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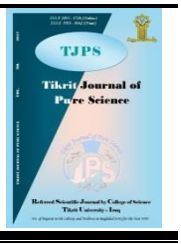

Study the Spectral Properties of the Molecule [Pentacene ($C_{22}H_{14}$)] by Using Semi-empirical Quantum Programs

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Abstract

The Study aims to determine the spectral properties of the molecule pentacene ($C_{22}H_{14}$) by using Semi-empirical quantum programs [Hyper Chem8.0, WinMopac7.21] by (MNDO–PM3) (Modified Neglect of Differential Overlap-Parameterization Model3). The study cover calculations of the space geometrical shape of pentacene molecule has been calculated by using initial and final matrixes, including length, the angle between bonds, dihedral angles and the charge of each atom in the pentacene molecules. Total energy, the electronic energy, zero point energy, energy gap, core-core repulsion, ionization energy, and dipole moment for molecule were calculate. Curved potential energy per molecule was drawn where it was adopted to change the length of the bonds (C_1-C_2),(C_1=C_4), and (C_1-H_{23}) in the pentacene molecule. As well, as have been obtained vibration frequencies of pentacene in (IR) region and electronic transition in (UV) region. The study's results were in agreement with the previous research.

1. Introduction

The molecule pentacene ($C_{22}H_{14}$) is considered aromatic hydrocarbons is composed of five benzene rings. Pentacene is an organic molecular semiconductor (O M S) of great interest for potential applications in thin film transistor [1,2] .While pentacene transistors exhibit good carrier mobility [3,4]. Pentacene shapes is solid blue-black color to the group of acinates has crimson Luster. There are many applications for pentacene ($C_{22}H_{14}$) and its derivatives in the field of electronic. Pentacene is used as a conductor in organic electronic devices and as a transistor including transistor of field effect. There are several ways to determine the total energy of predictive molecular structures are :(1-Ab-initio electronic structures calculations, 2- semi empirical methods, 3-Molecular mechanics, 4-Density functional theory).Using semi-empirical quantum programs by the method(MNDO-PM3) at a stable geometric structure, From the most significant molecular, modeling programs [WinMopac7.21, Hyper Chem8.0]. Hyperchem is a quantum mechanics program contains all the molecular modeling programs, through hyperchem 8.0 program is possible to draw the molecules by selecting the internal coordinates of the molecules (r,Θ,Φ), then their spectral properties,and the other programs WinMopac7.21 is an improved copy of MOPAC programs which is constantly evolved, To define Mopac: Mopac is an over all purpose, Semi-empirical molecular orbital program, have facilities to study of chemical reactions concerning molecules, linear polymers and ions. It applies the semi-empirical Hamiltonians (AM1, MNDO, MNDO/3, NDOPM3). This program present calculations of vibrational spectra, isotopic replacement effects, thermodynamic quantities, and force constants in an integrated program[5,6] .One of the most basic physics and chemistry problem is finding the molecular properties such as the energy and the balanced molecular arrangement, which would be in agreement with the Schrodinger equation :-

$H\psi = E\psi$ …(1)

H: is Hamiltonian-operator which is characterizes the total energy of any wave function for a system in a certain level.

E: is the numerical value of energy (eign value)

Ψ: is the wave function of the quantum system and describes the system status.

2. Theory

The total number of energy levels of any molecule very large and the total energy is divided between different energies as in the following equation [7].

$E_{total} = E_{rot} + E_{vib} + E_{elec}$…..(2)

Where E_{total} : Total energy ,E_{rot} :Rotation energy and E_{Vib}: Vibration energy, E_{elec}: electronic energy. In this research the focus is the vibrational energy, which represents the energy and kinetic energy that molecules possess which result from their vibrational movement and this energy is quantified. In order to approximate, we can imagine that there are two atoms linked by a chemical bond and vibrate along inter nuclear axis, if the atoms have the masses (m_1 and m_2) and the bond between them has zero mass helical spring, the two atoms would vibrate harmonically to the center of the mass[8]**.** According to the Hook's law the restoring force is:

$F = - k(r-re)$ …… (3)

Where (k) is the force constant, (r-re)is the displacement from the center of the mass

Both masses can move together as one (effective mass), and symbolizes them (μ).

$\frac{1}{\mu} = \frac{1}{m1} + \frac{1}{m2} \rightarrow \mu = \frac{m_1 . m_2}{m_1 + m_2}$ ….. (4)

or vibrate consonantly relative to the center of its mass at a frequency given by relationship

$v_{vib} = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ …. (5)

From this equation we can observe that the frequency increases with (k) (The force of the atom) and deceases with the increase of the effective mass (μ) and the force can be written in terms of potential energy as in equation [9].

$V(r) = \frac{1}{2}k(r - r_e)^2$ …. (6)

Where V(r) is the potential energy given by the harmonic model, and (r_e) equilibrium distance. According to quantum mechanics (Hamiltonian) for the harmonic oscillator in one dimension [7,10].

$H = \frac{-h^2}{2\mu}\nabla^2 + \frac{1}{2}k\,(r - re)^2$ ….. (7)

It is obvious from solving this equation that the total vibrational energy is quantitative and take the values:

$E_v = h\nu_{vib}\,(v + \frac{1}{2})$ …. (8)

Where ν_{vib} the total vibrational frequency, (v) it represents the number of vibrational quantum (v=0,1,2,3,4...) Since that (ν =cω) is why the equation becomes as follows.

$E_V = h\,c\omega\,(v + \frac{1}{2})$ …. (9)

Where as (ω) represent wave number and be unit is cm^{-1}, (c) represent speed of light in the vacuum.

An equation (9) can be written in terms of wave number, as is usual in the spectroscopy study ,as in the following equation .

$G(v) = \omega\,(v + \frac{1}{2})$ …. (10)

from this equation, we observe that the distances between adjacent vibrational levels are equal and equal (hcw) to that of main vibrational level (G_0) called (zero point energy). Which are calculated when (v=0) as in the equation.

$G(0) = \frac{1}{2}\omega_0$ …. (11)

Many of function of the Morse potential function have been proposed in relation to the proposed scientist, as in the following equation [11].

$Vm = De\,[1 - e^{-\beta(r-re)}]^2$……(12)

Where(D_e) is the dissociation energy of the molecule , and (V_m) represents the potential energy ,(β) is a special constant for each electronic state of the molecule. When the potential energy is substituted with the Morse potential function in the Schrorodinger equation , the vibrational energy levels is defined by [12].

$G(v) = (v + \frac{1}{2})\,\omega_e - (v + \frac{1}{2})^2\,\omega_e x_e$ …. (13)

Where (x_e) is the anharmonic constant , and G(v) represents the vibrational energy level (ω_e) is the vibrational frequency in an harmonic movement. The Morse equation, we can extract the number of vibrational energy levels (V= 1,2,3,…… V_{max}) [10].

$V_{max} = \frac{\omega e}{2\omega exe} - \frac{1}{2}$ … (14)

The zero point energy G (0) becomes zero point energy when (V= o) [9].

$G(o) = \frac{1}{2}\omega_e(1 - \frac{1}{2}x_e)$ …..(15)

And dissociation energy (De) Almost given by relationship [13] .

$De \cong \frac{\omega e^2}{4\omega_e x_e}$ ….. (16)

Vibrational frequency and normal coordinates of molecular calculations can also be made from the constants of molecular forces can be solved the abstract equation of Wilson. This is the most common method if the abstract equation of Wilson [14].

$\Sigma\, jLj\,(F_{ij} - \lambda M_{ij})$… (17)

Where (F_{ij}) in the equation (19) represents a matrix element of the force constants, and (M_{ij}) matrix masses of atoms, (λ) Eigen value, (L_i) values of Eigen vector coefficients. From the solution of the abstraction equation, we will obtain the basic vibrational frequencies of the molecule (3N-6) BY compensating the values of λ in equation [14,15] .

$\lambda = 4\pi v^2\,c^2$… (18)

Where (v) the harmonic frequency is represented by a unit (cm^{-1}), c:The speed of light .The dipole moment is the electrostatic force working between two equal and different charges by indicating the a mount of charge is **(q)** and the distance between two of them is (d), the equation of the dipole moment can be written as [15].

$\mu = q.d$…(19)

3. Electronic Transitions

The electronic transitions in organic compounds and some other compounds can be determined by ultraviolet-visible spectroscopy, provided that transitions in the ultraviolet (UV) or visible range of the electromagnetic spectrum exist for this compound [16,17].Electrons occupying a HOMO of a sigma bond can get excited to the LUMO of that bond. This process is denoted as a $\sigma \rightarrow \sigma^*$ transition

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to the Likewise promotion of an electron from a π-bonding orbital to an antibonding π orbital* is denoted as a $\pi \rightarrow \pi^*$ transition. The following molecular electronic transitions exist:

.σ (sigma) – orbital has symmetry about the bonding axes,lowest energy

• **π (pi)** – only one orbital plane passes through both nuclei involved

• **n (non-bonding)** – orbital involved is not involved in bonding, usually a lone pair, higher in energy

• **σ* , π* (anti-bonding)** – nadal planes exist between nuclei, high in energy, usually unpopulated in stable molecules. as show in figure (1).

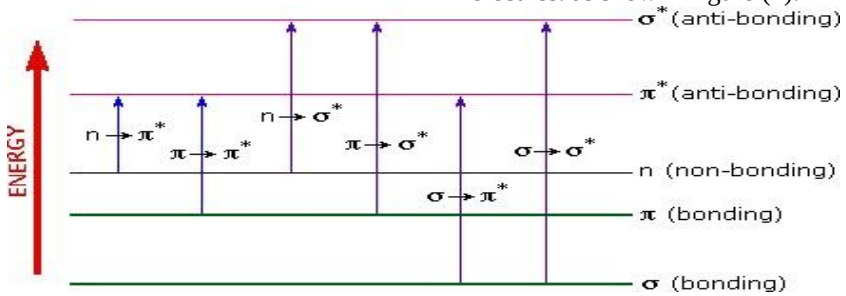

Fig.(1): illustrates the Levels of electronic energy in the molecules and the possibilities of transitions between them

4. Results and Discussion

4.1.The molecular structure (pentacene)

Pentacene ($C_{22}H_{14}$) represented by the shape in the figure (2), which drawn by hyperchem8.0 program, the calculation the program depends on the internal coordinates (r, θ, φ) [(r) the distance between these atoms, (θ°) represents an angle between three atoms, (φ°) They are dihedral- angle], and the geometric shape at the equilibrium state.

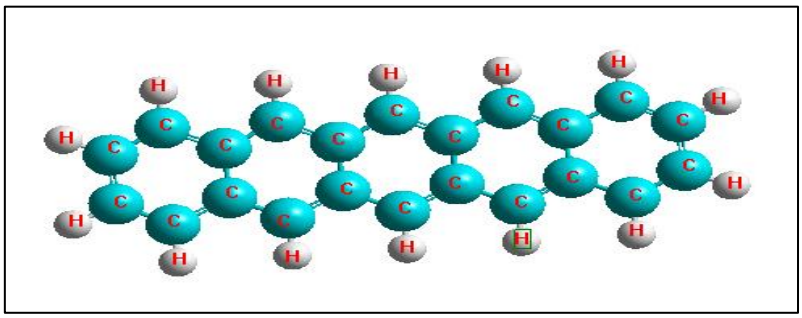

Fig. (2): the molecular structure of pentacene ($C_{22}H_{14}$) molecule drawn by the hyperchem 8.0 program.

Table (1) shows pentacene molecule matrix, which can obtained after the drawing molecule when reaching the optimization state for the best geometrical, position. The table illustrates the atoms of the molecule, the distance between these atoms (r), the best position of these atoms (opt). The values of the angles between bond (Θ°), and the dihedral angles (Φ°).

Table (1) The initial matrix of the pentacene molecule shows, the internal coordinates (r ,Θ,Φ) , by HyperChem. Program

ATOM	r (A)	OPT	θ^o	OPT	Φ^o	OPT	A B C
C	0	0	0	0	0	0	0 0 0
C	1.3537	1	0	0	0	0	1 0 0
C	1.4338	1	120.6799	1	0	0	2 1 0
C	1.4422	1	120.7493	1	359.7629	1	1 2 3
C	1.3537	1	120.6906	1	0.3892	1	3 2 1
C	1.4361	1	118.5670	1	359.6705	1	4 1 2
C	1.3772	1	121.4144	1	179.7419	1	4 1 2
C	1.4208	1	120.7985	1	359.2970	1	7 4 6
C	1.3772	1	120.0063	1	0.8624	1	6 4 7
C	1.4209	1	120.7964	1	359.9653	1	9 6 4
C	1.3985	1	121.2076	1	180.1803	1	8 7 4
C	1.3987	1	120.7727	1	178.6027	1	11 8 7
C	1.4283	1	119.6154	1	359.9154	1	12 11 8
C	1.3984	1	121.2023	1	178.6842	1	10 9 6
C	1.4206	1	121.2206	1	180.3178	1	12 11 8
C	1.4206	1	119.1918	1	181.4102	1	13 12 11
C	1.3774	1	120.8204	1	178.658	1	15 12 11
C	1.3774	1	120.8093	1	180.1881	1	16 13 14
C	1.4424	1	121.4378	1	180.1781	1	17 15 12
C	1.3537	1	120.7575	1	179.2160	1	19 17 15
C	1.4424	1	121.4405	1	179.1613	1	18 16 13
C	1.3537	1	120.7517	1	179.7172	1	21 18 16
H	1.0959	1	121.2736	1	179.9117	1	1 2 3
H	1.0949	1	120.9936	1	179.7924	1	2 1 4
H	1.0947	1	118.3084	1	180.3294	1	3 2 1
H	1.0959	1	121.2694	1	180.1269	1	5 3 2
H	1.0970	1	120.3194	1	179.5619	1	7 4 6
H	1.0972	1	120.3696	1	179.8076	1	9 6 4
H	1.0971	1	119.5637	1	0.0482	1	14 10 9

These properties were found after obtaining the initialize matrix and incorporated in to the matrix by using the (WinMopac7.21) program. These properties include (heat of formation, Dipole moment, Ionization Potential, zero point energy, molecular weight, No. of Filled level, electronic energy, Total energy, Binding Energy, Core –Core Repulsion). Table (2) illustrates some of the spectral properties that give full descriptions of the molecular structure.

Table (2) The results of the spectral properties of the pentacene ($C_{22}H_{14}$) molecule calculated by the (WinMopac 7.21) program

The spectral properties	The calculated values by winmopac7.21 program	The calculated values Hyper Chem program	Units
Heat of Formation	107.93209	107.4173660	KCal/mol
Total Energy	-2320.06238	-2820.0820274923	eV
Electronic Energy	-20512.35955	-20513.046973435	eV
Core-Core Repulsion	1792.29718	17692.964945943	eV
Dipole moment	0.039	0.039	Debyes

4.2. The Anharmonic Potential Energy Calculation (pentacen $C_{22}H_{14}$) .

The values for the length of the bonds and total energy values, where calculated by using WinMopac 7.21 program, when changing several distances of the,($C_1 - C_2$),($C_1 = C_4$) ,and($C_1 - H_{23}$) bonds were determined for the pentacene molecule, The an harmonic potential energy curve was plotted and distance at which we obtain the lowest total energy value as in Fig. (3),(4),(5), and the total energy values at the equilibrium position of the bonds, ($C_1 - C_2$), (C_1=C_4), (C_1-H_{23}) is respectively were (- 2820.062 eV) at the equilibrium distance r_{eq} = (1.35 A^O), (2820.02 eV) at the distance r_{eq} = 1.4 A^O, (- 2820. 06 eV) at the distance r_{eq} = 1.1 A. The curve in the fig. (3),(4),(5), showed, when atoms are rounded together less equilibrium was created after the equilibrium distance is very high and it accompanied by alarge potential energy that increases rapidly either when the atoms are removed some from each other more than after the equilibrium will appear weak attractiveness accompanying, them aweak potential energy which increases less rapidly. Then, start the effect of bond stretch (C_1-C_2) and the potential curve shifts from harmonic behavior to an harmonic behavior, and increasing the energy between (C_1-C_2) atoms until the molecule begins to dissociate, until the bond breaks down, and the energy at this point called the dissociation energy, so for the other bonds, (C_1= C_4), (C_1-H_{23}), and the other dissociation energies as

following: (C_1-C_2) (De = 8.9 eV) as shown in fig (3), (C_1= C_4) (De = 8.1 eV) as shown in fig (4), (C_1-H_{23}) (De= 6.127 eV) as shown in fig (5), when comparing the values of the dissociation energies of each of the bonds in the pentacene molecule, the difference is due to the difference in the length of the bonds due to the difference in the inertia determined by the difference in mass.

Table (3) the total energies of the pentacene molecule at different (C_1-C_2) Lengths

R(A^o)	Total energy (eV)
0.7	-2787.349
0.8	-2798.911
0.9	-2807.141
1	-2813.236
1.1	-2816.845
1.2	-2819.067
1.3	-2819.646
1.3337	-2820.037
1.3437	-2820.056
1.3537	-2820.062
1.3637	-2820.056
1.3737	-2820.042
1.4	-2820.0002
1.5	-2819.539
1.6	-2818.794
1.7	-2818.103
1.8	-2817.401
1.9	-2816.426
2	-2816.111
2.1	-2815.122
2.2	-2814.265
2.3	-2813.579
2.4	-2813.137
2.5	-2813.286
2.6	-2812.940
2.7	-2812.551
3	-2811.806
3.5	-2811.357
4	-2810.263
4.5	-2811.162

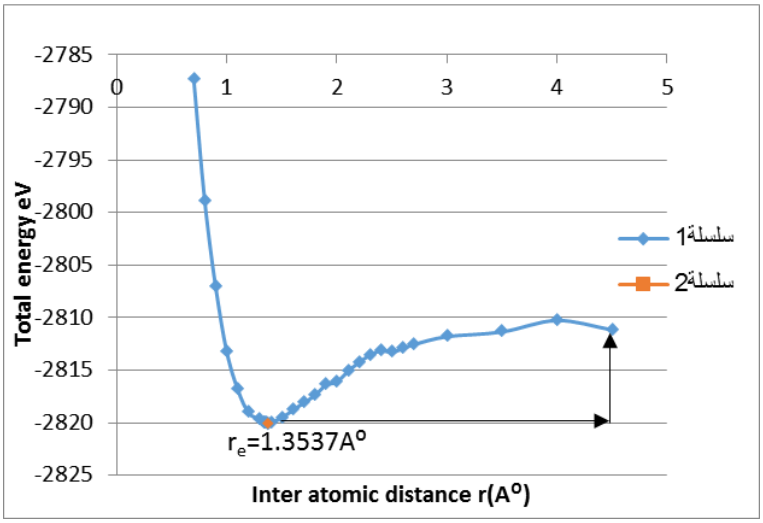

Fig.(3):The total energies of the pentacene molecule at different (C_1-C_2)Lengths.

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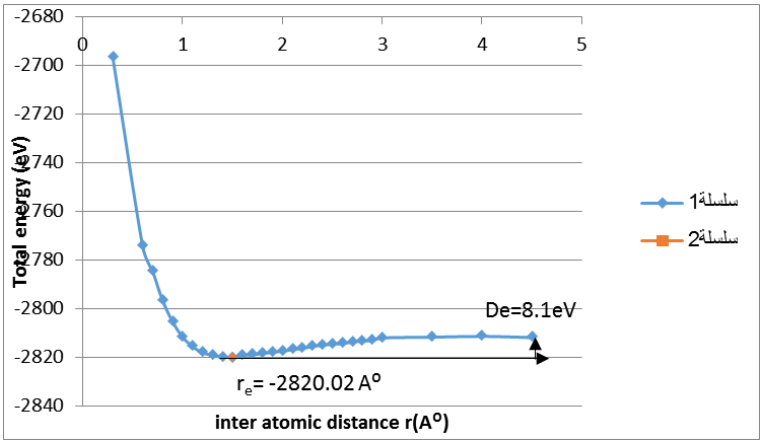

Fig.(4):the total energies of the pentacene molecule at different (C_1=C_4)Lengths

Table(4) the total energyies of the pentacene molecule at different (C_1=C_4).

Distance r(A°)	Total Energy (eV)
0.3	-2696.485
0.6	-2774.35
0.7	-2784.7
0.8	-2796.66
0.9	-2805.42
1	-2811.7
1.1	-2815.68
1.2	-2818.15
1.3	-2819.15
1.4	-2820.02
1.5	-2820
1.6	-2819.2
1.7	-2819.04
1.8	-2818.49
1.9	-2818.03
2	-2817.55
2.1	-2816.89
2.2	-2816.41
2.3	-2815.56
2.4	-2815.04
2.5	-2814.64
2.6	-2814.44
2.7	-2813.78
2.8	-2813.32
2.9	-2813.19
3	-2812.08
3.5	-2811.77
4	-2811.43
4.5	-2811.94

Table (5): the total energies of the pentacene molecule at different (C_1-H_{23}) Lengths.

Distance r(A°)	Total Energy (eV)
0.3	-2785.1
0.4	-2796.86
0.5	-2805.46
0.6	-2811.31
0.7	-2815.04
0.8	-2817.77
0.9	-2819.21
1	-2819.88
1.1	-2820.06
1.2	-2819.91
1.3	-2819.59
1.4	-2818.81
1.5	-2818.65
1.6	-2818.11
1.7	-2817.51
1.8	-2816.78
1.9	-2816.23
2	-2815.49
2.1	-2815.23
2.2	-2814.78
2.3	-2814.28
2.4	-2814.68
2.5	-2814.49
2.6	-2814.12
3	-2814.01
3.5	-2814.31
4	-2813.93

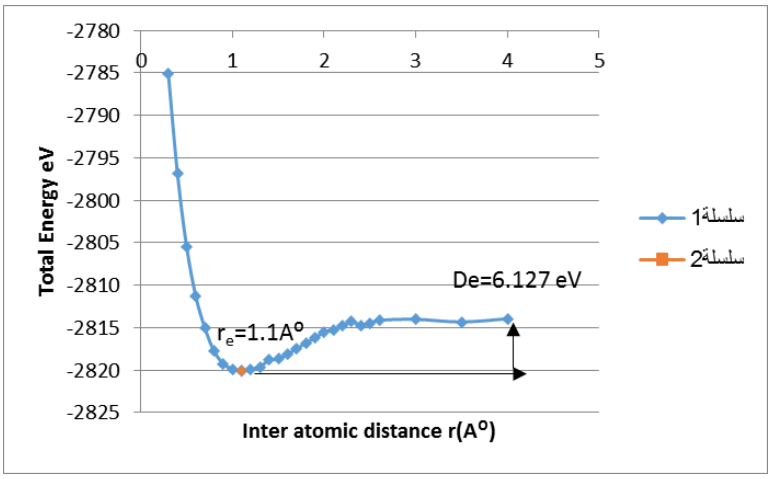

Fig.(5) :the total energies of the pentacene molecule at different (C_1-H_{23})Lengths.

4.3 The frequencies and Vibrational modes calculation

After drawing the curved potential for a practical pentacene ($C_{22}H_{14}$), in Table (6) illustrates the basic frequencies at the infrared (IR), region of the pentacene molecule with the intensity and the symmetry as their number was (102), according to the relationship (3N-6), where (N) represents the number of atom of the molecule. The table also (6) showed the frequencies (the wave number) of the molecule are close to the results of the (hyperchem 8.0 and WinMopac 7.21) programs .

Table (6): The vibrational frequencies of pentacene calculated by HyperChem and WinMopac programs

VIBRATION MODE	HYPERCHEM PROGRAM			WINMOPAC PROGRAM	Other work
	INTENSITY Km/mol	WAVE NUMBER 1/cm	SYMMETRY	WAVE NUMBER 1/cm	Wave number cal.[18]
1	0.10988	34.80	1 A		
2	0.00001	59.46	2 A	62.81	
3	0.00078	93.71	1 B	94.85	
4	0.01885	124.79	2 B	126.33	
5	0.08949	129.34	3 B	130.06	
6	0.26299	172.74	3 A	173.83	
7	0.00000	208.33	4 A	209.33	
8	0.00018	248.03	4 B	249.20	
9	0.00052	256.96	5 A	257.34	
10	0.00000	277.15	6 A	277.18	
11	0.00001	307.01	5 B	307.65	
12	0.00006	311.51	7 A	312.40	
13	0.00421	389.14	6 B	389.60	
14	17.04934	439.24	8 A	440.40	
15	0.01659	440.80	7 B	442.19	
16	0.33204	445.45	9 A	446.70	
17	0.00823	446.57	8 B	447.28	
18	0.00034	468.05	10 A	468.88	
19	0.05439	474.30	11 A	474.54	
20	0.00010	480.69	9 B	481.28	
21	0.44063	500.09	10 B	500.17	
22	0.00284	533.57	12 A	534.02	
23	0.79837	584.40	11 B	584.56	
24	0.00019	607.67	13 A	607.79	
25	0.32518	634.65	12 B	634.80	
26	0.00032	644.71	14 A	645.02	
27	0.00002	704.62	15 A	705.04	
28	0.00121	724.76	13 B	725.26	
29	0.00011	730.71	16 A	730.95	
30	0.00054	732.06	17 A	732.35	
31	0.04079	733.24	14 B	733.62	
32	38.57559	761.50	18 A	762.89	
33	0.06218	763.98	15 B	765.32	
34	0.01039	831.99	16 B	832.21	

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35	0.34906	841.09	17 B	842.91	
36	0.00025	851.36	18 B	852.07	
37	0.00011	858.36	19 A	859.15	
38	5.61856	872.41	20 A	873.07	
39	0.00236	872.87	21 A	873.20	876.85
40	0.24855	891.64	19 B	891.76	
41	0.00655	901.77	22 A	901.94	
42	0.00020	906.01	20 B	906.53	
43	0.01766	915.71	21 B	916.30	
44	0.22267	949.03	23 A	949.60	
45	28.01798	949.52	24 A	950.17	
46	0.00085	954.12	25 A	954.42	
47	0.01742	975.07	22 B	975.93	
48	22.96610	978.03	26 A	978.79	
49	0.01140	981.58	23 B	982.27	
50	0.00044	1010.29	27 A	1011.22	
51	0.00366	1011.80	24 B	1012.77	
52	2.94330	1026.73	25 B	1028.89	
53	0.46234	1038.93	26 B	1039.89	
54	0.23243	1089.86	27 B	1090.11	
55	0.00007	1090.59	28 A	1090.82	
56	0.51824	1126.81	28 B	1127.09	
57	0.00122	1128.00	29 A	1128.24	1136.97
58	0.00044	1147.34	30 A	1147.54	1144.18
59	0.00083	1157.08	31 A	1157.55	
60	0.14527	1158.35	29 B	1158.83	
61	0.11746	1172.30	30 B	1172.49	
62	13.21567	1202.55	31 B	1203.61	
63	0.00633	1204.89	32 A	1205.14	
64	0.00013	1210.25	33 A	1210.44	
65	0.00623	1239.01	32 B	1239.22	
66	0.00002	1258.18	34 A	1258.30	
67	1.07775	1299.57	33 B	1299.70	
68	0.00456	1383.85	35 A	1384.15	1376.7
69	0.01769	1396.82	34 B	1397.03	
70	13.21229	1401.45	35 B	1401.79	
71	0.00066	1420.16	36 A	1420.39	
72	1.59781	1446.03	36 B	1446.25	
73	0.00018	1457.24	37 A	1457.52	
74	0.00061	1515.24	38 A	1516.22	1509.36
75	0.13821	1600.56	37 B	1600.99	
76	0.00112	1605.14	39 A	1605.38	1601.08
77	0.85469	1617.93	38 B	1618.25	
78	0.04707	1637.32	39 B	1637.59	
79	0.00010	1651.94	40 A	1652.35	
80	0.35756	1717.56	40 B	1717.92	1700
81	0.00105	1737.74	41 A	1738.22	
82	0.27442	1749.10	41 B	1749.42	
83	0.00018	1750.87	42 A	1751.19	
84	0.00020	1778.75	43 A	1779.00	
85	0.07799	1812.28	42 B	1812.58	
86	0.00099	1814.21	44 A	1814.64	
87	0.00907	1842.55	45 A	1842.85	
88	2.43854	1846.13	43 B	1846.45	
89	46.45101	3043.75	89	3044.14	
90	5.54784	3044.68	90	3045.17	
91	1.16687	3045.45	91	3045.77	
92	0.40228	3046.24	92	3046.59	
93	5.35097	3046.57	93	3046.98	
94	0.01903	3047.64	94	3047.98	
95	0.48891	3049.72	95	3049.95	
96	5.28118	3049.74	96	3050.26	
97	3.18588	3051.46	97	3052.03	
98	3.10430	3051.78	98	3052.16	

99	9.42458	3065.38	99	3065.74	
100	9.82886	3065.52	100	3065.99	
101	33.30232	3076.36	101	3076.79	
102	11.81179	3076.63	102	3077.13	

Table (6) that the Vibrational frequencies between two the atoms (C - H) it were at the wave numbers 1147.34 cm^{-1}. This value was in agreement with the previous studies 1144.18 cm^{-1} [18].

Figure (6) illustrates some of Vibrational modes of the pentacene molecule and shows the atoms' motion directions, the figure also determines the intensity, the symmetry and frequency for each style.

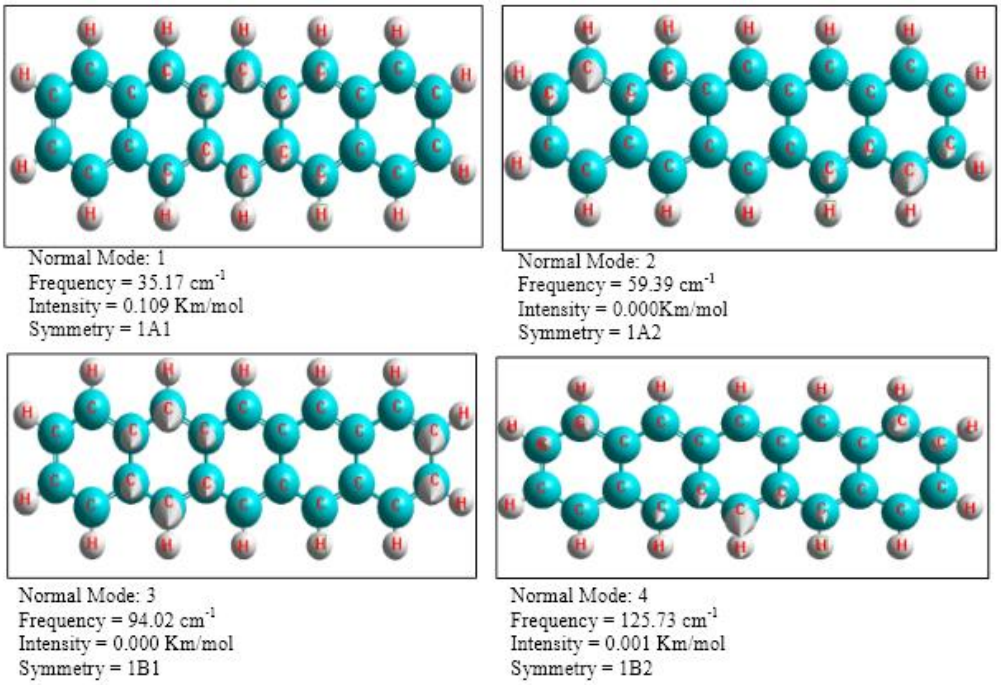

Fig. (6): The main vibrational modes, the frequency, the intensity and symmetry of Pentacene for each mode drown by hyperchem 8.0 program

4.4 Molecular Orbital Eigen Values.

Figure (7) illustrates the energy levels of the molecular orbitals and the symmetry level for the pentacene treated by hyperchem program 8.0 , the figure (7) shows (5) of the occupied orbitals and (8) unoccupied orbitals. The energy of the highest occupied molecular orbital (E_{HOMO}), and the energy of the lowest unoccupied molecular orbital (E_{LUMO}) were calculated by measuring the molecular according to the relationship (Egap= $E_{LUMO} - E_{HOMO}$), was equal to = 7.819 eV , and the ionized energy (I.P) was calculated from the absolte value of the highest occupied orbital and it was equal to (8.526 eV).

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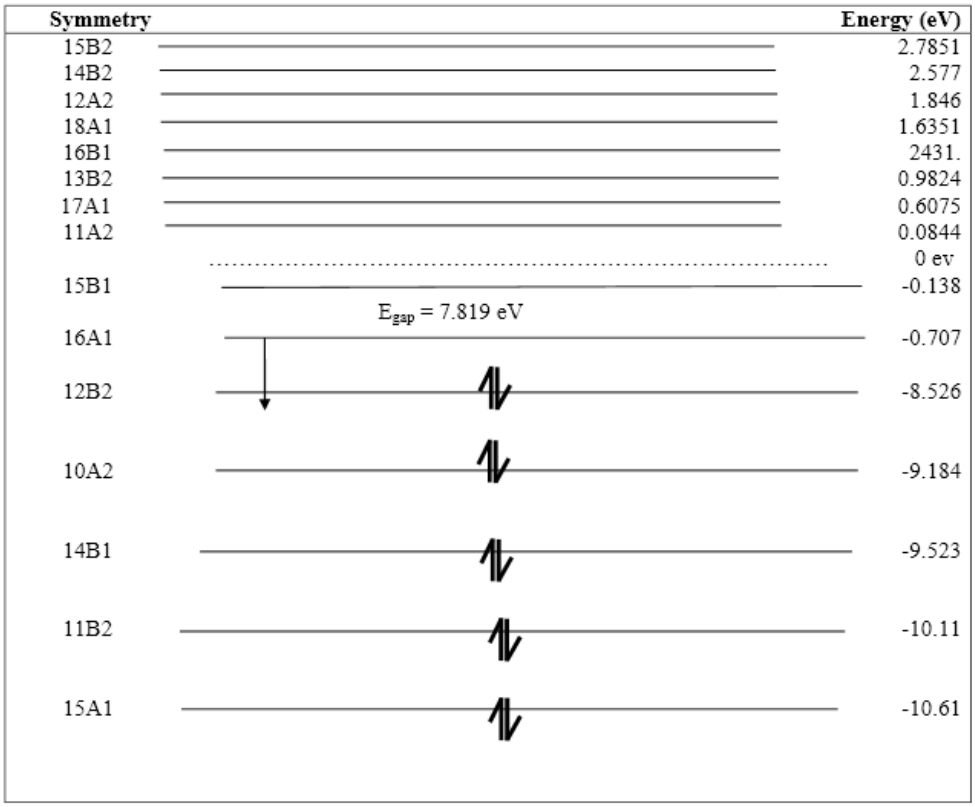

Fig. (7): Values of energy levels of a pentacene molecule and detection of the highest molecular orbital (E_{HOMO}), and lower orbital (E_{LUMO}) , and the symmetry of each orbital calculated by the HyperChem 8.0 program

2-6 UV spectroscopy of (pentacene $C_{22}H_{14}$).

Figure (8) illustrates the UV spectroscopy of pentacene, when to the results obtained from the programs hyperchem and winmopac, with giving spectral characteristics such as higher transition was (9), and the wave length (280.8nm), Oscillator strength (3.341), as shown in fig (8),(9).

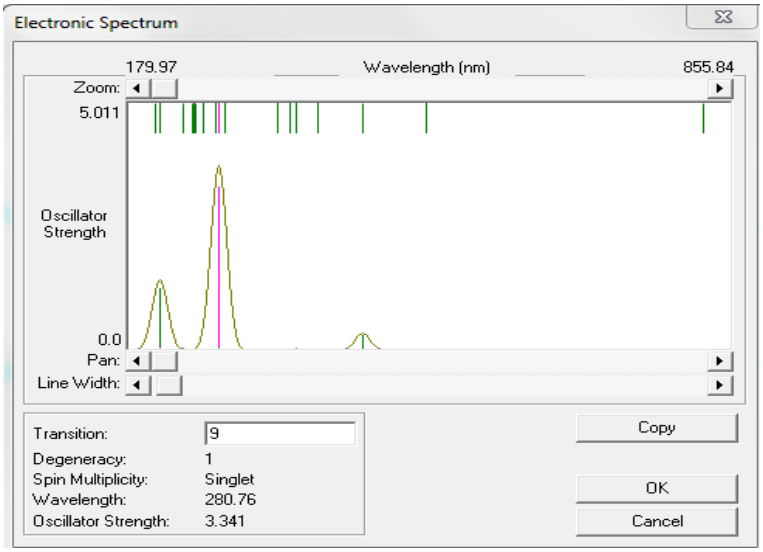

Fig. (8): UV Spectroscopy of pentacene calculated by the hyperchem 8.0 program

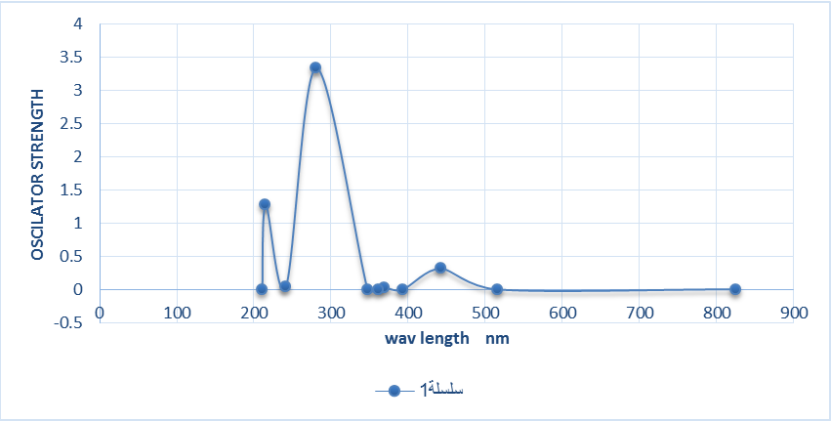

Fig. (9): illustrates the electronic spectrum of pentacene drawn by Excel program

It has been concluded from figure (8),(9) that the wave length (λmax =280.8nm) this was in agreement with the previous studies (λmax =303.5nm).[19].

5. Conculusions

From studying the molecular properties of the pentacen molecule, we have concluded that:

1-The lowest energy of pentacene molecule that make the molecule to be in the equilibrium state was [-2820.062eV,-2820.02eV,-2820.06eV] respectively.

2-The equilibrium distance (bond length) of pentacene is equal to (1.35A^{O},1.4 A^{O},1.1 A^{O}),
and the dissociation energy of the bonds, ($C_1 - C_2$), (C_1=C_4), (C_1-H_{23}) is respectively was (8.9eV ,8.1eV,6.12eV) the results confirmed that as the bond length increase, the molecule starts to dissociate when the bond length reaches to the point that breaks bond ,This was in agreement with previous studies.

3-Molecule (102) showed a vibrational mode in the infrared region due to the base (3N-6).

4-The molecule has 5 orbitals occupied by the electrons and 8 orbitals unoccupied by the electrons, the energy gap was 7.819 eV and the ionization energy was (7.819eV).

5-Electronic spectrum pentacene such as the wave length (280.8 nm), oscillator strength was (3.341).

6-The value of dipole moment of pentacene molecule was (0.039D).

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دراسة الخصائص الطيفية للجزيئة [البنتاسين ($C_{22}H_{14}$)] باستخدام برامج الكم شبه التجريبية

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الملخص

تهدف هذه الدراسة لايجاد الخواص الطيفية للبنتاسين خماسي باستعمال برامج الكم شبه التجريبية [HyperChem0.8,WinMopac7.21] بمعدل اهمال التداخل التفاضلي وقد تم الحساب الشكل هندسي لجزيئة البنتاسين تم حسابه باستعمال المصفوفات البدائية والنهائية والتي تتضمن الطول وزاوية بين أواصر، زاويا سطوح والشحنة لكل ذرة لجزيئة البنتاسين، الطاقة الكلية، طاقة الكترونية، طاقة نقطة الصفر ،فجوة الطاقة ،طاقة الالباب، طاقة التاين ,وعزم ثنائي القطب لجزيئة تم حسابه. تم رسم منحني طاقة الجهد للجزيئة حيث اعتمد رسم بتغير طول الاصرة (C_1-H_{23}) , (C_1=C_4), و (C_1-C_2) للجزيئة البنتاسين إضافة الى تم الحصول على ترددات الاهتزازية لبنتاسين في منطقة تحت الحمراء والانتقالات الكترونية في منطقة فوق البنفسجية نتائج هذه الدراسة متوافقة مع البحوث السابقة.