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The Influence of H_2O-attaching on the NMR Parameters In the Zigzag and Armchair AlN Nanotubes: A DFT study

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ABSTRACT

Zigzag (6,0) and armchair (3,3) Aluminum nitride nanotubes were investigated in perfect and H_2O-attach states by using density functional theory (DFT) in level of B3LYP and 6-31G(d) basis set. For this purpose, *Gaussian 09w* program of package was used and after final optimization, structural and NMR parameters were studied. However, GIAO method was used and effects of attaching of H_2O on values of chemical shift anisotropic and chemical shift isotropic were considered. Obtained results were shown that by attaching of H_2O group, value of CS^I and CS^A, in various nucleuses ^{7}N and ^{13}Al more changed and was caused to some changes in different property of AlNNTs.

Key words: AIN Nanotubes, CS^A, CS^I, DFT, NMR.

INTRODUCTION

In during recent decades research domain about nanostructure is developed a lot, and many studies are done about it. After discovery of fullerene [1] and carbon nanotubes in 1991 by Ijimia[2], many investigations were done about chemical and physical properties of these compounds and quality of their application in industry[3-6]. Carbon nanotubes are arranged as a cylindrical structure. It means that it's carbonic empty tube. These structures exist as a single-wall and multi-wall. The single-walls nanotubes involve chiral, armchair and zigzag models. Arrangement of carbon atoms in wall of cylindrical structure is similar to carbon arrangement in graphite sheets and includes weak von der vales bonds. In multi-wall models, upper layers are attached to sub layers. Other type of nanotubes, is non carbonic nanotubes made by noncarbonic elements. These kind of applicable and known nanotubes are involving elements of III and V group in periodic Table[7-8]. These nanotubes are studied theatrically and experimentally. In the early, these compounds were introduced by theoretical methods, and subsequently synthesized experimentally[9-10]. However, many properties of

Aluminum-Nitrogen Nano Tubes (AlNNTs) are considered theoretically and experimentally. By addition of various chemical groups to these compounds, structural parameters and chemical shift are changed that caused to changing of electrical conductivity, thermal conductivity and physicochemical properties of these structures as a semiconductor. NMR parameters have given lots information about chemical medium around of nucleus, and considered base on two basic parameters involving isotropic chemical shift (CS^I) and anisotropic chemical shift (CS^A)[11-12]. However, NMR values and coupling constant in different nucleus are changed by doping or attaching of various chemical groups on these nanotubes[13-14]. Obtained results are shown that some structural parameters like bond angles and bond lengths are changed by doping or attaching of various atoms on these compounds[13-14]. Because of these properties, new effects of H_2O groups are considered for AlNNTs in various models. Main aim of these changing and attaching of H_2O group is investigation of physicochemical effects of AlNNTs and quality of H_2O effects on specific properties of these compounds.

Computational Details

For investigation of structural property and NMR parameters at first, proposed AlNNTs were designed and for final optimization Gaussian 09 program of package was used[12]. Molecular formula of this structure in armchair (3,3) model is $Al_{21}H_{14}N_{21}O$ and in zigzag (6,0) model is $Al_{24}H_{14}N_{24}O$. Considered length of nanotube in various models is about 10 angstrom. All calculations were done in theory of the level B3LYP and 6-31G(d) basis set. The GIAO method was used for calculation of CS^I and CS^A values and these parameters for ^{13}Al and ^{7}N nucleuses were calculated as equation 1 and 2 [13-15]. CS tensors in the principal axes system (PAS) ($\sigma_{33} > \sigma_{22} > \sigma_{11}$) obtained by mechanic quantum calculation[16,17].

$$CS^I\ (ppm) = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3 \quad ...(1)$$

$$CS^A\ (ppm) = \sigma_{33} - (\sigma_{11} + \sigma_{22})/2 \quad ...(2)$$

All obtained results were calculated in gas phase condition, 298 K temperature and 1.0 atm pressure by pentium IV computer with Intel® core i7-1.73 GHz processor, 4G of memory in XP windows®.

RESULTS AND DISCUSSION

H_2O-attach and perfect AlNNTs structures were considered in zigzag (6,0) and armchair (3,3) models (see fig 1 to 4). After calculations, obtained results were reported in Table 1 to 4. In this study, DFT method was used in theory of the level B3LYP and 6-31G (d) basis set.

Geometrical parameter

Obtained results are reported after final optimization for bond lengths in Table 1 and 2. It is shown that bond lengths are different in various states and it is because of neighbor atom effects or additional atoms to main structure. In armchair (3,3) model of AlNNTs, H_2O is attached to $^{13}Al40$ atom by $^{8}O55$ and this linking is near to center of nanotube that this structure remains symmetric (Table 1). However in zigzag (6,0) model, like armchair (3,3) model, $^{8}O61$ is linked to $^{13}Al41$.

Bond length in (3,3) armchair AlNNTs

As a result, after final optimization, values of bond length is about 1.016 Angstrom for bond between ^{7}N and ^{8}O in perfect state, and it is about 1.584 Å for bond between ^{1}H and Al (Fig 1). After addition of H_2O, bond lengths of Al-^{1}H are changed and it is about 1.585 to 1.586 Å (Fig 2). But bond lengths of N-^{1}H aren't changed. Variation of bond lengths are high for ^{13}Al and ^{7}N. Before attaching of H_2O group, variation range of bond length is about 1.806 to 1.821 Å in different parts of AlNNTs and after attaching of H_2O group, it is about 1.860 to 1.805 Å. Maximum variation range is belong to $^{7}N12$-$^{13}Al40$ that bond length is changed to 1.860 Å. Similar changes are obtained for AlNNTs in armchair (4,4) that variation range of ^{7}N-Al, is about 1.820 to 1.830 Å[14]. In fact, these variation range is because of direct effect of $^{8}O55$ to $^{13}Al40$ and moreover because of high electro negativity of oxygen and high steric hindrance, have direct effect on length of nanotube in armchair model.

Bond length in (6,0) zigzag AlNNTs

In zigzag model, variation range of bond length of ^{13}Al-^{1}H is about 1.582 Å in perfect state

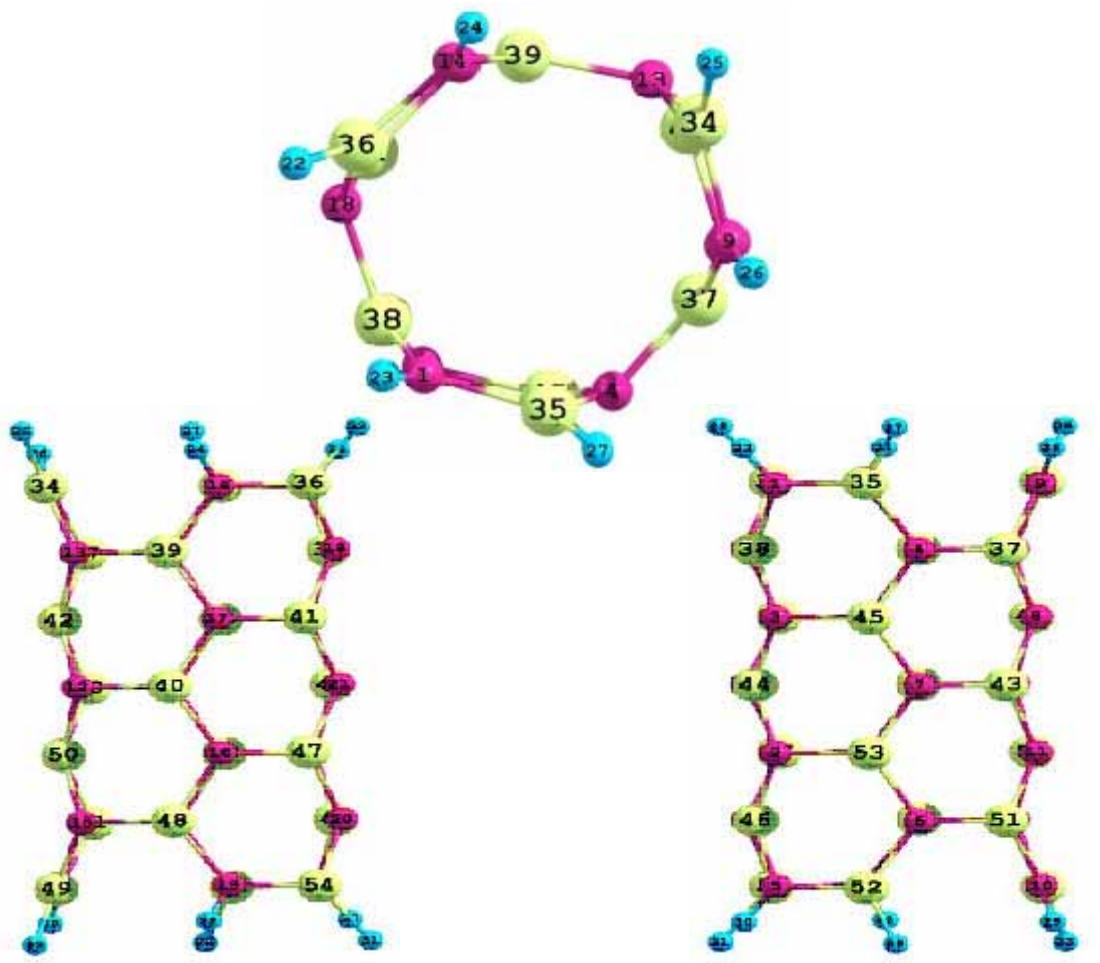

Fig 1. 2D views of the perfect in (3,3) armchair model of AlNNTs.

and 1.583 to 1.840 Å in H_2O-attach state (Table 2). Variation range of bond length of ^{7}N-^{1}H is about 1.019 Å in perfect state and after attaching of H_2O group, it is about 1.018 to 1.020 Å. But changing of bond length in ^{13}Al-^{7}N is different and its variation range is about 1.880 to 1.807 Å in perfect state that by attaching of H_2O group, it is about 1.783 to 1.821 Å (Fig 3 and 4). These obtained results are completely similar to zigzag (10,0) model of AlNNTs that is reported about 1.820 to 1.830 [11]. Maximum variation for $^{7}N10$- $^{13}Al40$, are varied from 1.807 to 1.788 Å and for $^{7}N14$-$^{13}Al59$ are varied from 1.807 to 1.873 Å. It is because that hydrogen in H_2O group is being near to $^{7}N13$ and it is in middle of $^{13}Al59$ and $^{13}Al60$ atoms and hydrogen atoms attract ^{7}N atom. By comparison of two nanotubes in perfect and armchair state, it is shown that, variation ranges aren't so much in two different state and results are similar approximately.

NMR properties

For calculation of NMR properties, at first all structures were optimized. After that, NMR parameters were considered by GIAO method for all proposed structures. So CS^{I} and CS^{A} were considered in different states of AlNNTs (Table 3, 4).

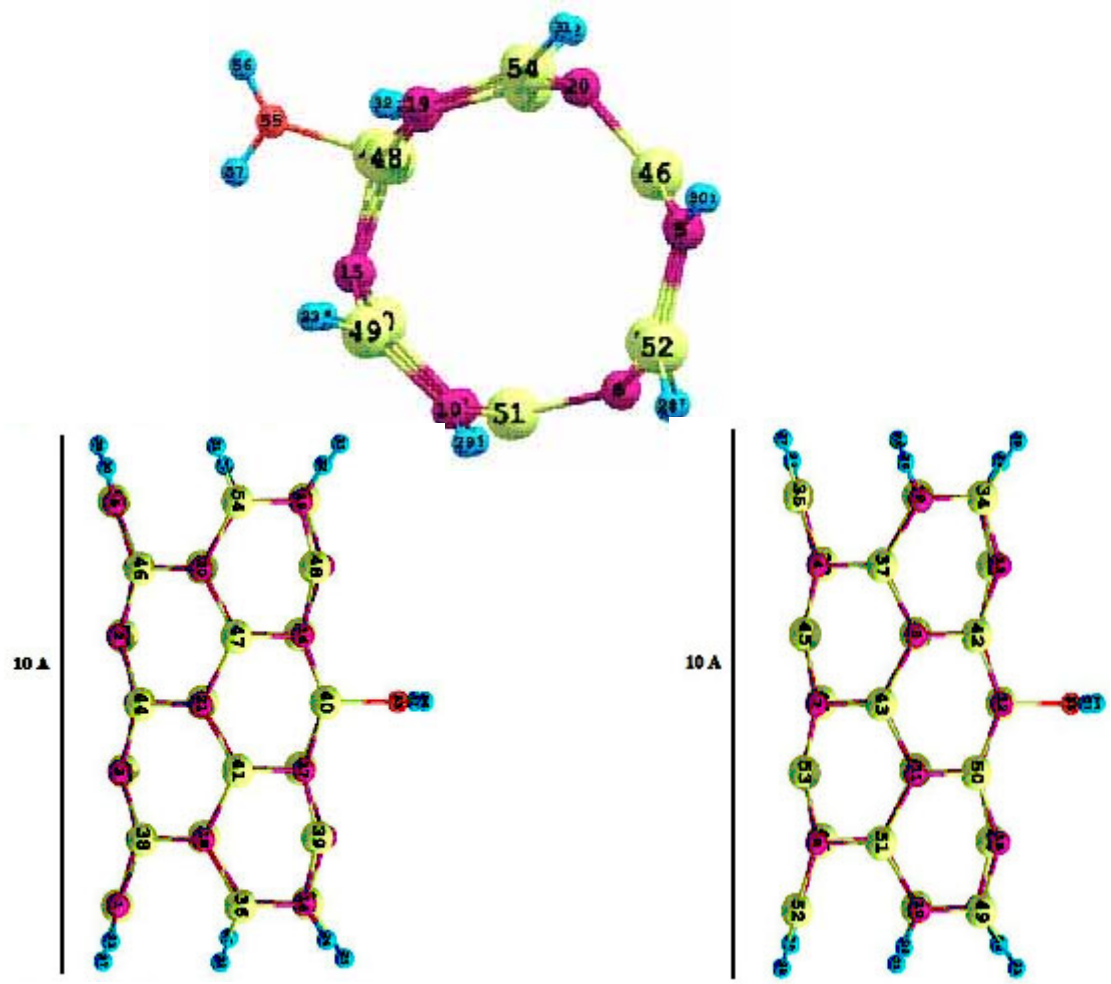

Fig 2. 2D views of the H_2O-attach in (3,3) armchair model of AlNNTs.

CS^I parameter

CS^I in armchair (3,3) AlNNTs in perfect and H_2O-attach

Quality of obtained results for chemical shift in different nucleus of oxygen, nitrogen and aluminum are reported in Table 3. AlNNTs is symmetric of chemical property in perfect state. Because of it, similar results are obtained for CS^I values in different parts of structure. The CS^I value for AlNNTs in armchair (3,3) model and without H_2O-attach, has minimum amount and it is about 168.08 ppm for ^{7}N8 nucleus and has maximum amount for ^{7}N19 and ^{7}N14 nucleuses, is 197.60 ppm (Fig 1). As a result, H_2O has no effect on CS^I value of ^{7}N nucleus but by investigation of CS^I value of ^{13}Al nucleus, maximum value of CS^I in perfect state in ^{13}Al34 nucleus is 440.31 ppm and maximum value of CS^I in ^{13}Al40 nucleus is 460.26 ppm. By addition of H_2O, some changes have been seen in this process and for ^{13}Al40 that attached to oxygen directly, CS^I has maximum amount and it's 501.36 ppm. In ^{13}Al35 and ^{13}Al52 nucleuses, minimum amount of CS^I has been seen and it's 439.89 ppm. Chemical shift for ^{8}O55 nucleus is 284.40 ppm. As obtained results, ^{13}Al has maximum amount of CS^I, ^{8}O has medium amount and ^{7}N and after that ^{1}H have minimum amount of CS^I. All obtained results depend on quality of field strength, shielding or deshielding groups and electron density of in different nucleus.

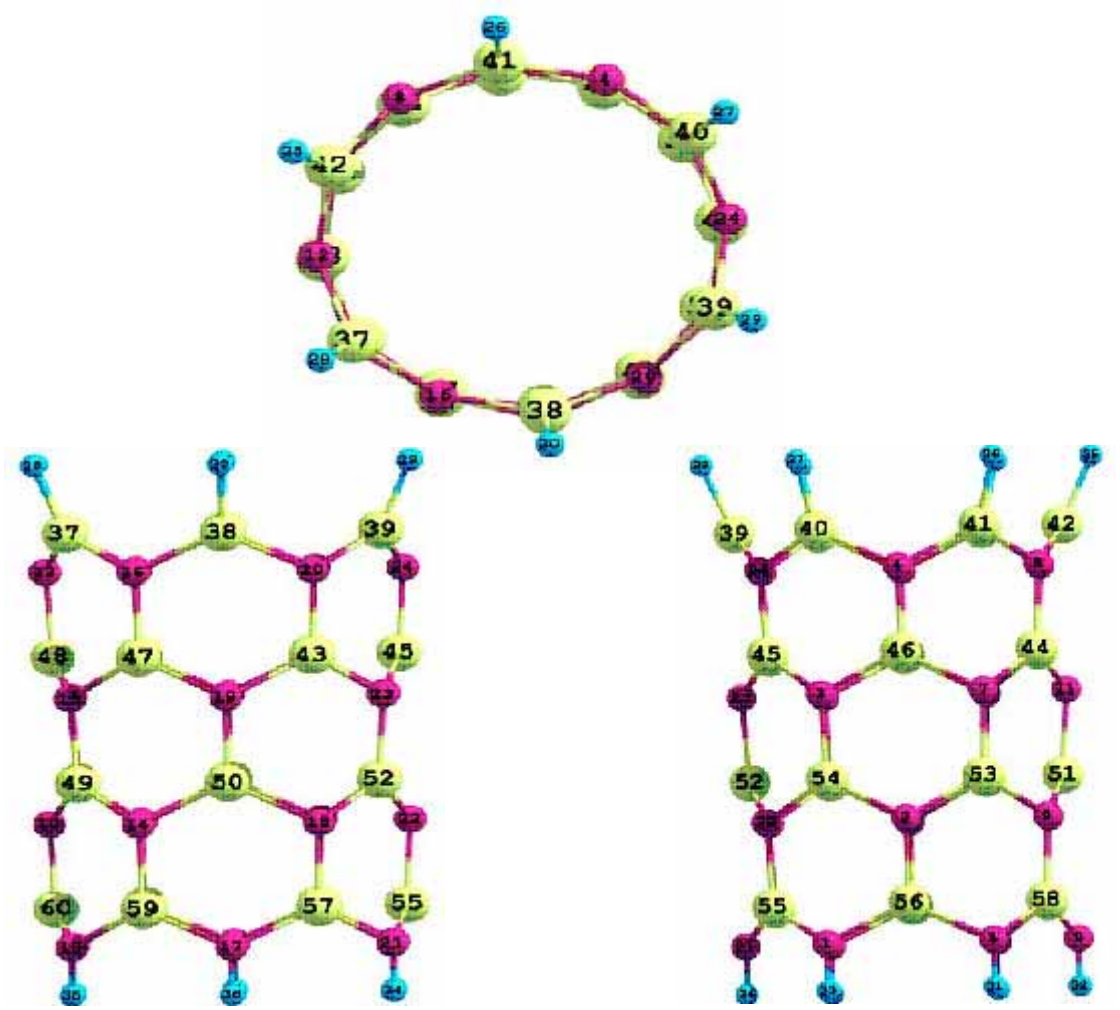

Fig 3. 2D views of the perfect in (6,0) zigzag model of AlNNTs.

CS^{I} in zigzag (6,0) AlNNTs in perfect and H_2O-attach

Investigating of AlNNTs zigzag (6,0) in perfect and H_2O-attach state, is shown that, changing of CS^{I} in this state, is different from armchair state (Table 4, Fig 3 and 4). Investigating of ^{7}N nucleus is shown that, before addition of H_2O, minimum amount of CS^{I} for $^{7}N8$ nucleus is 137.18 ppm and maximum amount of CS^{I} for $^{7}N1$, $^{7}N5$, $^{7}N9$, $^{7}N13$, $^{7}N17$, $^{7}N21$ nucleuses is 221.44 ppm (See table 4). However, value of CS^{I} is changed after attaching H_2O group and $^{7}N12$ nucleus of CS^{I} is minimum value and for $^{7}N5$ nucleus has maximum value. Investigating of CS^{I} in ^{13}Al nucleus is shown that before addition of H_2O, $^{13}Al40$ and $^{13}Al37$ have minimum amount of CS^{I} and it's about 433.37 ppm, $^{13}Al54$ and $^{13}Al49$ nucleuses have maximum amount of CS^{I}, it's about 454.54 ppm. Moreover after attaching of H_2O group, minimum value of chemical shift for $^{13}Al49$ nucleus, CS^{I} has maximum amount and it's 498.05 ppm. However, CS^{I} value for $^{8}O61$ nucleus is 255.67 ppm. Comparison of these two armchair and zigzag models, is shown that CS^{I} value in zigzag model is less than armchair model. In same nanotube, obtained CS^{I} value for ^{7}N nucleus, is in range of 129 to 213 ppm, and it's so close to obtained results[10].

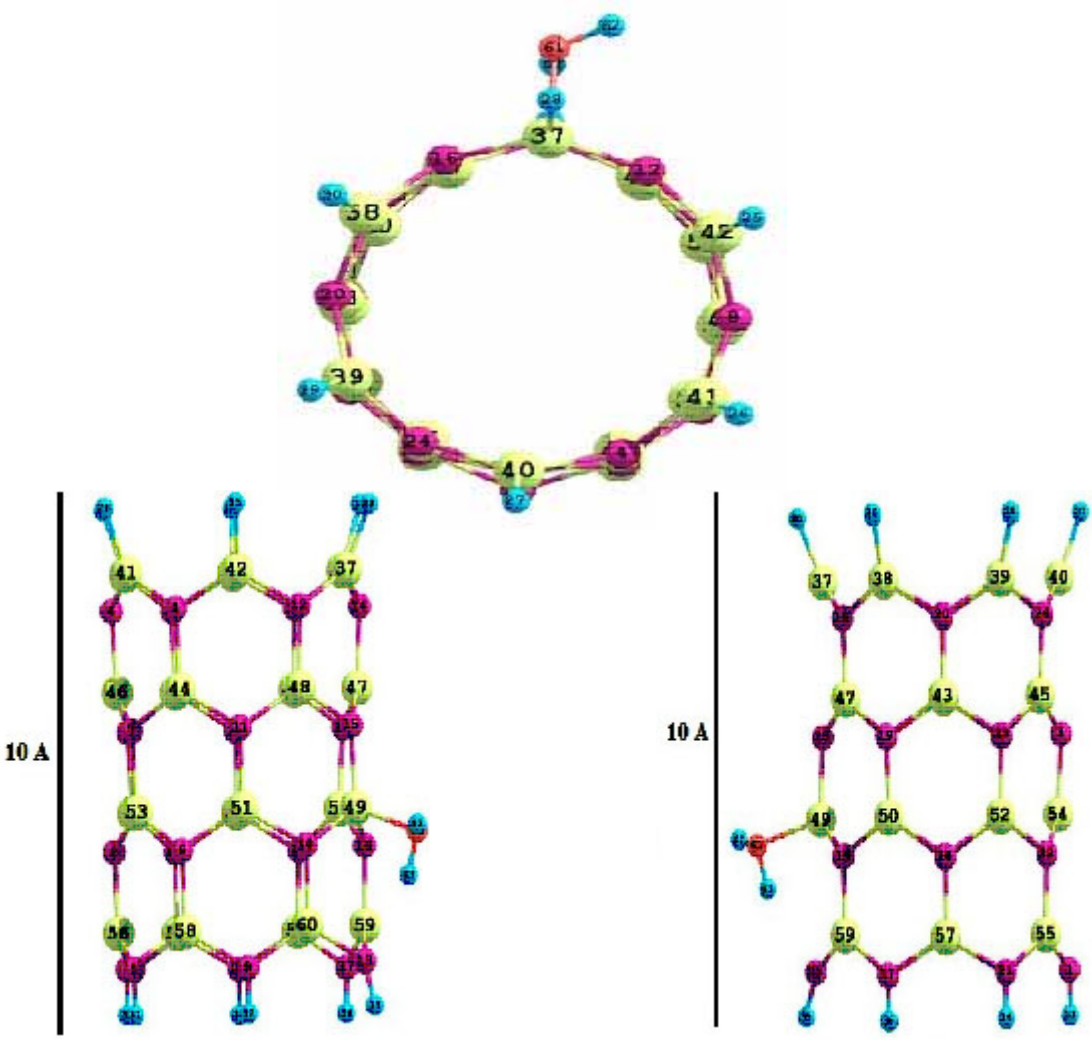

Fig 4. 2D views of the H_2O-attach in (6,0) zigzag model of AlNNTs.

CS^A parameter

CS^A in armchair (3,3) AlNNTs in perfect and H_2O-attach

Obtained results of CS^A analysis are shown that, in AlNNTs structure, obtained values of this parameter are different in armchair and zigzag models and addition of H_2O group has direct effect on this parameter (Table 3). Investigating of ^7N nucleus is shown that minimum amount of CS^A before attaching of H_2O is in $^7N16$ and $^7N17$ nucleuses, and it's about 52.36 ppm. But after addition of H_2O group, CS^A parameter is changed that minimum amount of CS^A in $^7N13$ nucleus is 52.62 ppm. But in ^{13}Al nucleus, before attaching of H_2O, maximum amount of CS^A in $^{13}Al53$ and $^{13}Al45$ nucleuses is 49.66 ppm and minimum amount of CS^A in $^{13}Al35$ and $^{13}Al52$ nucleuses is 23.50 ppm (Fig 3). After attaching of H_2O, this series are changed, that base of it, CS^A in $^{13}Al35$ and $^{13}Al52$ nucleuses is 22.62 ppm and for $^{13}Al40$ nucleus that attached to H_2O directly, is 66.87 ppm and it is maximum amount of CS^A. However CS^A value for $^8O55$ nucleus is obtained about 52.92 ppm

Table 1: Bond length (Angstrom) of perfect and H_2O-attach in (3,3) armchair model of AlNNTs.

Bond length	Armchair Perfect	Armchair H_2O attach	Bond length	Armchair Perfect	Armchair H_2O attach
N1- H23	1.016	1.016	N13- Al34	1.814	1.812
N1- Al35	1.807	1.805	N13- Al39	1.813	1.815
N1- Al38	1.813	1.815	N13- Al42	1.818	1.824
N2- Al44	1.812	1.814	N14- Al24	1.016	1.016
N2- Al46	1.815	1.815	N14- Al36	1.807	1.807
N2- Al53	1.820	1.819	N14- Al39	1.813	1.815
N3- Al38	1.815	1.815	N15- Al48	1.813	1.815
N3- Al44	1.812	1.814	N15- Al49	1.814	1.812
N3- Al45	1.820	1.819	N15- Al50	1.818	1.824
N4- Al35	1.814	1.814	N16- Al40	1.812	1.835
N4- Al37	1.812	1.813	N16- Al47	1.820	1.813
N4- Al45	1.818	1.820	N16- Al48	1.814	1.809
N5- Al30	1.016	1.016	N17- Al39	1.814	1.809
N5- Al46	1.813	1.815	N17- Al40	1.812	1.835
N5- Al52	1.807	1.805	N17- Al41	1.820	1.813
N6- Al51	1.812	1.813	N18- Al36	1.814	1.811
N6- Al52	1.814	1.814	N18- Al38	1.813	1.811
N6- Al53	1.818	1.820	N18- Al41	1.819	1.824
N7- Al43	1.821	1.821	N19- H32	1.016	1.016
N7- Al45	1.813	1.815	N19- Al48	1.813	1.815
N7- Al53	1.813	1.815	N19- Al54	1.807	1.807
N8- Al37	1.815	1.812	N20- Al46	1.813	1.811
N8- Al42	1.821	1.823	N20- Al47	1.819	1.824
N8- Al43	1.813	1.811	N20- Al54	1.814	1.811
N9- H26	1.016	1.016	N21- Al41	1.814	1.812
N9- Al34	1.806	1.807	N21- Al44	1.821	1.817
N9- Al37	1.813	1.813	N21- Al47	1.814	1.812
N10-H29	1.016	1.016	H22- Al36	1.584	1.585
N10- Al49	1.806	1.807	H25- Al34	1.584	1.586
N10- Al51	1.813	1.813	H27- Al35	1.584	1.585
N11- Al43	1.813	1.811	H28- Al52	1.584	1.585
N11- Al50	1.821	1.823	H31- Al54	1.584	1.585
N11- Al51	1.815	1.812	H33- Al49	1.584	1.586
N12- Al40	1.821	1.860	Al40- O55	-	2.007
N12- Al42	1.814	1.807	H56- O55	-	0.969
N12- Al50	1.814	1.807	H57- O55	-	0.972

Table 2: Bond length (Angstrom) of perfect and H_2O-attach in (6,0) zigzag model of AlNNTs

Bond length	Zigzag Perfect	Zigzag H_2O attach	Bond length	Zigzag Perfect	Zigzag H_2O attach
N1- H33	1.019	1.019	N14- Al59	1.807	1.783
N1- Al55	1.815	1.816	N15- Al47	1.815	1.816
N1- Al56	1.815	1.816	N15- Al48	1.815	1.815
N2- Al53	1.816	1.818	N15- Al49	1.811	1.835
N2- Al54	1.816	1.818	N16- Al37	1.818	1.817
N2- Al56	1.807	1.806	N16- Al38	1.818	1.815
N3- Al45	1.815	1.816	N16- Al47	1.814	1.819
N3- Al46	1.815	1.815	N17- H36	1.019	1.017
N3- Al54	1.811	1.810	N17- Al57	1.815	1.823
N4- Al40	1.818	1.818	N17- Al59	1.815	1.806
N4- Al41	1.818	1.818	N18- Al50	1.816	1.821
N4- Al46	1.814	1.814	N18- Al52	1.816	1.815
N5- H31	1.019	1.019	N18- Al57	1.807	1.806
N5- Al56	1.815	1.816	N19- Al43	1.815	1.808
N5- Al58	1.815	1.814	N19- Al47	1.815	1.816
N6- Al51	1.816	1.821	N19- Al50	1.811	1.808
N6- Al53	1.816	1.817	N20- Al38	1.818	1.818
N6- Al58	1.807	1.805	N20- Al39	1.818	1.815
N7- Al44	1.815	1.816	N20- Al43	1.814	1.814
N7- Al46	1.815	1.815	N21- H34	1.019	1.019
N7- Al53	1.811	1.812	N21- Al55	1.815	1.816
N8- Al41	1.818	1.816	N21- Al57	1.815	1.814
N8- Al42	1.818	1.818	N22- Al52	1.816	1.819
N8- Al44	1.814	1.814	N22- Al54	1.816	1.817
N9- H32	1.019	1.018	N22- Al55	1.807	1.806
N9- Al58	1.815	1.821	N23- Al43	1.815	1.817
N9- Al60	1.815	1.806	N23- Al45	1.815	1.815
N10- Al49	1.816	1.866	N23- Al52	1.811	1.812
N10- Al51	1.816	1.800	N24- Al39	1.818	1.819
N10- Al60	1.807	1.788	N24- Al40	1.818	1.817
N11- Al44	1.815	1.809	N24- Al45	1.814	1.814
N11- Al48	1.815	1.816	H25- Al42	1.582	1.584
N11- Al51	1.811	1.809	H26- Al41	1.582	1.583
N12- Al37	1.818	1.818	H27- Al40	1.582	1.583
N12- Al42	1.818	1.815	H28- Al37	1.582	1.583
N12- Al48	1.814	1.818	H29- Al39	1.582	1.583
N13- H35	1.019	1.020	H30- Al38	1.582	1.584
N13- Al59	1.815	1.856	O61- H62	-	0.973
N13- Al60	1.815	1.856	O61- H63	-	1.014
N14- Al49	1.816	1.851	O61- Al49	-	2.001
N14- Al50	1.816	1.796			

Table 3: Isotropic Chemical Shift (ppm) and Anisotropic Chemical Shift (ppm) values for various nucleus of perfect and H_2O-attach in (3,3) armchair model of AlNNTs

Armchair (3,3) AlNNTs	Perfect		H_2O-Attach	
	CS^I	CS^A	CS^I	CS^A
N1	197.13	51.19	196.60	52.62
N2	168.67	17.88	167.37	18.48
N3	168.67	17.88	167.37	18.48
N4	173.03	26.75	171.96	27.96
N5	197.13	51.19	196.60	52.62
N6	173.03	26.75	171.96	27.96
N7	174.42	18.33	173.34	19.97
N8	168.06	17.96	169.98	17.97
N9	197.35	52.36	197.45	52.52
N10	197.35	52.36	197.45	52.52
N11	168.06	17.96	169.98	17.97
N12	173.97	18.55	182.52	11.80
N13	172.17	27.57	170.07	27.18
N14	197.60	52.17	196.32	51.96
N15	172.17	27.57	170.07	27.18
N16	169.41	17.48	172.20	20.31
N17	169.41	17.48	172.21	20.31
N18	171.39	27.42	171.36	24.20
N19	197.60	52.17	196.32	51.96
N20	171.39	27.42	171.36	24.20
N21	173.25	18.15	176.97	22.03
Al34	440.31	23.56	441.21	26.25
Al35	440.89	23.50	439.89	22.62
Al36	440.56	23.68	441.31	26.86
Al37	460.26	34.20	459.95	35.98
Al38	460.01	33.36	459.91	34.69
Al39	460.13	34.59	456.30	43.51
Al40	458.14	49.13	501.36	66.87
Al41	460.16	48.47	457.69	43.02
Al42	460.12	48.38	460.00	57.13
Al43	458.86	48.26	457.14	48.60
Al44	458.65	48.22	458.95	44.57
Al45	459.55	49.69	460.00	46.16
Al46	460.01	33.36	459.90	34.69
Al47	460.16	48.47	457.69	43.02
Al48	460.13	34.59	456.29	43.51
Al49	440.31	23.56	441.21	26.25
Al50	460.12	48.38	460.00	57.13
Al51	460.26	34.20	459.95	35.98
Al52	440.89	23.50	439.89	22.62
Al53	459.55	49.69	460.00	46.16
Al54	440.56	23.68	441.31	26.87
O55	-	-	284.40	52.92
H56	-	-	29.09	21.59
H57	-	-	28.52	14.05

Table 4: Isotropic Chemical Shift (ppm) and Anisotropic Chemical Shift (ppm) values for various nucleus perfect and H_2O-attach in (6,0) zigzag model of AlNNTs

Zigzag (6,0) AlNNTs	Perfect		H_2O-Attach	
	CS^I	CS^A	CS^I	CS^A
N1	221.23	30.27	219.98	35.20
N2	183.63	28.82	182.47	29.86
N3	173.32	27.71	172.12	28.12
N4	137.58	67.26	137.08	67.16
N5	221.44	28.42	221.69	27.85
N6	183.28	30.43	184.64	24.58
N7	173.94	26.84	174.65	26.59
N8	137.18	67.86	138.00	66.83
N9	221.44	28.42	219.72	27.75
N10	183.63	28.82	177.58	31.01
N11	173.94	26.84	174.98	25.45
N12	137.58	67.26	134.61	67.96
N13	221.23	30.27	220.80	21.98
N14	183.63	28.82	181.62	31.86
N15	173.32	27.71	178.97	25.82
N16	137.58	67.26	134.72	68.16
N17	221.44	28.42	221.03	27.36
N18	183.28	30.43	184.61	26.18
N19	173.94	26.84	175.40	25.06
N20	137.18	67.86	138.25	67.03
N21	221.44	28.42	221.41	27.85
N22	183.63	28.82	182.22	29.98
N23	173.94	26.84	174.38	26.75
N24	137.58	67.26	137.02	67.20
Al37	437.37	9.08	435.55	9.54
Al38	437.52	9.08	439.17	12.12
Al39	437.52	9.08	437.44	9.85
Al40	437.37	9.08	437.16	8.70
Al41	437.52	9.08	437.35	9.54
Al42	437.52	9.08	439.06	11.79
Al43	454.53	28.30	454.56	31.62
Al44	454.53	28.30	454.53	30.85
Al45	454.40	28.19	453.75	27.87
Al46	454.40	28.19	453.88	28.00
Al47	454.40	28.19	454.61	37.07
Al48	454.40	28.19	453.47	37.33
Al49	454.54	36.33	498.05	65.52
Al50	454.01	36.68	455.23	42.03
Al51	454.01	36.68	454.57	42.82
Al52	454.01	36.68	454.06	37.68
Al53	454.01	36.68	454.12	38.15
Al54	454.54	36.33	453.44	37.16
Al55	450.48	34.89	449.38	37.32
Al56	450.48	34.89	449.33	37.23
Al57	450.67	35.40	453.07	46.78
Al58	450.67	35.40	452.91	46.30
Al59	450.48	34.89	444.45	63.48
Al60	450.48	34.89	442.35	62.81
O61	-	-	255.67	33.97
H62	-	-	30.11	15.86
H63	-	-	23.43	24.80

CS^A in zigzag (6,0) AlNNTs in perfect and h20 attach

Obtained results for CS^A value in AlNNTs in zigzag (6,0) model are similar to armchair model. However obtained values have few differences (Table 4). For ^7N nucleus in AlNNTs, before attaching of H_2O group, CS^A value for $^7N7$,$^7N11$,$^7N19$ and $^7N23$ nucleuses is similar to each other and it's 26.84 ppm that is minimum amount of CS^A. But when H_2O is attached to AlNNTs structure, minimum amount of CS^A for $^7N13$ nucleus is 21.98 and maximum amount of CS^A is in $^7N16$ nucleus. Obtained results are shown that, attaching of H_2O group has no effect on ^7N nucleus. However investigating of ^{13}Al nucleus before attaching of H_2O group is shown that minimum amount of CS^A in $^{13}Al37$, $^{13}Al38$, $^{13}Al39$, $^{13}Al40$, $^{13}Al41$ and $^{13}Al42$ is 2.08 ppm and $^{13}Al50$, ^{13}Al 51, $^{13}Al52$ and $^{13}Al53$ nucleuses (36.68 ppm) have maximum amount of CS^A (Fig 3). But after addition of H_2O, this process is changed. In $^{13}Al49$ nucleus that attached to Oxygen of H_2O group directly, has maximum amount of CS^A and it's 65.52 ppm but in $^{13}Al40$ nucleus, minimum amount of CS^A is 8.70 ppm. However, CS^A value for $^8O61$ is 33.97 ppm. For AlNNTs in zigzag (10,0) model, CS^A value for ^{13}Al nucleus is in range of 16 to 29 ppm and for ^1H nucleus is in range of 19 to 63 ppm that is in agreement to other results[13-20].

CONCLUSION

→ In perfect state, for each armchair and zigzag models, regular and symmetric processes exist for bond length and NMR parameters, that by attaching H_2O group, this regular changing will be changed and range of this changes increased regard to perfect state.

→ Investigating of CS^I value in different state is shown that by addition of H_2O group, this parameter is changed and CS^I value for ^{13}Al nucleus in AlNNTs is more than ^8O and ^7N nucleuses.

→ Investigating of CS^A process is shown that, this variation after attaching of H_2O in AlNNTs zigzag (6,0) model is more than AlNNTs armchair (3,3). However, by attaching of H_2O group, CS^A in different nucleus is changed strongly in armchair and zigzag models.

→ When hydrogen atom in H_2O group being near to AlNNTs structure, structural parameters are changed that is because of attraction effects of two hydrogen atoms and tendency for formation hydrogen bond.

→ In final by attaching of H_2O group to AlNNTs, electronic density, CS^A and CS^I value in various nucleuses, bond lengths and bond angles is changed and have more affected on nucleus that attach to H_2O group directly.

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