Comparison Study of Frequencies and Electronic Properties by Quantum Mechanical Calculation between Cyclacene and Carbon nanotube.

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Abstract: *Semi empirical quantum mechanical calculations were carried out on the most stable structure for calculating the vibration frequencies and IR absorption intensities for normal coordinates of the cyclacene named mono ($C_{56}H_{28}$) and Carbon nanotube named tetra ($C_{140}H_{28}$)– ring layer of (7,7) armchair single wall carbon nanotube (SWCNTs) at their equilibrium geometries which were all found to have D7d 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 which are active in IR spectra of the two molecules. , the results showed that C-H stretching vibration frequencies value increased with increased of length nano tube (rings layer SWCNT). The results include 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 .*

Key words: *SWCNT single wall carbon nano tube, γ: Out of plane of the molecule. δ: In- plane of the molecule, G03 aprogram for calculation.*

I. Introduction

Nanotechnologies are the engineered convergence of biology, chemistry, and informatics on a nanoscale that is, involving materials measured in billionths of a meter[1]. Graphite is a layered material that is very flexible, in which each layer is able to curve in order to form cages, nanotubes, nanocoils, nanocones, etc[1], Carbon nanotubes (CNTs) have become a paradigm in the physics of low-dimensional systems due to their fascinating properties [2]. Single wall carbon nanotubes (SWCNTs) are formed from sheets of annulated six membered aromatic rings [2]. The hybridization of each carbon atom in the sheet is sp2 (Fig. 1) [3]. They are of aromatic character, similar to graphite, and posse's conjugated C-C bonds [4]. Their aromaticity is graded according to the space distribution of the atoms, the nature of their molecular orbitals, their symmetry and chirality [5]. Various studies were done for the physical properties of the nanotubes [6-11]. The study of vibration of SWCNTs is for successful applications in nanotechnology. Specifically, some vibration modes of SWCNTs, e.g., radial breathing mode [12-15], beam-like bending mode, [16-17] and longitudinal mode [18], offers valuable probes for the molecular structures and the elastic properties of CNTs. On the other hand, CNTs consisting of straight concentric layers with circular cross-section could lose their structural symmetry due to the vibration in axial, circumferential and radial directions [19,20]. This could result in a sudden change in their physical properties (e.g., the electrical properties [21] and in turn, significantly affect their performance in nanostructures. Thus, similar to the buckling behaviour [22] the vibration of SWCNTs turns out to be a major topic of great interest in nanomechanics, considerable efforts [23] have been devoted to capturing the fundamental vibration behaviours of SWCNTs by using experimental techniques [12-13,17-18] and multi-scale modelling tools [14-15, 24-26].Recently, the interest of the mechanics of SWCNTs has been transferred from their fundamental behaviours to the effect of internal and external factors on the elastic properties [27-29], buckling [30-33] of SWCNTs. However no comparison study could be found in the literature for a normal coordinate analysis of the simplest type of nanotube i.e. the Cyclacene and Carbon nanotube (mono and tetra) rings-layer SWCNTs [34,36], the use of vibration measurements to characterize nanotube mechanical properties.
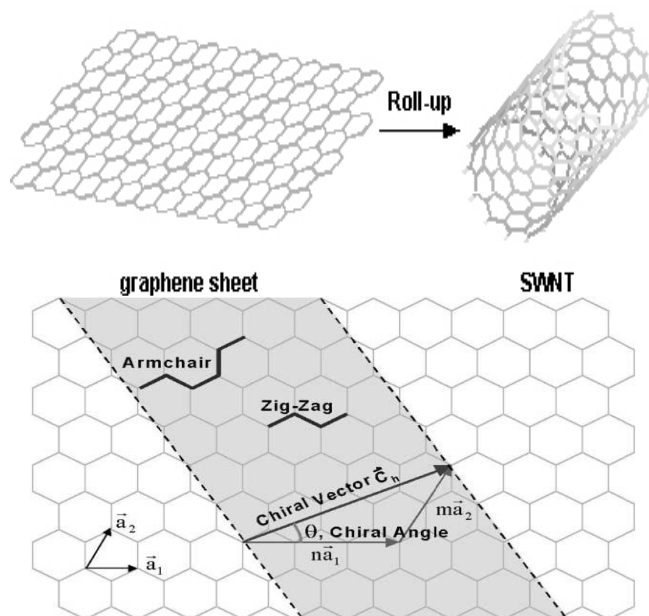
Fig. 1. Schematic diagram showing how a hexagonal sheet of graphite is 'rolled' to form a carbon nanotube.

asym. (γCCC) (puck.)   **asym. CH str.**   **sym. ring (C--C str.)**
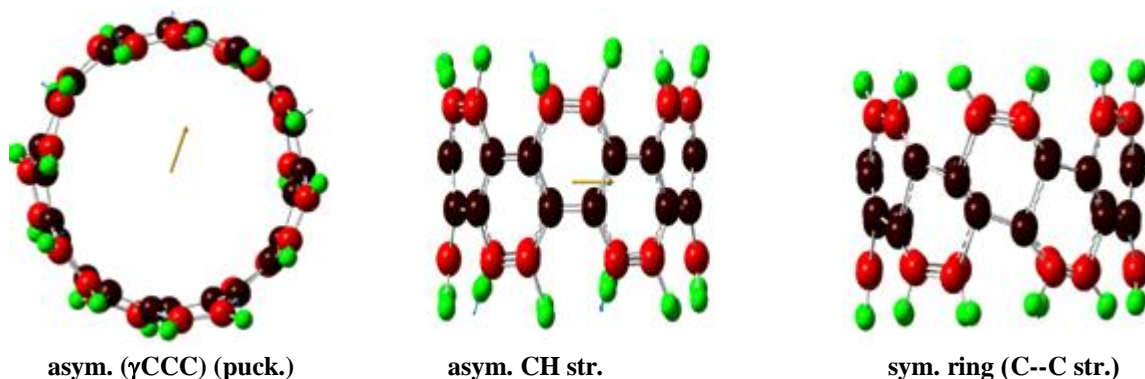*Fig.2: Structure deformation of a SWCNT as caused by its vibration motion.*

II. Methods of calculation

Both G03 program by PM3 method [37], 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 [38] 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.3) shows the two types of bonds in an armchair SWCNT [39].
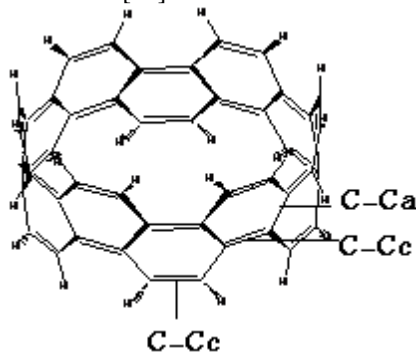

Fig. 3: Structure of armchair SWCNT, indicating the two types of C-C bonds; C-Caxial (C-Ca) and C-Ccircumferential (C-Cc).

Various quantum mechanical studies were done for the physical properties of the nanotubes [40-44]. 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 [45-46]. The active vibrations causes a change in its geometry structure (figure. 2), The calculation gives different geometry were done to study the impact of the puckering distortion on the electronic properties of CNTs [47-49]. 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 [50].
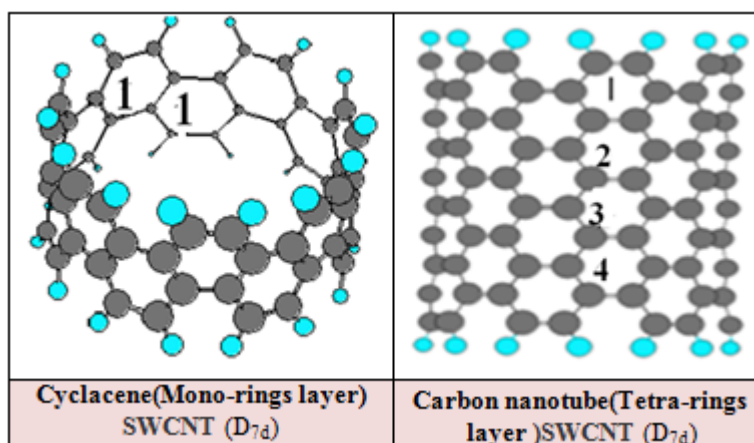

Fig. 4: Equilibrium geometry for (mono, and tetra)-rings layer for armchair (7,7) single wall carbon nanotube (SWCNT) by using Mopac2000 program.

Table 1, shows a repetitive sections of bonds. Table 2 shows comparison of their calculated geometric parameters.

The classifications of carbon nanotubes armchair (mono and tetra)-rings layer, determined by the different of the numbers of rings and the length of CNT, can also be described as single-walled nanotubes (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 is composed of annulated number of member aromatic rings molecules. The (mono and tetra)-rings layer SWCNTs are composed of annulated six member aromatic rings. Their (PM3) calculated equilibrium geometry shows D_7d symmetry [24-25], Figure 5.Due to their symmetry (D_{7d}) [51], figure 5 and table 1, shows a repetitive sections of bonds. Table 2 shows comparison of their calculated geometric parameters.
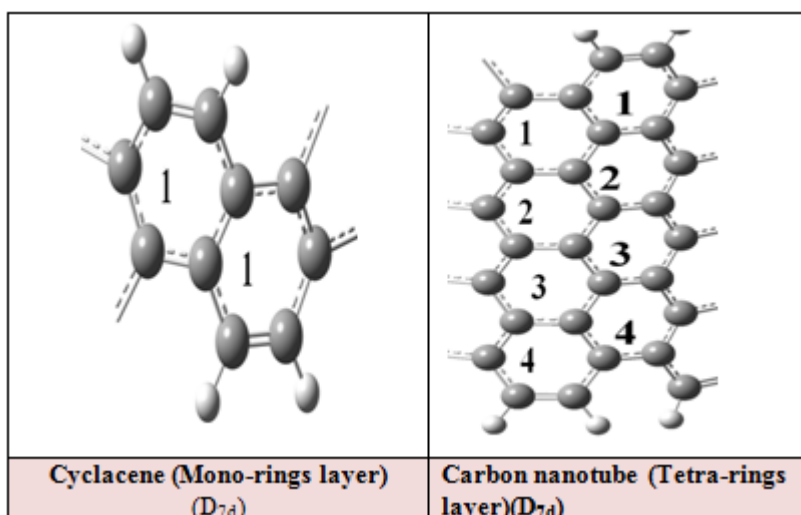

Fig.(5): Repetitive sections of bonds and angles for (mono and tetra) rings layer of armchair SWCNT at their equilibrium geometries according to their point group (D_{7d}).

Table 1: PM3 calculated bond distances of (mono and tetra) rings layer for ArmChair 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
Mono-ring layer D_{7d}	10.049	5.526	1.4302	--------	1.4005	1.3604	1.4351	--------	1.0997
Tetra-rings layer 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-Cc: circumferential bond   C-Ca: axial 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 for (mono and tetra)-rings layer SWCNT, and double or conjugated double bond or single bond for tetra-rings layer SWCNT.

The C=Cc bond increase with increasing numbers of rings layer.   For odd rings layer mono (C-H) and (C---Cc) bonds are longer in mono from that in tetra .

Also note that (...C...Ca), increase in length from outer to centre in mono rings layer, and decrease in length from outer to centre in tetra-rings layer. Figure 4, table 1.

Table 2 shows some physical properties of calculated (mono and tetra)-rings layer for armchair SWCNT at their equilibrium geometry.

Table 2: Some physical properties of the calculated (mono and tetra) rings layer for armchair SWCNT at their equilibrium geometry .

Arm Chair (SWCNT)	M. Wt. g/ mol	ΔH_f kcal/mol,(kJ)	μ (debye)	HOMO (eV)	LUMO (eV)	ΔE (eV) LUMO-HOMO
Mono-ring layer $C_{56}H_{28}$	700.837	300.346 1256.648	0.000	-8.054	-1.213	6.841
Tetra- rings layer $C_{140}H_{28}$	1709.761	721.486 3018.699	0.000	-7.403	-2.437	4.066

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

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

Vibration frequencies assignment of Cyclacene(Mono-rings layer)($C_{56}H_{28}$) armchair (SWCNT)
The Cyclacene (Mono-rings layer) SWCNT posses 246 fundamental vibrations (3N-6). Inspection of its irreducible representation, as defined by the symmetry (D_7d) character table, results in the following modes of vibration;
Γvibration = Γtotal - (Γrotation + Γtranslation) = 3N - 6 = 246
Γvibration=$18E_3u+18E_3g+18E_2g+18E_2u+17E_1u+17E_1g+9A_1u+8A_2g+9A_1g+8A_2u$= 246
There are 42 vibration modes (IR active) ($17E_1u$, and $8A_2u$). Their assignments are as follows:

CH stretching vibration
These are 28 in number, the displacement vectors of which are located at the H atoms. Their frequency values range from (3005.2-3029.4 cm^{-1}) (IR active), Inspecting the values in table 3 .
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 (1347.6-1809.5cm^{-1}), Inspecting the values in table 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 (237.5-1105,6 cm^{-1}),. Inspecting the values in table 3.

In-plane (CCC) bending vibration (δCCC)

Their calculated vibration frequencies (IR active) as modes range from (326.4-1011.7 cm^{-1}), Inspecting the values in table 3.

Out of plane CH bending vibration (γCH)

Their calculated vibration frequencies (IR active) as modes range from (572.8-1215.4 cm^{-1}), Inspecting the values in table 3.

Out of plane ring bending vibrations (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 (572.8-1215.4 cm^{-1}), Inspecting the values in table 3.

Table 3: Vibration frequencies and IR absorption intensities for Cyclacene (mono-rings layer) ($C_{56}H_{28}$) molecule as calculated applying G03 program.

EU	Symmetry & description	PM3 Freq. cm^{-1}	Intensity km/mol
ν_{237}	CH str.	3029.383	28.714
ν_{227}	CH str.	3005.239	107.300
ν_{215}	C=C str	1809.491	15.036
ν_{191}	ring (CC$_{str.}$)(elongation)	1625.087	0.0384
ν_{187}	C--C str	1593.311	12.2663
ν_{179}	C=C str	1526.865	17.4909
ν_{153}	γCH(wag.)	1197.14	16.559
ν_{136}	δCH(siccer.)	1105.650	0.4390
ν_{125}	δCH(rock)+δring (δCCC)	1011.752	0.2571
ν_{103}	γCH (wagg.)+ γring (γCCC)	890.496	18.575
ν_{94}	γCH (wagg.)+ γring (γCCC)	852.991	93.477
ν_{86}	δCH(rock)	812.674	137.946
ν_{74}	γCH (wagg)+ γring (γCCC)	702.001	1.791
ν_{60}	γCH (wagg)+ γring (γCCC)	572.863	13.074
ν_{34}	δCH(rock)	388.437	15.734
ν_{28}	δCH(rock)+δring (δCCC)	326.432	11.190
ν_{21}	δCH(rock)	237.476	10.236
A$_2$u			
ν_{231}	CH str.	3010.232	358.860
ν_{191}	C=C str	1695.497	8.1662
ν_{165}	C=C str	1347.570	7.2816
ν_{156}	γCH (wagg)+ γring (γCCC)	1215.372	48.906
ν_{132}	δCH(siccer.)	1077.490	0.6641
ν_{88}	δCH(rock)+δring (δCCC)	814.134	0.590
ν_{51}	δCH(rock)+δring (δCCC)	516.299	7.919

Vibration frequencies assignment of Carbon nanotube(tetra-rings layer) ($C_{140}H_{28}$) armchair SWCNT.

The Carbon nanotube (tetra-rings layer) 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;

Γvibration = Γ_{total} - (Γrotation + Γtranslation) = 3N - 6 = 498

Γvibration=36E$_3$u+36E$_3$g+36E$_2$g+36E$_2$u+35E$_1$u+35E$_1$g+18A$_1$u+17A$_2$g+18A$_1$g+**17A$_2$u**

 = 498

These are 87 IR active (35E$_1$u, and 17A$_2$u). Their assignments are as follow:

Relative to the 6$_h$ reflection the vibration modes are classified as symmetric and antisymmetric modes.

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 cm^{-1}), Inspecting the values in table 4.

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 cm^{-1}), Inspecting the values in table 4.

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 cm^{-1}), Inspecting the values in table 4.

In-plane (CCC) bending vibration (δCCC)
Their calculated vibration frequencies (IR active) as modes range from (149.7- 1343.7 cm^{-1}), Inspecting the values in table 4.

Out of plane CH bending vibration (γCH)
Their calculated vibration frequencies (IR active) as modes range from (270.1- 1288.6 cm^{-1}), Inspecting the values in table 4.

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 cm^{-1}), Inspecting the values in table 4.

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≠ 0.0) are allowed (IR active, Ramman inactive).

Table 4: Vibration frequencies and IR absorption intensities of Carbon nanotube (tetra-rings layer) (C$_{140}$H$_{28}$) molecule as calculated applying G03 program.

EU	Symmetry & description	PM3 Freq. cm^{-1}	Intensity km/mol
ν_{489}	CH str.	3029.030	9.0755
ν_{481}	CH str.	3004.260	117.430
ν_{461}	C-C str	1796.560	4.349
ν_{457}	C=C str	1793.220	14.884
ν_{435}	C=C str	1722.350	2.539
ν_{414}	C=C str	1675.170	0.278
ν_{403}	C-C str	1643.150	1.444
ν_{399}	ring (CCCstr.)	1602.760	0.019
ν_{369}	ring (CCCstr.)	1556.180	0.460
ν_{363}	C- C str	1536.560	8.336
ν_{352}	ring (CCCstr.)	1498.850	17.800
ν_{334}	ring (CCCstr.)	1409.130	30.762
ν_{321}	δring (δCCC)	1343.710	0.280
ν_{313}	γCH(wagg.)+ γring (γCCC)	1288.640	6.322
ν_{295}	γCH(wagg.)	1152.630	5.583
ν_{274}	δCH(siccer.)	1067.710	1.066
ν_{260}	δCH(siccer.)	1004.260	0.076
ν_{247}	γring (γCCC)+ γCH	964.564	1.237
ν_{241}	γCH(twiss.)+ γring (γCCC)	945.735	0.012
ν_{227}	γCH(twiss.)+γring (γCCC)	896.600	5.130
ν_{216}	δCH+δring (δCCC)	858.660	22.623
ν_{194}	δCH(rock)	812.820	125.337
ν_{153}	γCH(twiss.)+ γring (γCCC)	674.771	1.1662
ν_{150}	δCH+δring (δCCC)	664.392	11.594
ν_{143}	δCH(rock.)+ +δring (δCCC)	653.804	7.294
ν_{124}	γCH(wagg.)+ γring (γCCC)	602.856	3.092
ν_{99}	γCH(twiss.)+ γring (γCCC)	492.552	22.087
ν_{95}	γCH(twiss.)+ γring (γCCC)	481.314	1.576
ν_{82}	γCH(twiss.)+ γring (γCCC)	436.045	4.350
ν_{61}	γCH(twiss.)+ γring (γCCC)	357.166	2.910
ν_{59}	γCH(twiss.)+ γring (γCCC)	346.147	1.028
ν_{44}	γring (γCCC)+ γCH(wagg.)	284.641	0.935
ν_{38}	γCH(wagg.)+ γring (γCCC)	270.122	5.758
ν_{13}	δCH(rock.)+δring (δCCC)	149.751	6.048
A$_2$u			
ν_{483}	CH str.	3008.892	616.385
ν_{442}	C=C str	1765.630	14.298
ν_{409}	C=C str	1654.390	3.133
ν_{387}	ring (CCCstr.) elonga.	1600.180	4.349
ν_{367}	ring (CCCstr.) elonga.	1542.980	2.304

ν_{348}	ring (CCCstr.)elonga.	1480.570	0.208
ν_{329}	γring (γCCC)	1363.960	100.904
ν_{303}	ring (CCCstr.)	1193.150	5.645
ν_{284}	γCH(twist.)	1114.750	20.534
ν_{260}	γCH(twist.)	1028.510	1.906
ν_{188}	δCH(rock)	801.216	4.297
ν_{147}	γring (γCCC)+ γCH(breath.)	660.794	0.366
ν_{138}	γring (γCCC)+ γCH(breath.)	642.957	2.882
ν_{109}	δCH(rock)+δring (δCCC)	518.928	10.4807
ν_{67}	δCH(rock.)+δring (δCCC)	376.334	1.735
ν_{35}	γring (γCCC)(breath.)	256.287	0.431
ν_{15}	δCH(rock.)+δring (δCCC)	152.020	0.730

(Figure 5) shows the vibration pictures for some modes of the CNT (Armchair), as calculated applying semi-empirical methods (PM3) by Gaussian 03 program.

The results and Relations
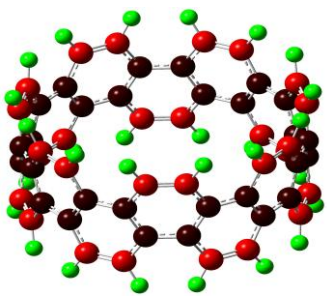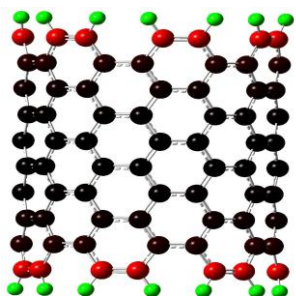
νCH$_{str.}$(mono-rings layer) > ν.CH$_{str.}$ (tetra-rings layer)

νCC$_{str.}$(mono-rings layer) > ν CC$_{str.}$(tetra-rings SWCNT)

$\nu\delta$ring (tetra-rings layer) >$\nu\delta$ring (mono-rings layer)

$\nu\gamma$ring(tetra-rings layer) > $\nu\gamma$ring(mono-rings layer)

$\nu\delta$CH(mono-rings layer) >$\nu\delta$CH(tetra-rings layer)

$\nu\gamma$ CH(tetra-rings layer) >$\nu\gamma$ CH(mono-rings layer)

νCC$_{str.}$(mono-rings layer) > ν CC$_{str.}$(tetra-rings)

νCH$_{str.}$(di-rings layer) $\approx$$\nu$CH$_{str.}$(terta-rings layer)

Finally, the calculated vibration frequencies (IR-active) show that vibration frequency values of (C-C stretching) , (γring, $\nu\delta$ring.) vibrations frequency shows higher frequency values with increased numbers of rings layer in length lead to many more electronic and mechanical applications.

Table 5: Calculated Vibration frequencies of (mono and tetra) rings layer for armchair SWCNTs
applying G03 program by PM3 method**.**

Arm Chair (SWCNT)	C-H$_{str.}$	C- Ca$_{str}$	C=Cc$_{str.}$	C--Cc$_{str}$
Mono-rings layer $C_{56}H_{28}$	3029.38 Eu	1625.08 Eu	1809.50 Eu	1593.30 Eu
Tetra-rings layer $C_{140}H_{28}$	3029.11 Eu	1602.70 Eu	1793.22 Eu	1796.50 Eu

Finally, the calculations show that, similar to the carbon nanotubes [52-53], the charge densities are mainly concentrated at the circumferential carbon and hydrogen atoms of mono and multi-rings layer 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. 6.

Cyclacene(Mono-rings layer)D$_{7d}$		**Tetra-rings layer D$_{7d}$** **nanoring C$_2$h**	
C—H 0.112		C—H 0.113	
C=C -0.091		C= C -0.088	
C---C -0.022		C—C -0.015	
		C---C -0.007	

		C---C -0.002	.
		C---C -0.001	

Fig. 6. Distribution of charge density at the atoms for (mono and tetra) rings layer of armchair SWCNT as calculated applying G03 program.

IV.   Conclusion

Quantum mechanics 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 three molecules Cyclacene and Carbon nanotube($C_{56}H_{28}$, $C_{140}H_{28}$) Vibrational motion of atoms decreases the electrical conductivity of nanotubes 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[54,55]. 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 operateat room temperature. Nanotubes possess extraordinary mechanical properties and are among the strongest materials known.

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