

Theoretical Study for Electronic and Vibrational properties of nano cylinder ($C_{140}H_{28}$).

Huda N. AL-Ani¹

¹Department of Chemistry, College of Science, University of Baghdad Jadiriya, Baghdad, Iraq

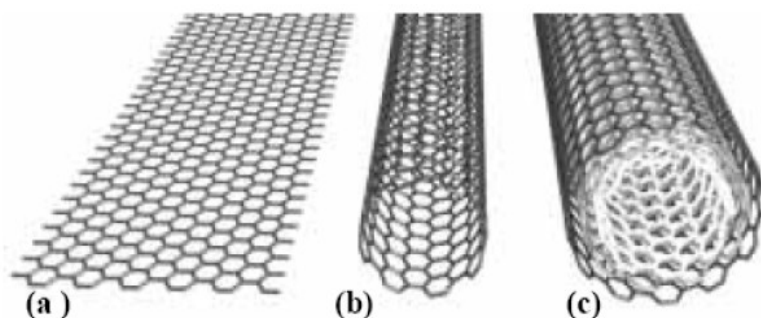
Abstract: Semi-empirical methods were applied for calculating the vibration frequencies and IR absorption intensities for normal coordinates of the (**armchair nano cylinder**) ($C_{140}H_{28}$) single wall carbon nanotube(SWCNT) at equilibrium geometry which was found to has D_{7d} symmetry point group. Assignment of the modes of vibration (3N-6) was done depending on the pictures of their modes by applying (Gaussian 03) program. Comparison of the vibration frequencies of the nanotube which are active in IR, and inactive in Ramman spectra. For C-H stretching vibrations. The results show the relation for axial bonds, which are the vertical C-C bonds (annular bonds) in the rings and for circumferential bonds which are the outer ring bonds. Also include the assignment of puckering, breathing and clock-anticlockwise bending vibrations. They allow a comparative view of the charge density at the carbon atom too.

Keywords: SWCNT single wall carbon nano tube; G03 aprogram for calculation. ; γ : Out of plane modes of the molecule; δ : In- plane modes of the molecule.

I. Introduction

Carbon nanotubes were discovered in 1991 by Iijima [1]. Since then, efforts in synthesis, characterization and theoretical investigation on nanotubes have grown exponentially. This is mostly due to their perceived novel mechanical and electronic properties and their tremendous potential for future technological applications. In 1993, the simplest kind of carbon nanotubes, single-walled carbon nanotubes (SWNTs), were discovered independently by the Iijima group [2] and an IBM team headed by Bethune [3]. These SWNTs can be regarded as a rolled-up graphite sheet in cylindrical form. Some specific defect-free forms of these SWNTs show remarkable mechanical properties and metallic behavior [4]. These materials present tremendous potential as components for use in nano-electronic and nano-mechanical device applications or as structural elements in various devices. New and exciting phenomena have been observed[5], including field emission [6], quantum conductance [7], superconductivity[8], and higher thermal conductivity than diamond[9]. Depending upon structure, the nanotubes are either metallic or insulating, which is a feature that has been intensively investigated and exploited in prototype devices [5]. CNTs are extraordinarily flexible and do not break upon mechanical deformation. For example, they can be bent mechanically by mechanical milling, or by embedding the tubes in a polymeric resin[10], [11-13].

The vibrational modes of nanoscale spheres and tubes have been of great interest recently with advances in techniques for fabricating or synthesizing these structures [14]. Even for such small systems, continuum models are known to yield useful approximate description and provide valuable insight. Continuum models have been successfully used to study embedded nanoscale structures in two and one dimension such as heterostructures[15] They have also been applied to nonembedded nanoscale structures. For example, the continuum model has been used in the study of the radial breathing mode frequencies of nanospheres, including the effects of damping due to environmental interactions[16-18]. Also, the model has been applied to the study of both the normal modes and the energetics of fullerenes. [19,20] In such continuum models, the nanoscale properties of a material are frequently described with adequate accuracy by its bulk elastic properties[21]. As discussed in the previous work, nanotube deformation has been examined experimentally. Recent investigations have shown that carbon nanotubes possess remarkable mechanical properties, such as exceptionally high elastic modulus [22,23], large elastic strain and fracture strain sustaining capability[24,25]. Similar conclusions have also been reached through some theoretical studies[26-29] although very few correlations between theoretical predictions and experimental studies have been made.



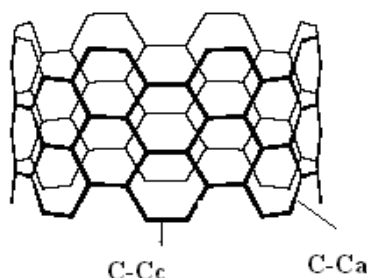
"Fig. 1": Carbon Nanotubes are made of single graphene sheets. (a) Shows cut-out part of a graphite lattice, (b) Shows a SWCNT, (c) Shows MWCNT where several CNTs are nested concentrically

II. Methods of calculation

Both G03 program by PM3 method [30], and Mopac 2000 program by PM3 method, Computational Packages have been employed throughout this study to compute the geometrical Parameters (bond lengths and bond angles) and the energetic properties [31] were applied throughout the present work.

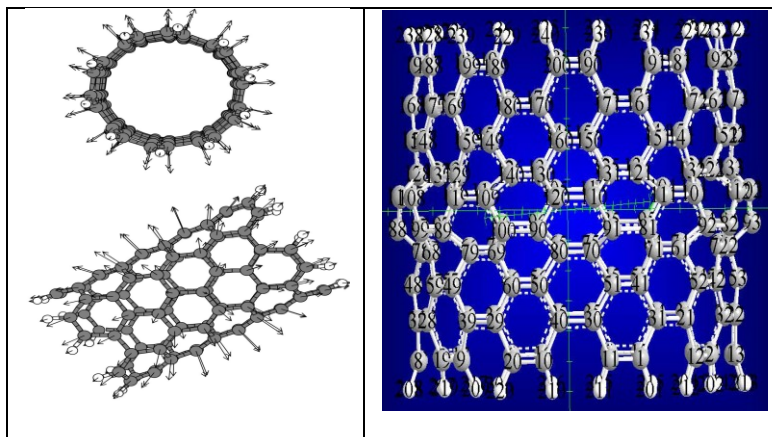
III. Results and Discussion.

To study the vibration motions of such molecules, one has to define its geometric parameters, and has to distinguish between the axial CC (C-Caxial) bonds and circumferential CC (C-Cc) bonds, (figure.2) shows the two types of bonds in an armchair CNT [32].



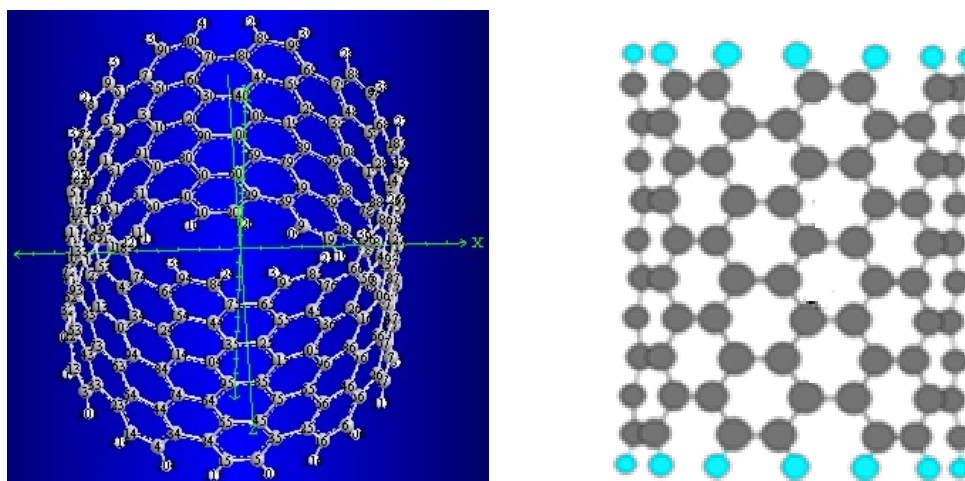
"Fig.2": Structure of armchair CNT, indicating the two types of C-C bonds; C-Caxial (C-Ca) and C-Ccircumferential (C-Cc).

Various quantum mechanical studies were done for the physical properties of the nanotubes [33-36]. Structure deformation is expected to change their thermal and electronic properties too. Basic vibrations of SWCNTs were measured and assigned as breathing, puckering and clock-anti-clockwise deformation modes [37]. They are considered as finger print vibrations for the carbon nanotubes (CNTs) [38]. The active vibrations causes a change in its geometry structure "Fig. 3", The calculation gives different geometry were done to study the impact of the puckering distortion on the electronic properties of CNTs [39-41]. For a normal mode of vibration to be infrared active, there must be a change in the dipole moment of the molecule during the course of vibration. During the vibration motion of a molecule, a regular fluctuation in the dipole moment occurs, and a field is established which can interact with the electrical field associated with radiation. For the absorption of infrared radiation, a molecule must undergo a net change in its dipole moment as a result of its vibrational or rotational motions [42].



"Fig. 3": Structure deformation of a SWCNT as caused by its vibration motion

The classifications of carbon nanotube (**armchair nano cylinder**), determined by the type (armchair) of the tube, can also be described as single-walled nanotube (SWNT), resembling by rolling a graphene sheet into a cylinder mathematically structures are uniquely defined by specifying the coordinates of the smallest folding vector (n,n), (armchair) molecule. The (PM3) calculated equilibrium geometry shows D_{7d} symmetry [43-44], "Fig. 4".



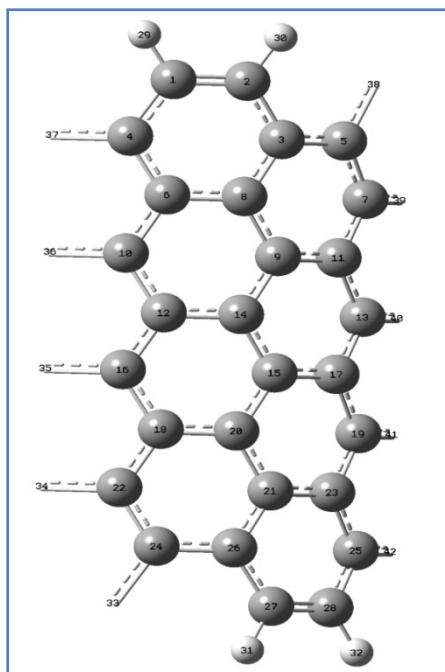
"Fig. 4": Equilibrium geometry of carbon nanotube

((**armchair nano cylinder**))single wall carbon nanotube (SWCNT) by using Mopac 2000 program. D_{7d} [45], "Fig. 5". and "Table 1", shows a repetitive sections of bonds. Due to their symmetry (Table 1: shows comparison of their calculated geometric parameters.

"Table 1": PM3 calculated bond distance and bond angles of (CNT) for (**armchair nano cylinder**)

Bond length (Å) and Bond angles (deg.)	nano tube $C_{140}H_{28}$
$C_1C_8^{**}$	1.3672
$C_1C_{22}^*$	1.4246
$C_8C_{21}^*$	1.4245
$C_{21}C_{36}^*$	1.4246
C_1H_{141}	1.0996
C_8H_{148}	1.0996
C_7H_{147}	1.0996
$C_{14}H_{156}$	1.0996
$C_7C_{14}^{**}$	1.3672
$C_7C_{28}^*$	1.4246
$C_{21}C_{28}^{**}$	1.43960
$C_{21}C_{36}^*$	1.40319

$C_{28}C_{35}^*$	1.40318
$\langle C_8C_1C_{22}$	120.2804
$\langle C_8C_1H_{141}$	121.6814
$\langle C_{22}C_1H_{141}$	117.8105
$\langle C_{14}C_7 H_{147}$	121.6904
$\langle C_{28}C_7 H_{147}$	117.8027
$\langle C_{14}C_7C_{28}$	120.2812
$\langle C_1C_8C_{21}$	120.2816
$\langle C_1C_8H_{148}$	121.6866
$\langle C_{21}C_8H_{148}$	117.8055
$\langle C_8C_{21}C_{28}$	121.3644
$\langle C_8C_{21}C_{36}$	118.374
$\langle C_{28}C_{21}C_{36}$	118.8102
$\langle C_3C_{24}C_{17}$	121.3676
$\langle C_3C_{24}C_{31}$	118.3696
$\langle C_{17}C_{24}C_{31}$	118.8098



"Fig.5": Repetitive sections of bonds and angles for (CNT) of (armchair nano cylinder) SWCNT at their equilibrium geometries according to point group(D_{7d}). SWCNT.

"Table 2": PM3 calculated bond distances of axial bond and circumferential bond for (armchair nano cylinder) SWCNT.

Arm Chair (SWCNT)	Diameter (Å)	CNT Length (Å)	Bond length (Å)						
			=C...Ca	-C...Ca	...C...Ca	C=Cc	C...Cc	C-Cc	C-H
(7,7) Arm Chair SWCNT D_{7d}	10.041	12.901	1.4246	-----	1.4031 1.4346 1.4301 1.4044	1.3670	1.4276 1.4292 1.3974 1.4395	-----	1.0996

C-Ca: axial bond.

C-Cc: circumferential bond

Noting that the C-Ca bonds in the angular SWCNTs are conjugated double bonds for all of different rings layer, but it may be connect to (CC double or single or conjugated double bond). The C-Cc bonds are

double or conjugated double bond of carbon (armchair nano cylinder) SWCNT, and double or conjugated double bond or single bond of carbon nanotube.

The C=Cc bond decrease with increasing of rings layer. For (C-H) and (C-Cc) bonds are longer in SWCNT.

Also note that (...C...Ca), increase in length from outer to centre in CNT, and decrease in length from outer to centre in CNT. "Fig. 5", "Table 1".

"Table 3": shows some physical properties of calculated for (nano cylinder) armchair SWCNT at the equilibrium geometry.

"Table 3": Some physical properties of the calculated for (armchair nano cylinder) SWCNT at the equilibrium geometry by using Mopac2000 program.

ΔH_f =heat of formation, HOMO=Highest Occupied molecular orbital, LUMO=Lowest Unoccupied molecular orbital, ΔE = The difference in energy levels.

ΔH_f increase with increasing the length of CNT, ΔE (LUMO-HOMO) decrease with increasing the length of CNT that prove their electrical conductivity increased with increasing number of rings layer. Dipole moment μ is zero for all, because the CNT has center of inversion symmetry element. same relation noticed for vibrations modes (IR active).

Arm Chair (SWCNT)	M. Wt. g/ mol	ΔH_f kcal/mol,(kJ)	μ (debye)	HOMO (eV)	LUMO (eV)	ΔE (eV) LUMO-HOMO
Nano cylinder $C_{140}H_{28}$	1709.761	721.486 3018.699	0.000	-7.403	-2.437	4.066

3.1.Vibration frequencies assignment of armchair nano cylinder ($C_{140}H_{28}$) SWCNT.

The armchair CNT posses 498 fundamental vibrations ($3N-6$). Inspection of its irreducible representation, as defined by the symmetry character table, results in the following modes of vibration;

$$\Gamma_{\text{vibration}} = \Gamma_{\text{total}} - (\Gamma_{\text{rotation}} + \Gamma_{\text{translation}}) = 3N - 6 = 498$$

$$\Gamma_{\text{vibration}} = 36E_3u + 36E_3g + 36E_2g + 36E_2u + 35E_1u + 35E_1g + 18A_1u + 17A_2g + 18A_1g + 17A_2u = 498$$

These are 87 IR active ($35E_1u$, and $17A_2u$). Their assignments are as follow:

Relative to the σ_h reflection the vibration modes are classified as symmetric and antisymmetric modes.

3.1.1.CH stretching vibration

These are 28 in number, the displacement vectors of which are located at the H atoms. Their calculated vibration frequencies (IR active) as modes range from ($3004.3- 3029.0 \text{ cm}^{-1}$), Inspecting the values in "Table 4".

3.1.2.Ring (CCC) stretching vibration

Their displacement vectors are not located at definite C atoms as could be seen from the atomic displacement vectors. Their calculated vibration frequencies (IR active) as modes range from ($1409.13- 1796.6 \text{ cm}^{-1}$), Inspecting the values in "Table 4".

3.1.3.In-plane CH bending vibration (δCH)

There are as few as the C-H bonds. Their displacement vectors are mainly located at the corresponding H atoms. Their calculated vibration frequencies (IR active) as modes range from ($149.7- 1067.7 \text{ cm}^{-1}$), Inspecting the values in "Table 4".

3.1.4.In-plane (CCC) bending vibration (δCCC)

Their calculated vibration frequencies (IR active) as modes range from ($149.7- 1343.7 \text{ cm}^{-1}$), Inspecting the values in "Table 4".

3.1.5.Out of plane CH bending vibration (γCH)

Their calculated vibration frequencies (IR active) as modes range from ($270.1- 1288.6 \text{ cm}^{-1}$), Inspecting the values in "Table 4".

3.1.6.Out of plane ring bending vibration (γCCC)

The modes include puckering deformations, as well as breathing vibrations of the whole ring. Their calculated vibration frequencies (IR active) as modes range from ($256.3- 1363.9 \text{ cm}^{-1}$), Inspecting the values in "Table 4". includes the calculated frequencies as calculated applying semi-empirical methods (PM3) by Gaussian03 program and IR absorption intensities of the vibration modes. Commonly known, the vibrations

with (intensity= 0.0) are forbidden (IR inactive, Ramman active), those with (intensity \neq 0.0) are allowed (IR active, Ramman inactive).

"Table 4".Vibration frequencies and IR absorption intensities for CNT ($C_{140}H_{28}$) molecule as calculated applying G03 program.

$E_{1u}(in)$	Symmetry & description	PM3 Freq. cm^{-1}	Intensity km/mol
V489	CH str.	3029.03	9.0755
V481	CH str.	3004.26	117.43
V461	C-C str	1796.56	4.349
V457	C=C str	1793.22	14.884
V435	C=C str	1722.35	2.539
V414	C=C str	1675.17	0.278
V403	C-C str	1643.15	1.444
V399	ring (CCC _{str.})	1602.76	0.0197
V369	ring (CCC _{str.})	1556.18	0.4601
V363	C- C str	1536.56	8.336
V352	ring (CCC _{str.})	1498.85	17.8001
V334	ring (CCC _{str.})	1409.13	30.762
V321	δ ring (δ CCC)	1343.71	0.2808
V313	γ CH(wagg.)+ γ ring (γ CCC)	1288.64	6.322
V295	γ CH(wagg.)	1152.63	5.5834
V274	δ CH(siccer.)	1067.71	1.0663
V260	δ CH(siccer.)	1004.26	0.076
V247	γ ring (γ CCC)+ γ CH	964.564	1.2371
V241	γ CH(twiss.)+ γ ring (γ CCC)	945.735	0.0122
V227	γ CH(twiss.)+ γ ring (γ CCC)	896.6	5.1302
V216	δ CH+ δ ring (δ CCC)	858.66	22.623
V204	γ CH(wagg.)+ γ ring (γ CCC)	830.641	46.341
V194	δ CH(rock)	812.82	125.337
V153	γ CH(twiss.)+ γ ring (γ CCC)	674.771	1.1662
V150	δ CH+ δ ring (δ CCC)	664.392	11.594
V143	δ CH(rock.)+ δ ring (δ CCC)	653.804	7.2941
V124	γ CH(wagg.)+ γ ring (γ CCC)	602.856	3.0915
V99	γ CH(twiss.)+ γ ring (γ CCC)	492.552	22.087
V95	γ CH(twiss.)+ γ ring (γ CCC)	481.314	1.5762
V82	γ CH(twiss.)+ γ ring (γ CCC)	436.045	4.3508
V61	γ CH(twiss.)+ γ ring (γ CCC)	357.166	2.9102
V59	γ CH(twiss.)+ γ ring (γ CCC)	346.147	1.0289
V44	γ ring (γ CCC)+ γ CH(wagg.)	284.641	0.935
V38	γ CH(wagg.)+ γ ring (γ CCC)	270.122	5.758
V13	δ CH(rock.)+ δ ring (δ CCC)	149.751	6.048
A _{2u}	Out plan		
V483	CH str.	3008.892	616.385
V442	C=C str	1765.63	14.298
V409	C=C str	1654.39	3.1335
V387	ring (CCC _{str.}) elonga.	1600.18	4.349
V367	ring (CCC _{str.}) elonga.	1542.98	2.304
V348	ring (CCC _{str.})elonga.	1480.57	0.2087
V329	γ ring (γ CCC)	1363.96	100.904
V303	ring (CCC _{str.})	1193.15	5.645
V284	γ CH(twist.)	1114.75	20.534
V260	γ CH(twist.)	1028.51	1.906
V188	δ CH(rock)	801.216	4.297
V147	γ ring (γ CCC)+ γ CH(breath.)	660.794	0.366
V138	γ ring (γ CCC)+ γ CH(breath.)	642.957	2.8819
V109	δ CH(rock)+ δ ring (δ CCC)	518.928	10.4807
V67	δ CH(rock.)+ δ ring (δ CCC)	376.334	1.735
V35	γ ring (γ CCC)(breath.)	256.287	0.4318
V15	δ CH(rock.)+ δ ring (δ CCC)	152.02	0.7306

"Fig. 6":Shows the vibration pictures for some modes of the (nano cylinder) CNT (Armchair), as calculated applying semi-empirical methods (PM3) by Gaussian 03 program.

3.2. The whole relations of (armchair nano cylinder) CNT.

The C-C frequencies different values are calculated for the different bonds of CNT. As expected the differences in the vibration frequencies are due to the different C-C force constants, The frequencies of the vibration modes in "Table 4", point to systematic correlations between the frequencies of different species. This is mostly obvious in the case of the C-H stretching vibrations, for which the following general relation holds:

$$\begin{aligned} \nu_{\text{sym}} \text{CHstr.} (3029.03 \text{ cm}^{-1}) &> \nu_{\text{asym.}} \text{CHstr.} (3008.892 \text{ cm}^{-1}) \\ \nu_{\text{sym}} \text{CC}_{\text{str.}} (1796.56 \text{ cm}^{-1}) &> \nu_{\text{asym}} \text{CC}_{\text{str.}} (1765.6 \text{ cm}^{-1}) \\ \nu_{\text{sym}} \delta \text{ring} (664.39 \text{ cm}^{-1}) &> \nu_{\text{asym.}} \delta \text{ring} (518.928 \text{ cm}^{-1}) \\ \nu_{\text{sym}} \gamma \text{ ring} (1288.64 \text{ cm}^{-1}) &< \nu_{\text{asym}} \gamma \text{ ring} (1363.96 \text{ cm}^{-1}) \\ \nu_{\text{sym}} \delta \text{CH} (1067.71 \text{ cm}^{-1}) &> \nu_{\text{asym}} \delta \text{CH} (801.216 \text{ cm}^{-1}) \\ \nu_{\text{sym}} \gamma \text{ CH} (1288.64 \text{ cm}^{-1}) &> \nu_{\text{asym}} \gamma \text{ CH} (1114.75 \text{ cm}^{-1}) \end{aligned}$$

This interesting result shows that in general the C-H and C-C stretching frequencies of the CNT for symmetric modes are higher than those of the asymmetric modes of CNT molecule.

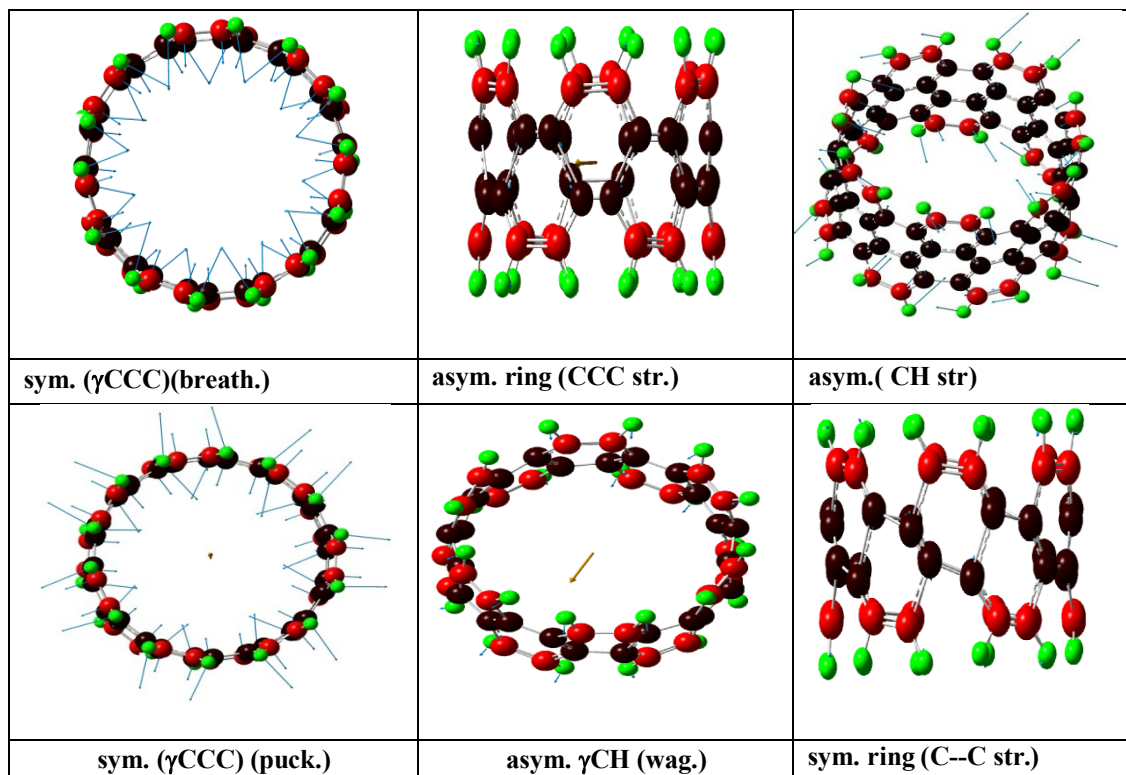
3.3. The results include the relation for IR absorption intensities.

The calculated IR absorption intensities values range from (125.337_ 0.0122 km/mol) for symmetric mods (E_{1u}), and the calculated IR absorption intensities values range from (100.94 - 0.298 km/mol) for asymmetric mods (A_{2u}).

Finally, the calculated vibration frequencies (IR-active) show that vibration frequency values of (C-C stretching), (γ ring, ν ring) vibrations frequency shows higher frequency values in CNT($C_{140}H_{28}$) lead to many more electronic and mechanical applications.

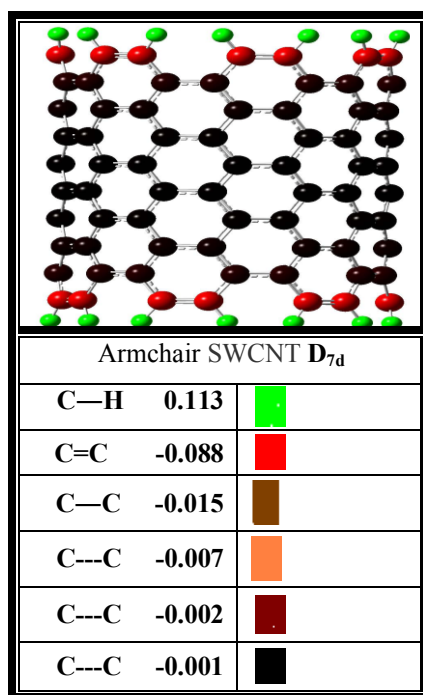
"Table 5": Calculated Vibration frequencies of (nano cylinder) armchair SWCNT applying G03 program by PM3 method.

Arm Chair (SWCNT)	C-H _{str.}	C-C _{str.}	C=C _{str.}	C--C _{str.}
(nano cylinder) armchair SWCNT $C_{140}H_{28}$	3029.11 E_{1u}	1602.70 E_{1u}	1793.22 E_{1u}	1796.50 E_{1u}



"Fig. 6". The graphical pictures of some vibration modes for CNT (armchair) as calculated applying G03 program.

Finally, the calculations show that, similar to the carbon nanotubes [46-47], the charge densities are mainly concentrated at the circumferential carbon and hydrogen atoms of SWCNT, parallel with their physical properties for electrical conductivity. The axial carbon atoms have diminishing charges from outer to centre. The H atoms are positively charged, the C atoms are of the negative charge, "Fig. 7".



"Fig. 7". Distribution of charge density at the atoms of (nano cylinder) armchair SWCNT as calculated applying G03 program.

Note. All calculations were done applying the G03 program of Pople et al . [30].

IV. Conclusion

Quantum mechanics semi-empirical (PM3) calculations were carried out with Gaussian 03 program, for investigated the result In order to calculate the vibration frequencies modes that active in infrared. Comparison of the Vibration modes which were active in IR for the (nano cylinder) armchair nanotube ($C_{140}H_{28}$). Vibrational motion of atoms decreases the electrical conductivity of nanotube and limits the performance of nanotransistors and other electronic devices based on them. Similarly, the stiffness of a nanotube and its capability for transporting heat is reduced with increasing defect density[48,49] They allow a comparative view of the charge density at the carbon atom too. The calculations show that, the charge densities are mainly concentrated at the hydrogen atoms (positively charged) and at the outer circumferential carbon atoms (negatively charge). The axial carbon atoms and the circumferential carbon atoms have diminishing charges from outer to the centre of the CNTs. They can have metallic properties (armchair, some zigzag) depending on their structure. CNTs are much better conductors of electricity than copper nanowires because there is less scatter of electrons. Nanotubes are exceptional ballistic conductors, which can be used in a variety of nanodevices that can operate at room temperature. Nanotubes possess extraordinary mechanical properties and are among the strongest materials known.

Acknowledgements

The calculated vibration frequencies (IR-active) show that vibration frequency values of (C-C stretching), (γ ring, ν ring.) vibrations frequency shows higher frequency values in CNT($C_{140}H_{28}$) lead to many more electronic and mechanical applications. Vibrational motion of atoms decreases the electrical conductivity of nanotube.

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