNNT zigzag model by means of DFT calculations. The calculated results showed that the average values of the B–N bond lengths are almost the same in the investigation of (6,0) zigzag Al-BNNT model. For the SCN-Al-BNNT model (Fig. 1a) the diameters are decreased, whereas in the NCS -Al-BNNT model (Fig. 1b) the changes of the diameter values were negligible. The dipole moments (μ) of the Al-doped BNNT structures Figs. 1a, b, and c show minor changes due to the Al-doping with respect to the pristine model. In comparison with the pristine model, the band gaps of the models shown in Figs.1. a, b and c are reduced, whereas their electrical conductance is increased. The NMR parameters for the pristine model are separated into four layers, and the NMR values for the 11-B and 15-N atoms that are directly bonded to the SCN and NCS atom in the Al-doped models are significantly SCN and NCS is resulting in a significant change in the both of these models. Comparison of the calculated NMR parameters in the SCN-Al-BNNT and NCS-Al-BNNT complexes shows that the properties of the electronic structure of the NCS-Al-BNNT model (Fig. 1.b) of the (6, 0) zigzag Al-BNNT that are more strongly influenced than those of the SCN-Al-BNNT model (Fig. 1.a). The NQR values of the first to those B atoms are located at the surface of the Al-BNNT connected to the SCN of the tube, showing the dominant role of these SCN and NCS for the determination of the electronic behavior of the Al-BNNT. The electronic sites of the B and N atoms in the NCS-Al-BNNT model (Fig. 1b) of the (6, 0) zigzag Al-BNNT showed greater changes than that of the SCN-Al-BNNT model (Fig. 1a). The NMR and NQR results show that the NCS-Al-BNNT model is a more reactive material than either the pristine or the SCN-Al-BNNT model of the (6, 0) zigzag Al-BNNT. Since the Al and B atoms have the lowest electronic density and N atom has the highest electronic density, respectively, indicating an electron acceptor-electron donor in the doped model of Al-BNNT.

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