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

Galsan T. Kamal¹, Abdul Hakim Sh. Mohammed², N. K. Hassan¹

¹ Physics Department, College of Education for pure Sciences, University of Tikrit, Tikrit, Iraq
² Physics Department, College of Science, Kirkuk University, Kirkuk, Iraq

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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 [HyperChem8.0, 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_3) 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.
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].

\[ E_{\text{total}} = E_{\text{rot}} + E_{\text{vib}} + E_{\text{elec}} \]  

Where \( E_{\text{rot}} \) : Total energy , \( E_{\text{vib}} \) : Vibration energy, \( E_{\text{elec}} \) : 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:

\[ F = -k(r-re) \]  

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 (\( \mu \)).

\[ \frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \Rightarrow \mu = \frac{m_1 m_2}{m_1 + m_2} \]  

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

\[ \nu_{\text{vib}} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \]  

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 (\( \mu \)) and the force can be written in terms of potential energy as in equation [9].

\[ V(r) = \frac{1}{2}k(r-r_e)^2 \]  

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].

\[ H = -\frac{h^2}{2\mu} \frac{\partial^2}{\partial \nu^2} + \frac{1}{2}k(r-re)^2 \]  

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

\[ E_v = \hbar \nu_{\text{vib}} (v+\frac{1}{2}) \]  

Where \( \nu_{\text{vib}} \) the total vibrational frequency, (\( \nu \)) it represents the number of vibrational quantum (\( v=0,1,2,3,4,... \)) Since that (\( v=\nu_0 \)) is why the equation becomes as follows.

\[ E_v = \hbar \nu_0 (v+\frac{1}{2}) \]  

Where as (\( \nu_0 \)) represent wave number and be unit is \( \text{cm}^{-1} \), (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.

\[ G(\nu) = \nu_0 (v+\frac{1}{2}) \]  

from this equation, we observe that the distances between adjacent vibrational levels are equal and equal (hc\( \nu \)) to that of main vibrational level (\( \nu_0 \)) called (zero point energy). Which are calculated when (\( v=0 \)) as in the equation.

\[ \nu(0) = \frac{1}{2} \nu_0 \]  

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

\[ V_m = D_e [1 - e^{-\beta (r-r_e)}]^2 \]  

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

\[ G(\nu) = (v+\frac{1}{2}) \nu_0 - (v+\frac{1}{2})^2 \nu_0 \nu_e \]  

Where (\( \nu_e \)) is the anharmonic constant , and (\( G(\nu) \)) represents the vibrational energy level (\( \nu_0 \)) is the vibrational frequency in an harmonic movement. The Morse equation, we can extract the number of vibrational energy levels (\( V=1,2,3,...... \)) [10].

\[ \nu_{\text{max}} = \frac{\hbar}{2 \omega_{\text{vib}}} \]  

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

\[ G(0) = \frac{1}{2} \nu_0 (1 - 2 \times \beta \nu_e) \]  

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

\[ \text{De} = \frac{\hbar \omega_{\text{vib}}}{4 \nu_0 \beta \nu_e} \]  

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].

\[ \Sigma \lambda L_j (F_{ij} - \lambda M_{ij}) \]  

Where (\( F_{ij} \)) in the equation (19) represents a matrix element of the force constants, and (\( M_{ij} \)) matrix masses of atoms, (\( \lambda \)) Eigen value, (\( L_{ij} \)) 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 \( \lambda \) in equation [14,15].

\[ \lambda = 4\pi^2 \nu_e^2 \]  

Where (\( \nu \)) the harmonic frequency is represented by a unit (\( \text{cm}^{-1} \)), 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].

\[ \mu = qd \]  

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

- $\sigma$ (sigma) – orbital has symmetry about the bonding axes, lowest energy
- $\pi$ (pi) – only one orbital plane passes through both nuclei involved
- $\sigma^*$ (anti-bonding) – orbital involved is not involved in bonding, usually a lone pair, higher in energy
- $\pi^*$ (anti-bonding) – nodal planes exist between nuclei, high in energy, usually unpopulated in stable molecules, as show in figure (1).

![Energy Levels](image)

**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 ($r, \theta, \phi$) ($r$ the distance between these atoms, $\theta$ represents an angle between three atoms, $\phi$) They are dihedral- angle, and the geometric shape at the equilibrium state.

![Molecular Structure](image)

**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 ($\theta$), and the dihedral angles ($\phi$).
Table 1: The initial matrix of the pentacene molecule shows, the internal coordinates (r, Θ, Φ), by HyperChem. Program

| ATOM | r (Å) | Θ° | φ° | OPT | A | B | C |
|------|-------|----|----|-----|---|---|---|
| C    | 1.3537| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4353| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4422| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3537| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4361| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3772| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4208| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3772| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4209| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3985| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3987| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4283| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3984| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4206| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4206| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3774| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4424| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3537| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.4424| 1   | 0  | 0   | 0 | 0 | 0  |
| C    | 1.3537| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0959| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0959| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0947| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0959| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0970| 1   | 0  | 0   | 0 | 0 | 0  |
| H    | 1.0972| 1   | 0  | 0   | 0 | 0 | 0  |
| Dipole moment | 0.039 | 0.039 | Debyes |

These properties were found after obtaining the initialize matrix and incorporated into 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_{25}H_{14}) molecule calculated by the (WinMopac 7.21 ) program

| The spectral properties | The calculated values by winmopac7.21 program | The calculated values by HyperChem program | Units |
|-------------------------|-----------------------------------------------|-------------------------------------------|-------|
| Heat of Formation       | 107.93209                                      | 107.417366                                 | KCal/mol |
| Total Energy            | -2320.06238                                    | -2820.082074923                            | 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 (pentacene C_{25}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 anharmonic 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 Å^0), (2820.02 eV) at the distance r_{opt} = 1.4 Å^0, (- 2820.06 eV ) at the distance r_{eq} = 1.1 Å. 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 a large 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 a weak 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°) | 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.
Fig. (4): the total energies of the pentacene molecule at different \( (C_1=C_4) \) Lengths

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

| Distance \( r(\text{Å}) \) | 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 \( r(\text{Å}) \) | 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 | 0.00001 | 59.46 | 1 A | 62.81 |
| 2 | 0.00001 | 93.71 | 1 B | 94.85 |
| 3 | 0.01885 | 124.79 | 2 B | 126.33 |
| 4 | 0.08949 | 129.34 | 3 B | 130.06 |
| 5 | 0.26299 | 172.74 | 1 A | 173.83 |
| 6 | 0.00001 | 248.03 | 4 B | 249.20 |
| 7 | 0.00001 | 256.96 | 5 A | 257.34 |
| 8 | 0.00001 | 277.15 | 6 A | 277.18 |
| 9 | 0.00001 | 307.01 | 5 B | 307.65 |
| 10 | 0.00001 | 311.51 | 7 A | 312.40 |
| 11 | 0.00421 | 389.14 | 6 B | 389.60 |
| 12 | 0.01659 | 446.45 | 9 A | 446.70 |
| 13 | 0.00823 | 446.57 | 8 B | 447.28 |
| 14 | 0.00034 | 468.05 | 10 A | 468.88 |
| 15 | 0.05439 | 474.30 | 11 A | 474.54 |
| 16 | 0.00010 | 480.69 | 9 B | 481.28 |
| 17 | 0.00001 | 500.09 | 10 B | 500.17 |
| 18 | 0.00284 | 533.57 | 12 B | 534.02 |
| 19 | 0.79387 | 584.40 | 11 B | 584.56 |
| 20 | 0.00019 | 607.67 | 13 A | 607.79 |
| 21 | 0.32518 | 634.65 | 12 B | 634.80 |
| 22 | 0.00032 | 644.71 | 14 A | 645.02 |
| 23 | 0.00002 | 704.62 | 15 A | 705.04 |
| 24 | 0.00121 | 724.76 | 13 B | 725.26 |
| 25 | 0.00011 | 730.71 | 16 A | 730.95 |
| 26 | 0.00054 | 732.06 | 17 A | 732.35 |
| 27 | 0.04079 | 733.24 | 14 B | 733.62 |
| 28 | 38.57559 | 764.50 | 18 A | 765.84 |
| 29 | 0.06218 | 763.98 | 15 B | 765.32 |
| 30 | 0.01039 | 831.99 | 16 B | 832.21 |
|   |   |   |   |   |
|---|---|---|---|---|
| 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 | 13.21299 | 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 | 1457.42 |
| 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 | 5.35979 | 3046.57 | 93 | 3046.98 |
| 94 | 0.01003 | 3047.64 | 94 | 3047.84 |
| 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 |
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].

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

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 drawn 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 (E_{gap} = E_{LUMO} - E_{HOMO}), was equal to = 7.819 eV, and the ionized energy (I.P) was calculated from the absolute value of the highest occupied orbital and it was equal to (8.526 eV).
Fig. (7): Values of energy levels of a pentacene molecule and detection of the highest molecular orbital ($E_{\text{HOMO}}$), and lower orbital ($E_{\text{LUMO}}$), 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 winnopac, 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 ($\lambda_{max}$=280.8nm) this was in agreement with the previous studies ($\lambda_{max}$=303.5nm).[19].

5. Conclusions
From studying the molecular properties of the pentacene 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 (1.35Å,1.4 Å,1.1 Å), and the dissociation energy of the bonds, (C–C), (C–C), (C–H) is respectively was (8.9eV, 6.12eV, 7.819 eV, 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 \([\text{البنتاسين} (\text{C}_{22}\text{H}_{14})]\) باستخدام برامج الكم شبه التجريبية

كمس طلال كمال 1، عبد الحكيم شكور محمد 2، نديم خالد حسن 1
قسم الفيزياء، كلية التربية للعلوم الصرفة، جامعة كركوك، كركوك، العراق
قسم الفيزياء، كلية العلوم، جامعة كركوك، كركوك، العراق

الملخص

هذا الدراسة تهدف لإيجاد الخواص الطيفية للبنتاسين خماسي باستخدام برامج الكم شبه التجريبية [21] بمعدل التداخل التفاضلي وقد تم الحساب الشكل هندسي لجزيئة البنتاسين ثم حسابه باستعمال المصروفات البدائية والنهائية والتي تتضمن الطول وزاوية بين أواصر زاوية حجم الحاجة لكل ذرة لجزيئة البنتاسين، طاقة الإلكترونية، طاقة الكتلة، طاقة الكتلة، طاقة الطاقة، فجوة الطاقة، طاقة الفجوة، طاقة محسية، طاقة الكتلة، طاقة الكتلة، طاقة التالين وعزم ثاني الفصل لجزيئة البنتاسين، هامش مسالمة، تم رسم منحنى حجم الصفر لجزيئة حيث اعتمد رسم منحنى الطاقة النقطة طاقة لجزيئة البنتاسين إضافة إلى ترددات الاهتزازات لجزيء البنتاسين في منطقة تحت الحمراء، وانحلالات الكهرمنية في منطقة فوق البنفسجية، وناتج هذه الدراسة متوافق مع البحوث السابقة.