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NMR Study of Gases Adsorption on Single–Walled Carbon Nano Tubes-A Review

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Abstract: In this study computational Nuclear Magnetic Resonance (NMR) study are performed to investigate the electronic structure properties of Single-Wall Carbon Nanotubes. The electronic structure, NMR spectrum, dipole moment of nitrogen, oxygen, and carbon nuclei's are thoroughly studied. The computational results indicate that rich adsorption patterns may result from the interaction of oxygen and nitrogen with two types, (5, 0) zigzag and (4, 4) arm chair, of carbon nano-tubes¹⁻². The chemical-shielding ($_{ij}$) tensors were converted to isotropic chemical-shielding ($_{iso}$) and anisotropic chemical shielding ($_{0}$) and asymmetrical (μ_{j}) parameters of ¹³C, ¹⁵N and ¹⁷O nucleus for the optimized structures. The nitrogen molecules adsorb with a comparatively lower rate and almost never a chemical binding is formed with the SWCNTs. Behavior of a single NH3 molecule adsorbed on external surface of single-walled carbon nanotubes (SWCNTs) is studied. ¹³C, ¹⁵N and ¹H chemical shielding of (8,0) is more sensitive to NH3 adsorption compared to (5,5), (6,6) and (5,0)tubes. ¹⁵N and ¹H chemical shielding correlate noticeably with diameter of the nanotubes. Gaussian 98 software has been used to carry out quantum chemistry calculations ³.

Keywords: NMR, SWCNTs, chemical shielding, GIAO, Gaussian98 software.

Introduction

Since discovered in 1991(Iijima, 1991), carbon nanotube has attracted great research attention owing to their unique structure and mechanical and electric properties⁴. The most popularly studied carbon nanotube is single walled nanotube (SWNT). Carbon nanotubes have many fascinating properties 5-6. And numerous studies have been conducted on their synthesis⁷⁻⁸, treatments ⁹⁻¹⁰. And properties¹¹⁻¹². physical Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool for structural and dynamic analysis in physical, chemical and biological systems. So far, varieties of NMR techniques have been developed with a very wide range of applications including magnetic resonance imaging. NMR spectroscopy is based on the study of nuclear spinning. A nuclear is characterized by a nuclear spin quantum number I. In some nuclei (such as ¹² C) the spin is zero. However, most nuclei (such as ¹H, ¹⁵N and ¹³C) possess an overall spin. The rules for determining the net spin of a nucleus are as follows: If the number of neutrons and the number of protons are both even, then the nucleus has no spin. If the number of neutrons plus the number of protons is odd, then the nucleus has a half-integer spin (i.e. 1/2, 3/2, 5/2). If the number of neutrons and the number of protons are both odd, then the nucleus has an integer spin (i.e. 1, 2, and 3). For nuclei with

I=0, there is no nuclear spin, thus no NMR phenomenon¹³. However, only a limited number of studies have been made on the adsorption of gases in carbon nanotubes; these include theoretical studies¹⁴⁻¹⁵. work¹⁶⁻¹⁷. experimental Manv researchers studied endohedral adsorption of nitrogen in single walled nanotubes of 10.2 of diameters ¹⁸⁻¹⁹. A large number of experimental studies have been carried out thus far on the adsorption of nitrogen ²⁰⁻²¹, oxygen ²²⁻²³, and carbon nanotubes single-walled. In this study, electronic structure properties of (5, 0) SWCNT involved with an O₂ and N₂ molecules are investigated. Nuclear magnetic resonance NMR properties are calculated in order to obtain useful information about the nature of interactions in nano-tubes. Consequently, the bond strength of O_2 is greater than N_2 species adsorbed on CNTs. In our study, oxygen and Nitrogen electronic structure modification effects on NMR chemical shielding and dipole moment (5, 0) of CNT, the influence of hydrogen doping (Hdoping) on the electrostatic properties of the zigzag SWCNTs is studied by means of the CS tensor

Materials And Methods

2.1. Software

GAUSSIAN 98 package program

2.2. Computational details

In the present study, O_2 and N_2 molecules adsorption behaviors on the SWCNT is taken in to consideration. A (5, 0) CNT containing 40 carbon atoms with length of 7.1 has chosen for the purpose. NMR chemical shielding calculations were carried out of theory using gauge independent atomic orbital's (GIAO) approach ³¹. We have performed experiments on single-wall carbon nanotube SWCNT networks and compared with DFT calculations to identify the microscopic origin of the observed sensitivity of the network conductivity to physisorbed O₂ and N₂. Previous DFT calculations of the transmission function for isolated pristine SWNTs have found physisorbed molecules have a little influence on their conductivity. However, by calculating we show that, physisorbed O₂ and N₂ affect the junction's conductance. This may be understood as an increase in tunneling probability due to hopping via molecular orbitals. We find the effect is substantially larger for O2 than for N2 SWNTs junctions, in agreement with experiment³². This may be understood as an increase in tunneling probability due to hopping via molecular orbital.

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calculations at the sites of ¹³C nuclei in representative model including H-doped of 7.1 nm long (5, 0) zigzag SWCNTs²⁴, (Table 1 and Figure 1)¹. NMR measures the local magnetic fields on nuclei, generated by response of electrons to an external uniform magnetic field. Solid-state ¹³C NMR has been applied to characterize nanotube carbons in the functionalized SWCNT samples ²⁵⁻²⁶. The signals corresponding to sp^2 carbons of nanotube are generally broad, centered around120-130ppm, and similar to those of unfunctionalized SWNTs²⁷⁻³⁰. In contrast to ¹³C NMR, calculation of nitrogen chemical shifts is much easier than experimental analysis. ¹⁵N with natural abundance of 0.365% and I=1/2 is applied for NMR studies. In the present work, electronic structure properties of (5, 5), (6, 6), (5, 0) and (8, 0) single-walled carbon nanotubes (SWCNTs) are studied by DFT method. Nuclear magnetic resonance (NMR) properties are calculated to obtain useful information about the nature of interactions.

We find the effect is substantially larger for O_2 than for N_2 SWNTs junctions, in agreement with experiment ³³. Components of CS tensor are defined by following relation ³⁴:

_{ij} = $(2E/B_i \mu_j) \mu_j B_i$

Where *E* is energy of the system and μ j and Bi are components of magnetic moment and external magnetic field, respectively. C_S tensor in the principal axes system (PAS) ($_{33}$ > $_{22}$ > $_{11}$) is diagonal and thus, principal values for specification of shielding is defined for this coordinate system:

Where $_{iso}$, and are isotropic, anisotropic and asymmetric parts of C_s tensor, respectively, in which in certain cases vanishes.

NH3 molecule adsorption behaviors on (5, 5), (6, 6), (5, 0) and (8, 0) single-walled carbon nanotubes (SWCNTs) is taken in to consideration. NMR chemical shielding calculations were carried out of theory using gauge independent atomic orbital's (GIAO) approach ³¹.

Results and Discussion

3.1. The ¹³C NMR chemical shifts

Tables1 exhibit the calculated ¹³C chemical shielding for CNTs. O₂ and N₂ adsorption on the CNT has a remarkable in flounce on ¹³C NMR tensors which is in complete accordance with the facts mentioned above Previously, it has been indicated that for the H-capped CNTs, the calculated ¹³C chemical shielding value sat the ends are smaller than in the tube's center if the carbon is directly bound to a hydrogen; otherwise it is larger³⁵. It is also depicted that chemical shielding components converge in a way similar to that of the chemical shifts when increasing the tube length albeit not as smoothly as the isotropic shielding. On the other hand, the calculated ¹³C chemical shielding values in the middle of the (5, 0) CNT seem to approach values 149.1757 and 149.1663 ppm (Table1)¹. It may be noted that 13C chemical shielding tensor the carbon sites depends remarkably on the tube size and nature of frontier orbital's ³⁵. The NMR chemical shielding of finite SWCNTs were found to converge very slowly, to the in finite limit, indicating that hydrogen capped tube fragments are not necessarily good models of infinite systems. For the hydrogen capped (9, 0) tube case, all of the frontier orbital's have carbon ps character, they are localized at each end of the tube³⁵. As the length of the fragment increases, these orbital's do not yield a contribution to the electron density along the tube (except at the ends) and must therefore be regarded as artifacts due to treating the finite sized systems. According to GIAO calculations performed after adsorption of O₂ ¹³C NMR parameters of those interacted carbon atoms are also modified. As understood by comparison of sites A_1 , A_2 , A_3 and A_4 , the carbon atoms included in O2 adsorption become more shielded. Among the two NMR principal components, intermediate shielding component, ₂₂, shows more change from nanotube to the O₂-CNT system. The results are consistent with strong interaction between the tube and O₂ molecule. The discrepancy between the ¹³C chemical shielding tensor for the site CNT, A₁, A₂, A₃ and A₄ systems must be attributed to the different nature of the frontier orbital.



Fig.1. (A) The (5, 0) SWCNT, (A_1) and (A_2) adsorption configurations of an N_2 molecule (sites A_1 and A_2 , respectively) (A₃) and (A₄) adsorption configurations of an O₂ molecule (sites A₃ and A₄,respectively).

Table 1. Calculated ⁻ C NMR parameters for CN1, N2–CN1, O2–CN1 system							
Model	atoms	11	22	33	iso		
CNT(A)	C1	-27.4749	155.3869	319.6152	149.1757	255.6593	1.0729
	C2	-27.4737	155.3875	319.5851	149.1663	255.6282	1.0730
	C3	-166.2046	-4.1528	153.1572	-5.7334	238.3359	1.0199
CNT(5,0)-O2(A1)	C1	74.4312	77.7044	155.3112	102.4823	79.2434	0.0620
	C2	74.6323	77.7154	155.0228	102.4568	79.2720	0.0637
CNT(5,0)-O2(A2)	C1	42.8507	97.3469	149.1738	96.4571	79.0751	1.0338
	C2	47.6078	104.8761	127.8227	93.4355	51.5808	1.6654
CNT(5,0)-N2(A3)	C1	76.1071	96.5323	143.1071	105.2245	56.8239	0.5411
	C2	76.0659	96.4950	143.0751	105.2120	56.7946	0.5396
CNT(5,0)-N2(A4)	C1	48.7700	48.7700	127.2600	74.9305	78.4943	0.0000
	C2	34.5201	76.2487	118.0313	76.2667	62.6469	0.9991

1 C.L. 1. 1¹³C ND/D

^aCalculated _{ii}, _{iso}, values in ppm. Table 2 exhibits the calculated ¹³C chemical shielding tensors for various CNTs³. NH3 molecule adsorption on external surface of CNTs has a remarkable influence on ¹³C NMR tensors, which is in complete accordance with the facts mentioned above .Previously, it has been indicated that for H-capped fragments, the calculated ¹³C chemical shielding values are smaller at the ends of tube, compared to the center, if the carbon is directly bound to hydrogen; otherwise, it is larger ³⁶. To assess the dependence of NMR results on carbon atom position, ¹³C chemical shielding isotropy values of armchair and zigzag tubes are examined before and after NH3 adsorption (Fig. 2). Three different parts of tube axis are considered (two ends and middle parts). Interesting trends are evidenced: For (5, 0) CNTs, the isotropy of 13 C shielding tensor are larger at the ends compared to the center. The values seem to approach 65 or 42 ppm in the middle of tube. For semiconductor (8, 0)tube, the carbon shielding at the ends deviates slightly from the middle values. Furthermore, after NH3 adsorption, a considerable increase in isotropy value is evidenced at the end parts. It can be also seen from Fig. 4 that ¹³C chemical shielding of (5, 5) and (6, 6) CNTs are separable at the three parts. The shifts are clearly sensitive to the nanotube radius. According to GIAO calculations performed after adsorption of NH_3 molecule on (5,0) CNT, the isotropy value of the ¹³C NMR shielding tensor increases, approximately by 3.16, 2.16, 7.35, 5.04, 2.39 ppm, at the C_1 , C_2 , C_3 , C_4 , C_5 , C_6 sites, whereas an opposite trend is evidenced for C_3 (Table 2). These shifts are much smaller than those calculated for N-H functionalized finite (11, 0), (13, 0) and

(14, 0) CNTs (ca.44ppm) ³⁷. For the (8, 0) CNT, the isotropy value decreases for C_3 (25%), C_4 (1.7%) and C₅ (24%) while an increasing is detected for other carbons .However, the increase is more significant for C_2 (35%) and C_6 (33%) sites. As for the armchair (5, 5) CNT, the 13C chemical shielding isotropy values are slightly deshielded for all carbon atoms after NH₃ adsorption. In case of (6, 6) CNT, ¹³C NMR tensors of interacted carbon atoms are also modified as a result of NH₃ adsorption. Comparing pristine (6, 6) and tubemolecule, it becomes clear that the C_1 and C_2 atoms included in NH₃ adsorption are slightly shielded. The results are consistent with the weak interaction between the tube and NH3 molecule. Thus, based on chemical shielding calculations upon NH₃ ^{13}C chemical adsorption. shielding of semiconductor (8, 0) is more sensitive than metallic (5, 5), (6, 6) and (5, 0) tubes. The discrepancy between the 13C chemical shielding tensor variation for the zigzag and armchair nanotubes can be attributed to the different nature of the frontier orbital. However, it is obvious that there is a large effect of the HOMO on the energies of the HOMO-1 etc. ${}^{13}C$ shielding tensor orientation for the (5, 0) system is shown in Fig. 3. It is qualitatively the same as that obtained previously for finite (9, 0)and (8, 0) SWNT CNTs³⁸⁻³⁹. The ₃₃ component is perpendicular to the tube's surface, while 22 component is along the tube's length. Such orientations are also compatible with those of infinite (9, 0) CNT^{38} indicating that the ${}^{13}C$ shielding tensor orientation does not depend on tube length.

 Table 2 .Calculated ¹³C chemical shielding isotropy values (in ppm) for SWCNT

Spacing	C1	<u> </u>		<u> </u>	C5	<u>C6</u>
species	CI	C2		C4	05	CO
Tube (5,0)	39.92	43.93	65.86	43.69	39.89	40.02
Tube(5,0)+NH3	3.08	46.09	57.82	51.04	44.93	42.41
Tube (8,0)	52.14	51.88	85.57	83.17	85.68	51.96
Tube 8,0)+NH3	52.59	69.85	64.51	81.74	65.17	69.29
Tube (5,5)	73.23	73.21	73.33	66.78	66.84	73.26
Tube(5,5)+NH3	73.02	70.14	72.93	65.84	66.72	72.35
Tube (6,6)	75.69	67.24	67.15	75.68	75.74	75.83
Tube(6,6)+NH3	75.79	67.43	66.54	74.18	74.09	75.56

3.2. The chemisorption and physisorption ¹⁷O and ¹⁵N NMR parameter modeled of armchair (4, 4) the surface and open end

Table 3 and 4 exhibits the calculated ¹³C chemical shielding tensors for SWCNTs. Nitrogen and Oxygen molecules chemisorption and physisorption on external surface and open ended of CNTs has a significant influence on ¹³C NMR tensors, which is in complete accordance with the facts mentioned above previously². Consequently, it has been ¹⁷O and ¹⁵N indicated that for the H-capped SWCNTs, the calculated ¹³C chemical shielding values physisorption are smaller at the open ended of tube, compared to the surface, if the carbon is directly bound to hydrogen, unless, it is larger. Adsorption configurations of Oxygen and nitrogen molecules are shown in Fig. (2,3). To assess the dependence of NMR results on carbon atom position, ¹³C chemical shielding isotropy values of armchair (4, 4) CNTs have calculated on surface and open ended ¹⁵N and ¹⁷O of ¹³C adsorption. Two different parts of surface tube axis and open ended are considered. Interesting open end is evidenced: for armchair (4, 4) CNTs, the isotropy physisorption ¹⁷O and ¹⁵N of ¹³C shielding tensor are larger at the surface compared to the open end. It is also showing that the chemical shielding components converge in a way similar to that of the chemical shifts when increasing the tube length even though not as smoothly as the isotropic shielding. Chemical shielding tensors and chemical shifts are efficient parameters for characterization of single walled

carbon nano tubes. The calculated ¹⁷O and ¹⁵N chemical shielding values in the middle of the open ended CNT (4, 4) and surface seem close to the values -3.58 ppm, -5.83ppm and 10.84 ppm, 96.46 ppm, respectively (Table 3). The calculated ¹⁷O and ¹⁵N chemical shielding of the surface CNTs armchair (4, 4) and open ended seem close to the values 53.8495, 54.1090, 78.5398 and 149.1663 ppm, respectively (Table 4). More recently, it is indicated that introduction of oxygen atoms is theoretically predicted to give rise to chiral current flow along the nanotube 37 due to symmetry breaking 40 . The results deduced from comparison of sites $(A_1, A_2, D_1 \text{ and } D_2)$, show that the carbon atoms included in oxygen and nitrogen molecular chemisorption and physisorption become more shielded. Among the six NMR principal components, intermediate shielding component, ₂₂, shows more change from SWCNTs compared with surface and open ended the oxygen-CNTs and nitrogen- CNTs system. The interest of oxygen and nitrogen CNTs in terms of application is the control of the type of charge carriers within the CNTs. Oxygen-CNTs and nitrogen- CNTs should show significant advantages over CNTs for gas sensor applications, due to their reactive tube surfaces and open ended and the sensitivity of their transport characteristics in relation with the presence, distribution and chemistry of oxygen. The molecular oxygen and nitrogen in the CNTs can be seen as regular defects which change the chemical and physical behavior of the CNTs.

model	¹⁵ N, ¹⁷ O	Atom	ij (11, 22, 33)	iso		
	01	Cı	-94.7701; 0.8185; 83.1939	-3.5859	130.1683	1.1015
CNT4,4-O ₂ D ₁	O 2	C ₂	-94.7683;0.8351;83.1889	-3.5814	119.4113	1.2009
NT4,4-N2 D2	N1	C1	-128.6994;28.0706;83.1526	-5.8312	133.4757	1.7620
	N_2	C ₂	-128.6994;28.2120;83.0000	-5.8291	133.2437	1.7664
CNT4,4-O2 A	01	Cı	-80.4572; 10.7847; 102.7393	11.0223	137.5755	0.9948
	O 2	C2	-80.8301; 10.9026; 102.4569	10.8431	137.4207	1.0013
CNT4,4-O2 A2	01	Cı	40.2230; 40.2230; 141.8900	96.4600	68.1450	0.0000
	O 2	C2	64.9425; 91.1836; 133.1339	96.4200	55.0709	0.7147
CNT4,4-N2 A1	N1	Cı	-88.7059; 38.8741; 95.3872	15.1851	120.3032	1.5907
	N_2	C ₂	-88.7419; 38.8274; 95.3910	15.1588	120.3483	1.5900
CNT4,4-N2 A 2	N1	C1	85.6400; 85.6400; 120.5500	97.2764	34.9100	0.0000
	N_2	C2	86.0700; 86.0700; 125.8100	99.3120	39.7400	0.0000

Table 3: Comparison of chemical shielding and chemical shift tensors physisorption on the surface and open ended ¹⁵N, ¹⁷O NMR parameters for CNTs, Nitrogen-CNTs (4, 4) and Oxygen-CNTs (4, 4) systems ^{a2}.

^a:Calculated $_{ii}$, $_{iso}$, values in ppm; ^b: In each raw, the first number is for $_{11}$, the second number is for $_{22}$, and the third number is for $_{33}$.

model	¹⁵ N, ¹⁷ O	Atom	ij (11, 22, 33)	iso		
	Nı	C1	85.6400; 85.6400; 120.5500	47.2827	176.1143	0.1897
CNT4,4-N2 D1	N2	C_2	86.0700; 86.0700; 125.8100	46.5658	182.5256	0.1729
	O 1	Cı	-8.9800;- 8.9800;103.1800	28.4067	98.6900	0.0000
CNT4,4-O2 D2	O_2	C_2	-8.9700;-8.9700;103.2000	28.4200	112.1700	0.0000
CNT4,4-N2 A 1	Nı	Cı	-65.7148; 14.9561;129.4085	26.2166	154.7878	4.6156
	N_2	C_2	-65.6491; 14.9320;129.3856	26.2228	154.7442	4.6094
		C_4	-65.6564; 14.9540; 29.4354	26.2443	66154.7472	4.6073
CNT4,4-N2 A2	Nı	C1	-34.9738; 44.0376; 17.5517	42.2052	113.0197	2.8081
	N_2	C_2	-76.9772;-39.0220;120.5170	1.5059	178.51	37.8064
		C3	-76.2848; -20.9271; 30.6033	11.1305	179.2092	7.4603
		C_4	-55.4982; 63.6156;121.5112	43.2095	117.4526	4.1350
CNT 4,4- O2	O 1	Cı	-66.8441; 54.0845;83.9711	23.7372	90.3508	2.0077
Aı	O_2	C_2	-66.4764; 53.8616; 84.4001	239229	90.7075	1.9900
		C3	-66.7714; 54.0846; 83.9711	23.7491	90.3313	2.0063
		C_4	-66.3669; 54.0373; 84.4001	23.9226	90.262	2.0009
CNT4,4-O2 A	O 1	Cı	-53.8794; 39.8243 ;95.9593	27.3014	102.9869	1.3648
2	O_2	C_2	-43.5238; 12.7128;100.4479	1.5456	118.3535	0.7761
		C3	-29.8179;7.3599;103.6236	27.0552	114.8526	0.4856
		C4	-66.1822;56.8643;97.6708	29.4509	102.3298	1.8037

Table 4: Comparison of chemical shielding and chemical shift tensors chemisorption on the surface and open ended ¹⁵N, ¹⁷O NMR parameters for CNTs, Nitrogen-CNTs and Oxygen-CNTs armchair(4, 4) systems ^a

^a:Calculated $_{ii}$, $_{iso}$, values in ppm; ^b: In each raw, the first number is for $_{11}$, the second number is for $_{22}$, and the third number is for $_{33}$.







с



CNT (4,4)

a

CNT (4,4)-02 D1

CNT (4,4)-O2 D2

b

CNT (4,4)-O2 A1

 $\operatorname{CNT}\left(4,4\right)\text{-}\operatorname{O}_2A_2$



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CNT(4,4)-O2(A2)

d

Fig.2.(a) Carbon nanotube armchair (4, 4) model, (b) Oxygen molecules chemisorption and physisorption on open ended of SWCNTs of armchair (4, 4), (c) Oxygen molecules chemisorption and physisorption on external surface of SWCNTs of armchair (4, 4), (d) Oxygen molecules chemisorption and physisorption on external surface of SWCNTs of armchair (4, 4).



Fig.3.(a) Nitrogen molecules chemisorption and Physisorption on open ended of SWCNTs of armchair (4, 4),(b) Nitrogen molecules chemisorption and physisorption on external surface of SWCNTs of armchair (4, 4), (c) Nitrogen molecules chemisorption and physisorption on external surface of SWCNTs of armchair (4, 4).

3.3. The ¹⁵N and ¹H chemical shielding

The ¹⁵N and ¹H chemical shielding tensors of adsorbed NH₃ molecule on external surface of zigzag and armchair CNTs are shown in Table 5. Results indicate that the ¹⁵N and ¹H NMR chemical shielding are also dependent upon the nanotube family, and radius. More especially, the ¹⁵N NMR isotropy value reduces from NH₃ to NH₃-tube and

the amount of reduction is more evident for (5, 0) CNTs. However, the ¹⁵N chemical shielding tensor increases with the tube diameter. Small differences are detected in proton NMR calculations of the nanotubes. This is mainly due to the limited interaction of hydrogen atoms with nanotubes².

Table 5. Calculated ¹⁵N and ¹H chemical shielding isotropy values (in ppm) for SWCNTs and a single NH₃ molecule

Species	¹⁵ N	${}^{1}\mathbf{H}$	${}^{1}\mathbf{H}$	${}^{1}\mathbf{H}$
Tube (5,0)+NH3	254.35	32.24	32.49	32.80
Tube (8,0)+NH3	258.35	33.98	34.00	34.02
Tube (5,5)+NH3	259.54	33.81	33.79	34.05
Tube (6,6)+NH3	260.32	34.21	34.02	34.08
Single NH3	260.96	32.67	32.67	32.67



Fig. 4. ¹³C chemical shielding isotropy values versus carbon atoms number (a) (5,0) ,(b) (8,0) ,(c) (5,5) and (d) (6,6) CNTs.

Conclusion

Adsorptions of O2, N2 on the CNT 13C NMR parameters are modified. It is found that ¹³C chemical shielding is appropriate parameter to investigate the nature of interactions in (5, 0)SWCNT. The ¹³C chemical shielding isotropy and anisotropy values vary remarkably from CNT to the CNT-O₂ and CNT-N₂ systems for two O₂, N₂ adsorption sites¹. Calculation of chemical shielding tensors and chemical shifts for oxygen and nitrogen nucleus reveals that increasing length and diameter of CNTs (4, 4) chemical shielding will cause oxygen and nitrogen nucleus converge on the single walled nanotube surface and open ended. The results are consistent with strong interaction physisorption between the tube and oxygen molecules in CNT (4, 4)-N₂ (A₂)². The results also

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show that the chemical shielding tensors and chemical shifts are efficient parameters for characterization of single walled carbon nanotubes. The equilibrium tube NH3 distance exhibits considerable sensitivity to the type of tube. The calculated NH3-tube bond lengths are 3.12, 3.67, 3.42 and 3.60 A° for (5,0), (8,0), (5,5)and (6,6), respectively. According to GIAO calculations, performed after NH₃ adsorption on (5, 0) CNT, isotropy value of ¹³C NMR shielding tensors increases, approximately by 3.16, 2.16, 7.35, 5.04, 2.39 ppm, at the C1, C2, C4, C5, C6 sites, whereas an opposite trend is evidenced for C₃.The ¹H and ¹⁵N NMR results reveal that chemical shielding due to NH₃ molecule adsorption are also dependent upon the nanotube family, and radius³.

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