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## Study of the Electronic and Spectroscopic Properties for Pyrene: B3LYP / DFT Calculations

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### ABSTRACT

Theoretical study for calculating molecular structure parameters of pyrene and its simplest derivatives with electron-donating groups (hydroxyl) in different positions were performed using DFT. B3LYP functional with 6-31G(d, p) basis set was used to investigate the effect on the electronic and structural properties for the positional variation of the hydroxyl subgroup in the pyrene. The optimized structures, total energies, electronic states, energy gaps, ionization potentials, electron affinities, chemical potential, global hardness, softness, global electrophilic index, dipole moment and dipole polarizability were calculated. The harmonic vibration frequencies calculated and compared with available experimental data. The results showed a decrease in energy gap and the presence of the electron-donating groups leads to easy oxidation.

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## INTRODUCTION

Aromatic compounds are a large class of conjugated  $\pi$ -electron systems of great importance in many research areas, such as materials science, astrochemistry (P.V.R. Schleyer, 2001) and molecular electronics (J. McMurry, 2000), (H.S. Nalwa, 2006), (B.A. Saleha *et al*, 2011). In the last case molecules with electron-accepting (high electron affinity) and electron-donating (low ionization potential) properties strongly effecting charge-transporting properties of thin films based on these materials are often used. In contrast to inorganic materials that consist of covalent or ionic bonds of atoms over the entire solids, organic materials are based on independent molecules and are characterized by weak intermolecular interactions. As a result, characteristics of energy levels and energy transformation for single molecules and condensed media differ a little, while the difference among these characteristics for inorganic compounds is much stronger. Thus, the properties of individual molecules can be used to describe molecular solids in the 1st approximation. Molecular electronics is one of the most important developments in modern-day technology (A.V. Kukhta *et al*, 2008).

Pyrene is a material in the dye manufacturing and rubber industry. pyrene can be oxidized by chromic acid into pyreonequinone which is the fundamental ring structure.

Di- amino naphthalene used for determination of selenium. Also used in the production of polymers and in organic semiconductor (R.T. Morrison *et al* 2005).

Organic semiconductors have been portably used since the time of their discovery (C.W. Tang *et al*, 1987) due to their flexibility, low cost (B. Zhenan, 2007), and intrinsic properties such as light emission. Some applications of organic semiconductors include: organic light emitting diodes (OLEDs), photovoltaic cells, thin film transistors, and biosensors. It is important to mention that most of the materials used for these applications contain conjugated p systems (D. Glossman-Mitnik (D. Glossman-Mitnik *et al* 2008).

The theoretical study of the electronic structure has proved to be very conducive to predict physicochemical properties of a large number of donor-acceptor systems. Moreover, theoretical calculations such as geometry optimizations are very important for understanding the pathways of electron and/or energy transfer processes in photoactive assemblies (B.A. Saleh 2009). The substituent attached to the molecular framework can enhance or diminish the reactivity. The mechanistic conclusions based on the linear relationships with free energy have been extremely fruitful. Accordingly, changes in reactivity in one reaction series caused by changes in

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substitution are related to changes in equilibrium or reactivity in another series caused by the same changes in substitution (B.A. Saleha *et al* 2011).

The goal of this work is the theoretical investigation of the effect of substitution groups (hydroxyl) on electronic and structural properties and the reactivity of pyrene molecular and the evaluation of their dipole polarizability by DFT method and comparison with experimental results.

### Computational Details:

Figure 1 represents the molecules under study. All the computational studies were carried out using the density functional theory (DFT) implemented in the Gaussian 09 suite of programs (M.J. Frisch *et al* 2009). The molecular properties of the compounds have been computed by DFT using the standard 6-31G(d, p) basis set. In the DFT calculations the Lee, Yang and Parr correlation functional (G. Robert *et al* 1994) is used together with Becke's three parameters (A.K.B. Bender 2000) exchange functional B3LYP. Conformational analysis of the molecules has been performed to have an idea about the lowest energy structures of the species.

The geometry optimization was performed at the B3LYP density functional theory with the same basis set (P. Romaniello 2006). Harmonic vibration frequencies were computed at the same level of theory. The hybrid functional B3LYP has shown to be highly successful for calculation the electronic properties such as ionization potential, electron affinity, electronic states and energy gap (J. Engelberts *et al* 2005). The DFT partitions the electronic energy as (A.M. Ali 2009):

$$E = E_T + E_V + E_J + E_{XC}$$

where  $E_T$ ,  $E_V$  and  $E_J$  are the electronic kinetic energy, the electron nuclear attraction and the electron-electron repulsion terms respectively. The electron correlation is taken into account in DFT via the exchange correlation term  $E_{XC}$ , which includes the exchange energy arising from the anti-symmetry of the quantum mechanical wave function and the dynamic correlation in the motion of individual electrons; it makes DFT dominant over the conventional HF procedure.

The geometry optimized structures in figure 1 are obtained without any symmetry restriction, and vibration analysis for each structure does not yield any imaginary frequencies, which indicates that the structure of each molecule corresponds to a local minimum on the potential energy surface (A.J. Camargo *et al.*, 2003).

In this investigation, ionization potential IP and the electron affinity EA are calculated depending on the Koopmans' theorem: (K. Sadasivam *et al* 2011).

$$IP = E_{HOMO} \quad , \quad EA = E_{LUMO} \quad (1)$$

Within the framework of the density functional theory (DFT), one of the global quantities is the chemical potential ( $\mu$ ), which is measures the escaping tendency of an electronic cloud, and equals (M. Oftadeh *et al* 2011):

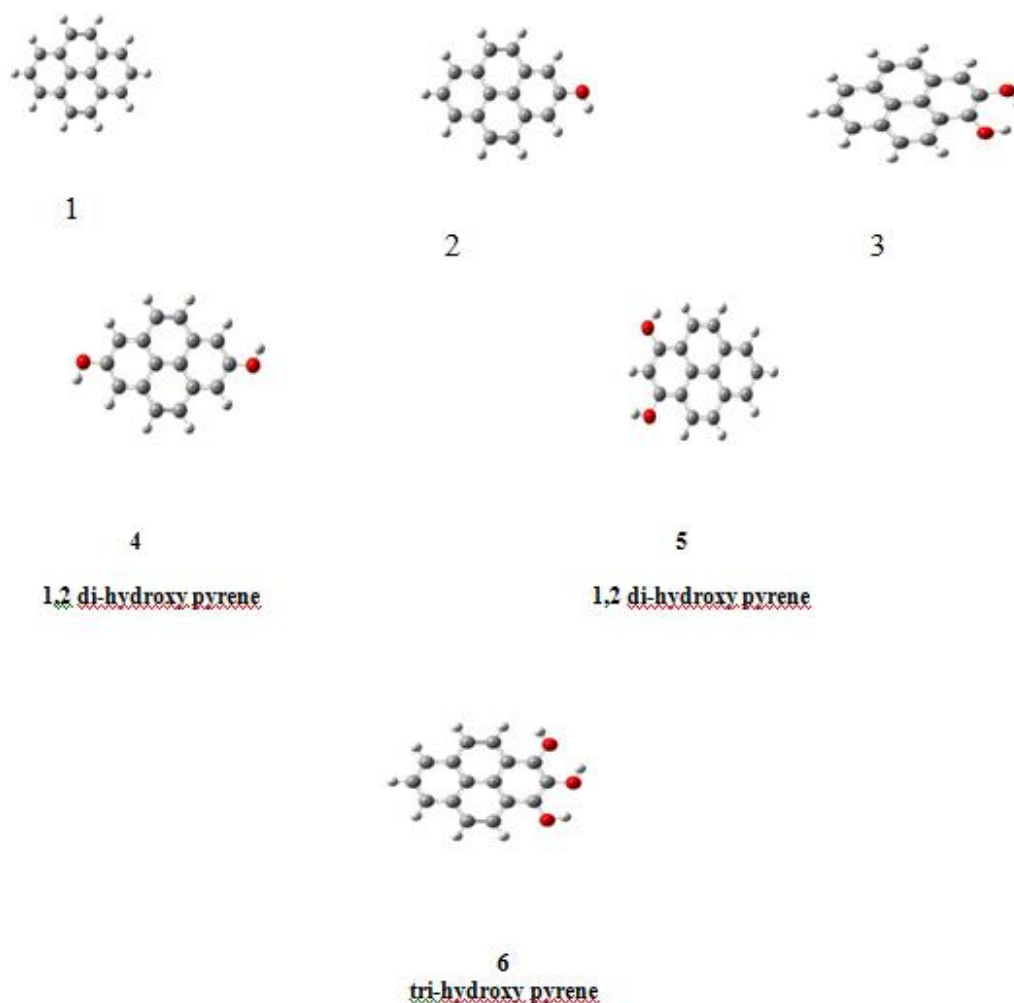
$$\mu \approx -\chi = -\frac{(IP + EA)}{2} \quad (2)$$

The theoretical definition of chemical hardness has been provided by the density functional theory as the second derivative of electronic energy with respect to the number of electrons N, for a constant external potential  $v(r)$  and the finite difference approximation to chemical hardness gives (M. Oftadeh *et al* 2011):

$$\eta = -\frac{(IP - EA)}{2} \quad (4)$$

And the softness is given as:

$$S = \frac{1}{2\eta} = \left[ \frac{\partial^2 N}{\partial E^2} \right]_{v(r)} = \left[ \frac{\partial N}{\partial \mu} \right]_{v(r)} \quad (5)$$



**Fig. 1:** Structures of pyrene and its derivatives discussed in this work.

*Electrophilic index is a measure of energy lowering due to maximal electron flow between donor and acceptor. Electrophilic index ( $\omega$ ) is defined as (M. Oftadeh 2009):*

$$\omega = \frac{\mu^2}{2\eta} \quad (6)$$

*If some of applied molecules are planar and some are not, it will be useful to report polarizability quantities that are invariant to the choice of coordinate system. One of them is the mean polarizability  $\langle\alpha\rangle$  is evaluated using the equation (M. Oftadeh 2009) :*

$$\langle\alpha\rangle = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (7)$$

Where  $(\alpha_{xx} \leq \alpha_{yy} \leq \alpha_{zz})$  are the eigenvalues of the polarizability tensor.

## RESULTS AND DISCUSSIONS

### **Molecular Geometry:**

The optimized structure parameters of molecules calculated by DFT-B3LYP levels with the 6-31G(d, p) basis set are listed in table 1 in accordance with the atom numbering scheme given in figure 1. Table 1 shows

the calculated bond lengths and angles for (1 – 6) molecules with the experimentally available from X-ray diffraction data for the original molecule (H. Dorsett *et al* 2000).

From the theoretical values, we can find that most of the optimized bond angles are slightly larger than the experimental values, due to the theoretical calculations belong to isolated molecules in gaseous phase and the experimental results belong to molecules in solid state.

**Table1:** Optimized geometrical parameters of molecules, bond length R ( $\text{\AA}$ ), Interaxial angles ( $^\circ$ ).

Molecules	Bond length	Our data	Exp.	Interaxial angles	Our data	Exp.
1	R(C <sub>3</sub> -C <sub>4</sub> )	1.426	1.412	A(C <sub>10</sub> -C <sub>3</sub> -C <sub>4</sub> )	120.441	119.5
	R(C <sub>3</sub> -C <sub>10</sub> )	1.430	1.422	A(C <sub>15</sub> -C <sub>10</sub> -C <sub>3</sub> )	121.804	120.2
	R(C <sub>14</sub> -C <sub>15</sub> )	1.445	1.417	A(C <sub>10</sub> -C <sub>15</sub> -C <sub>14</sub> )	119.098	120.5
	R(C <sub>11</sub> -H <sub>16</sub> )	1.400	1.092	A(H <sub>7</sub> -C <sub>10</sub> -C <sub>3</sub> )	120.155	117.0
	R(C <sub>15</sub> -H <sub>18</sub> )	1.087	1.092	A(H <sub>18</sub> -C <sub>15</sub> -C <sub>10</sub> )	118.469	119.9
2	R(C <sub>1</sub> -C <sub>2</sub> )	1.378		A(C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> )	119.606	
	R(C <sub>1</sub> -C <sub>6</sub> )	1.437		A(C <sub>1</sub> -C <sub>6</sub> -N <sub>20</sub> )	116.860	
	R(C <sub>1</sub> -N <sub>17</sub> )	1.420		A(C <sub>1</sub> -C <sub>2</sub> -H <sub>8</sub> )	119.476	
	R(C <sub>2</sub> -H <sub>8</sub> )	1.088		A(C <sub>1</sub> -N <sub>17</sub> -H <sub>16</sub> )	113.145	
	R(N <sub>17</sub> -H <sub>18</sub> )	1.013		A(H <sub>21</sub> -N <sub>20</sub> -H <sub>22</sub> )	110.370	
3	R(C <sub>1</sub> -C <sub>2</sub> )	1.384		A(C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> )	118.689	
	R(C <sub>9</sub> -C <sub>14</sub> )	1.374		A(C <sub>6</sub> -C <sub>1</sub> -N <sub>17</sub> )	119.25	
	R(C <sub>1</sub> -N <sub>17</sub> )	1.402		A(C <sub>1</sub> -C <sub>2</sub> -H <sub>8</sub> )	119.877	
	R(C <sub>2</sub> -H <sub>8</sub> )	1.088		A(C <sub>13</sub> -N <sub>20</sub> -H <sub>22</sub> )	114.269	
	R(N <sub>17</sub> -H <sub>18</sub> )	1.012		A(H <sub>21</sub> -N <sub>20</sub> -H <sub>22</sub> )	110.885	
4	R(C <sub>1</sub> -C <sub>2</sub> )	1.382		A(C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> )	121.722	
	R(C <sub>9</sub> -C <sub>13</sub> )	1.379		A(C <sub>1</sub> -C <sub>2</sub> -N <sub>17</sub> )	120.614	
	R(C <sub>6</sub> -N <sub>20</sub> )	1.397		A(C <sub>2</sub> -C <sub>1</sub> -H <sub>8</sub> )	119.390	
	R(C <sub>1</sub> -H <sub>8</sub> )	1.088		A(C <sub>6</sub> -N <sub>20</sub> -H <sub>22</sub> )	115.030	
	R(N <sub>17</sub> -H <sub>18</sub> )	1.011		A(H <sub>21</sub> -N <sub>20</sub> -H <sub>22</sub> )	111.609	
5	R(C <sub>1</sub> -C <sub>2</sub> )	1.381		A(C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> )	121.604	
	R(C <sub>1</sub> -C <sub>6</sub> )	1.411		A(C <sub>6</sub> -C <sub>5</sub> -N <sub>20</sub> )	121.679	
	R(C <sub>2</sub> -N <sub>17</sub> )	1.410		A(C <sub>9</sub> -C <sub>13</sub> -H <sub>16</sub> )	119.999	
	R(C <sub>13</sub> -H <sub>16</sub> )	1.086		A(C <sub>2</sub> -N <sub>17</sub> -H <sub>19</sub> )	117.223	
	R(N <sub>17</sub> -H <sub>19</sub> )	1.013		A(H <sub>21</sub> -N <sub>20</sub> -H <sub>22</sub> )	109.247	
6	R(C <sub>1</sub> -C <sub>2</sub> )	1.386		A(C <sub>2</sub> -C <sub>1</sub> -C <sub>6</sub> )	120.887	
	R(C <sub>1</sub> -C <sub>6</sub> )	1.408		A(C <sub>13</sub> -C <sub>10</sub> -N <sub>20</sub> )	120.802	
	R(C <sub>10</sub> -N <sub>20</sub> )	1.400		A(C <sub>9</sub> -C <sub>14</sub> -H <sub>18</sub> )	120.028	
	R(C <sub>1</sub> -H <sub>8</sub> )	1.087		A(C <sub>2</sub> -N <sub>17</sub> -H <sub>19</sub> )	113.506	
	R(N <sub>17</sub> -H <sub>19</sub> )	1.012		A(H <sub>21</sub> -N <sub>20</sub> -H <sub>22</sub> )	110.704	

### Energies:

Table (2) shows the values of the total energy and electronic states for the analyzed structures and the energy gap ( $E_{LUMO} - E_{HOMO}$ ) of the studied molecules. The total energy for all studied molecules as a linear function of the hydroxyl side group number adding to the molecule. The final total energy of the product is the collection of total energy of all small molecules which build the product molecule.

It is clear that from table 2, the total energy for all di-hydroxyl pyrene molecules is approximately the same in which this refers to that the total energy is independent on the position of the di-hydroxyl sub group in the ring, and it is observed that substitution of these groups causes increasing the HOMO and LUMO energy, it is known that the electron donating substituent increasing the LUMO and HOMO energies (M. Oftadeh *et al* 2011), and energy gap decreased. Therefore, the presence of substituent decreases the energy gap improves the conductivity and also enhances the solubility of these molecules.

The LUMO-HOMO energy gaps of di-hydroxyl pyrene molecules is small than that of the original molecule, with decreasing energy gap, electrons can be easily excited from the ground state [26,25]. This effect of the side group was the largest in molecule 2, it has energy gap of (3.069 eV). The energy gap of pyrene equals (3.796 eV) is agreements with experiment value (3.721eV). Table 2 shows also the symmetry of studied molecules, the molecule 1 (pyrene) is a planar and it from D<sub>2h</sub> point group (high symmetry), it contains 2-fold axis of rotation and two 2-fold rotations about axes perpendicular to principal axis and it have higher electro negativity, while molecules 4 and 6 are both C<sub>2h</sub> point group contains 2-fold axis of rotation and a horizontal reflection plane. The others all C<sub>s</sub> point group of low symmetry contain only the plane of reflection. This change in molecular symmetry comes from the presence of the substituent in the ring.

### Some Electronic Variables:

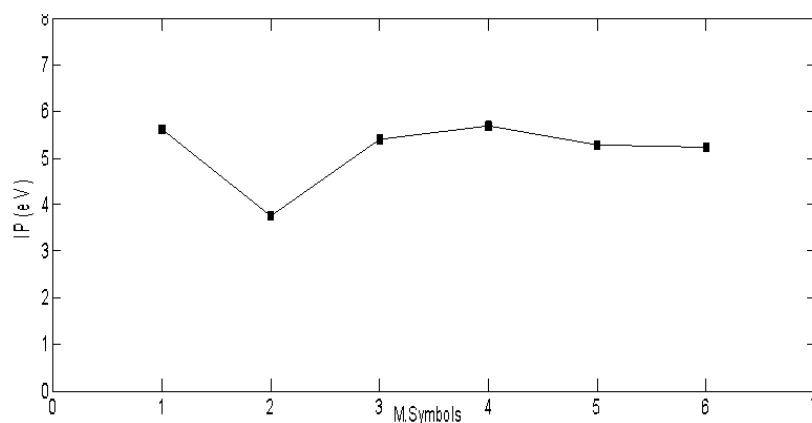
The properties that are displayed in figures (2-7) for each electronic variable are computed by Koopmans' theorem, in which it is based on the differences between the HOMO and the LUMO energies of the neutral

molecule and is known as orbital-vertical method.

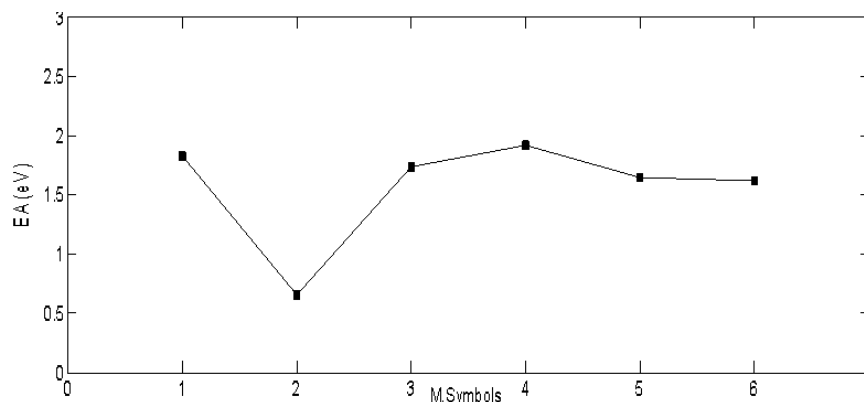
The calculated properties for each variable as shown in figures (2-7) clearly reveal that these di-hydroxyl pyrene compounds have a tendency to donate electrons instead of capturing them. The ionization potential for the di-hydroxyl pyrene molecules group is higher than that for the mono-hydroxyl pyrene molecule, but molecule (4) has the larger value of ionization potential, this indicates that this di-hydroxyl pyrene molecule needs high energy to become cation comparing with the others, it has the same behavior of the original molecule. While mono-hydroxyl pyrene molecule needs small energy to donating its electron. The strength of a donor molecule is measured by its electron affinity (EA) which the energy released when adding one electron to LUMO. A donor must have a low EA, adding the sub group to the ring leads to reduce the ability of the electron affinity for the molecule; EA for molecule 2 is the lowest, as we see in figure 5. The behavior of chemical potential for the studied structures likes the ionization potential and electron affinity, as we see in figure 4. Figure 6 showed that mono-hydroxyl pyrene molecule has good value of electronic softness and corresponds to its energy gap and electrophilic index values, this molecule has the smallest energy gap and the largest value of electrophilic index in which this indicates to that this molecule is more reactive than the others and has large chance to interact with the surrounding species in comparison with the other studied structures. In general, the results obtained by the calculation of electro negativity and electrophilic index are agreed very well with the other results.

**Table 2:** Total energy, electronic states and energy gap for molecules.

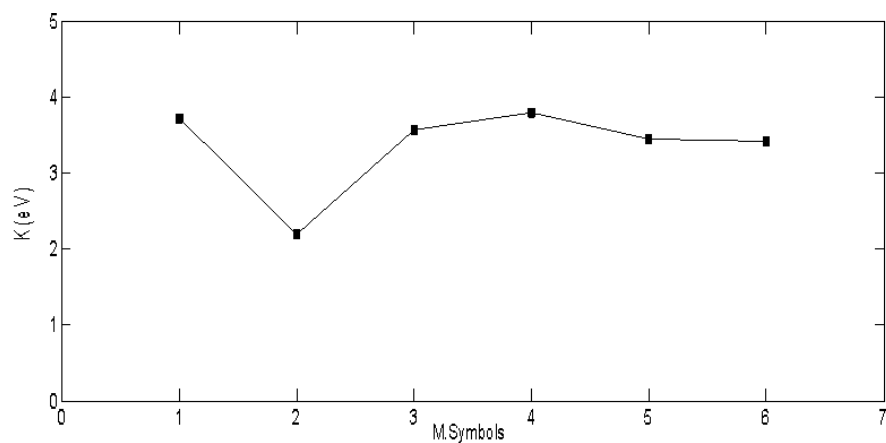
Structure	Energy(a.u)	Symmetry	Electronic States(eV)		Energy Gaps (eV) Our data	Energy Gaps (eV) Expt.
			HOMO	LUMO		
1	-615.83689	$D_{2h/c1}$	-5.62233	-1.82558	3.79675	3.721[28]
2	-691.06866	$C_{s/c1}$	-3.75076	-0.65388	3.09688	-
3	-766.29008	$C_s$	-5.41281	-1.73279	3.68002	-
4	-766.30193	$C_{2h/c1}$	-5.69934	-1.91293	3.78641	-
5	-766.30076	$C_s$	-5.22505	-1.61578	3.60927	-
6	-841.53513	$C_{2h/c1}$	-5.26968	-1.64300	3.62668	-



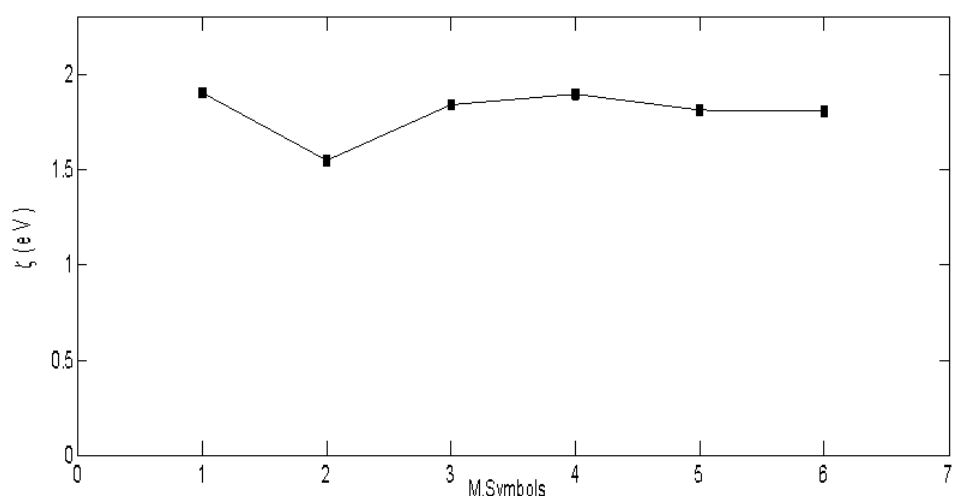
**Fig. 2:** The calculated ionization potential for molecules under study.



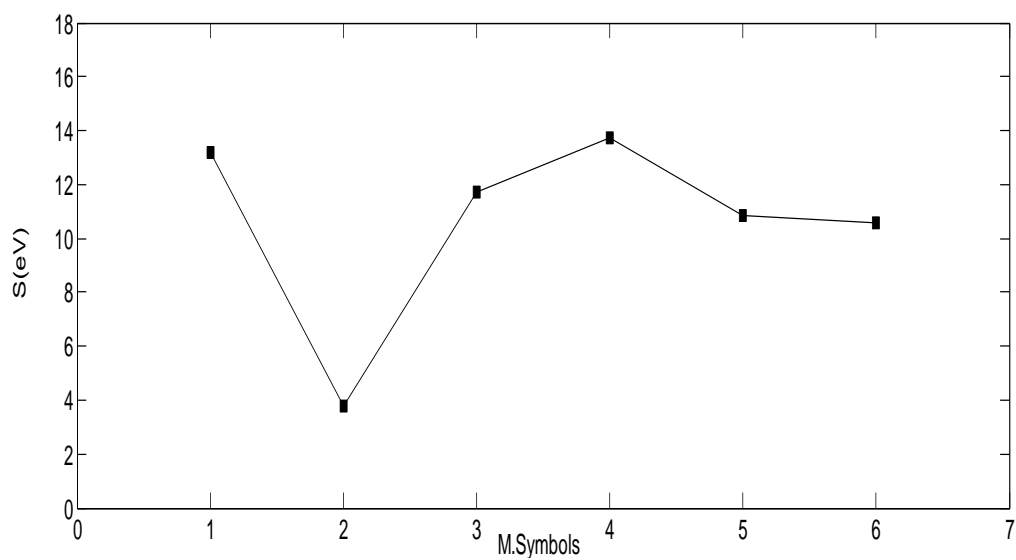
**Fig. 3:** The calculated electron affinity for molecules under study.



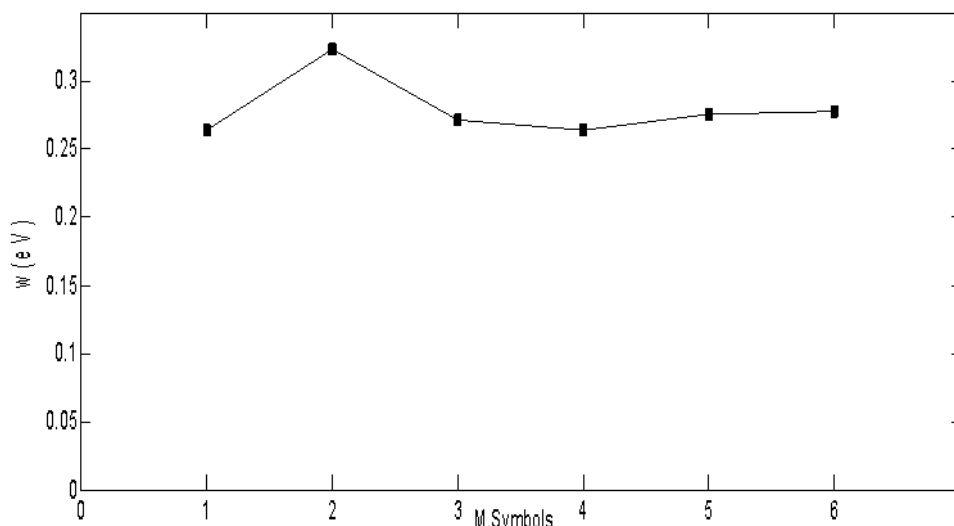
**Fig. (4):** The calculated chemical potential for molecules under study.



**Fig. (5):** The calculated absolute hardness for molecules under study.



**Fig. (6):** The calculated absolute softness for molecules under study.



**Fig. (7):** shows the calculated electrophilic index for molecules under study.

The molecules dipole moment represents a generalized measure of bond properties and charge densities in a molecule. Molecule with electron acceptor group due to better charge distribution and increasing distance have higher dipole moment, from table 4 molecule 4 has higher dipole moment (2.904 Debye) .

The results of the calculated polarizability for (1 – 6) molecules in table 4 showed that all substitution groups leads to increase the average polarizability and cause more reactive than the original molecule. The molecules 3 and 6 have average dipole polarizability equal 216.25 and 220.41 a.u, they have the highest polarizability and have highest reactivity. This due to the ring delocalizing  $\pi$  electron resonance from the phenyl groups(M. Oftadeh *et al* 2011).

**Table 4:** Calculated dipole moment  $\mu$  (Debye) and average polarizability  $\langle\alpha\rangle$  in atomic units for Molecules.

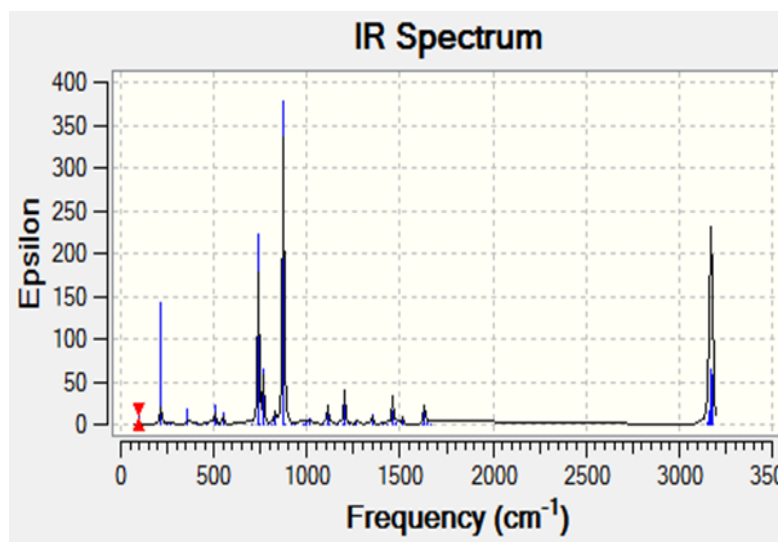
molecules	$\mu$	$\alpha_{xx}$	$\alpha_{yy}$	$\alpha_{zz}$	$\langle\alpha\rangle$
1	0.000	94.586	214.377	297.938	202.30
2	2.247	96.314 98.189	217.372 264.318	316.159 286.260	209.94
3	0.0035	96.855	219.080	330.597	216.25
4	2.904	97.136	229.760	317.298	215.51
5	2.448	98.730	232.014	330.506	214.73
6	2.223				220.41

### IR Spectra:

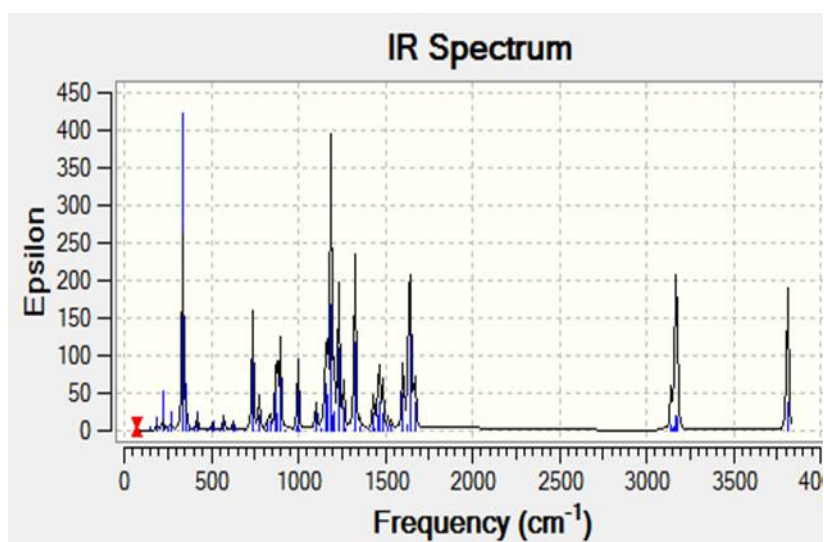
The harmonic vibration frequencies and the IR intensities calculated for the studied molecules at B3LYP level using the 6-31(d, p) basis set are shown in figure 8. As we know, the (C – H) stretching vibrations of aromatic molecules in the region (2900 – 3250)  $\text{cm}^{-1}$  which is characteristic region for ready identification of (C – H) stretching vibrations and particularly the region (3250 – 3100)  $\text{cm}^{-1}$  for asymmetric stretching and (3100 – 2900)  $\text{cm}^{-1}$  for symmetric stretching modes of vibration (R.R. Gotwals *et al* 2008).

The present work gives the frequency values at 3185, 3142.45 and 3225  $\text{cm}^{-1}$  for pyrene which are consistent with experimental results of 3085, 3110, 3136 and 3182  $\text{cm}^{-1}$ , and the aromatic molecules frequency has both in-plane (1100 – 1700)  $\text{cm}^{-1}$  and out-of-plane (below 1000  $\text{cm}^{-1}$ ) (C – H) bending vibrations, the in plane vibration for pyrene calculated at 885.5  $\text{cm}^{-1}$  and 975.34  $\text{cm}^{-1}$  which a good agreement with experimental results 878.3 and 954.9  $\text{cm}^{-1}$ [20], and the out-of-plane (C – H) deformation vibrations calculated at 612.87  $\text{cm}^{-1}$  and 734.67  $\text{cm}^{-1}$  is agreement with experimentally predicted in 603  $\text{cm}^{-1}$  and 726  $\text{cm}^{-1}$ (A.J. Camargo *et al* 2003).

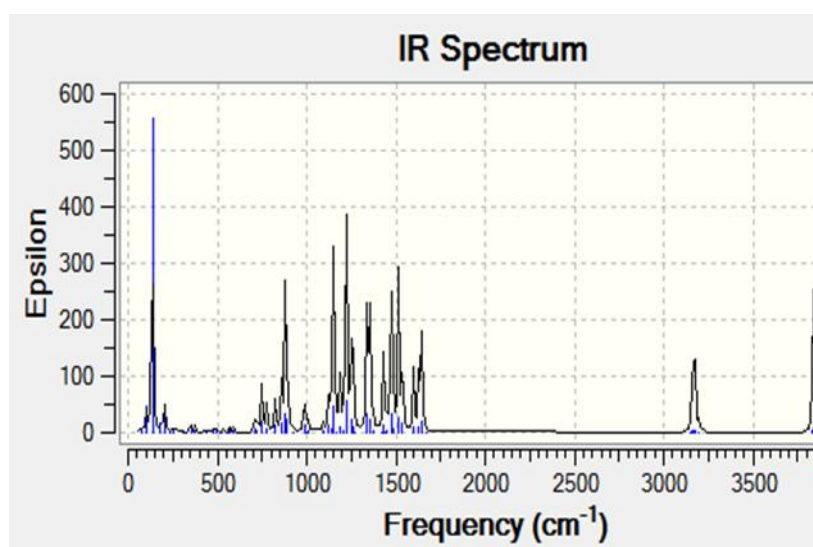
It is clear from figure 8 that the IR spectrum for hydroxyl pyrene molecules characters from that of pyrene by multiply the vibration mode due to existing of (O – H) , (C – O) bonds, (C = C) stretching and (C – H) stretching, for (2 – 6) molecules the stretching of (O – H) bond has been observed at (1322 – 1402)  $\text{cm}^{-1}$ , the (C – H) stretching stay in the region (3108 – 3305)  $\text{cm}^{-1}$ , the stretching of (C – O) bond has been observed at (1312 – 1422)  $\text{cm}^{-1}$  and the stretching of (C = C) bond at the range (1410 – 1520)  $\text{cm}^{-1}$ , while the bending of (O – H) bond appeared at (1565 – 1675)  $\text{cm}^{-1}$ . The stretching (O–H) bond for molecules are calculated at 1635.45  $\text{cm}^{-1}$ . The  $\pi$ -electron density on the aromatic ring was delocalized the presence of the –OH sub groups, which reduced the strength of (C = C) bond and depending on the position of hydroxyl group. The torsion vibrations appear at very low frequency for (2 – 6) molecules at below 100  $\text{cm}^{-1}$ . Generally, the number of vibration modes for each structure was agree with the calculations for non-linear molecular system according to the relation  $3N-6$ , where N is the number of atoms that the structure included.



1

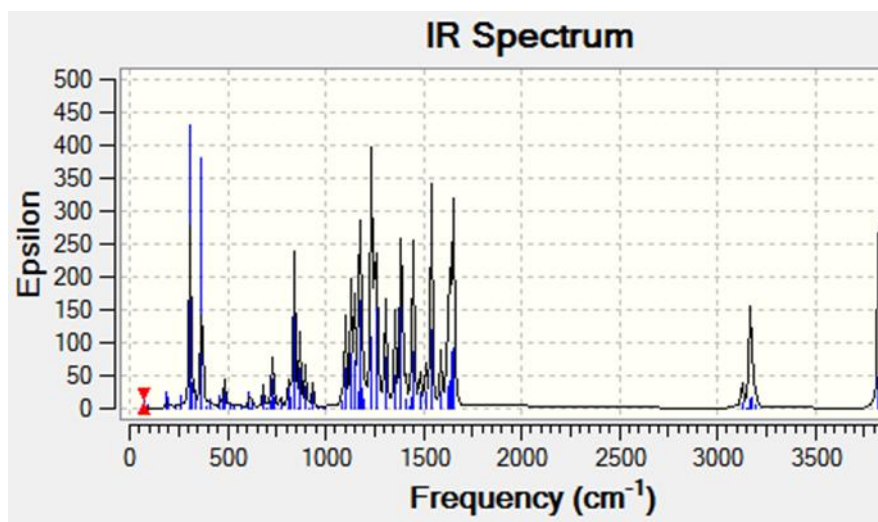


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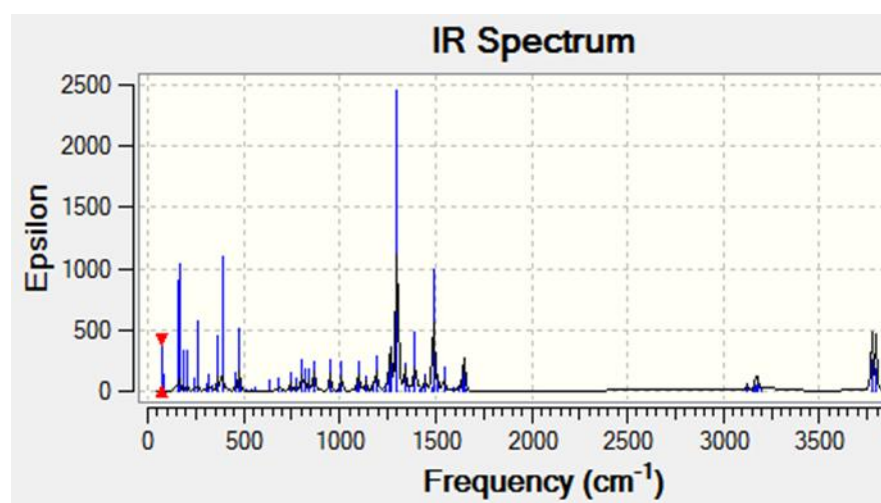


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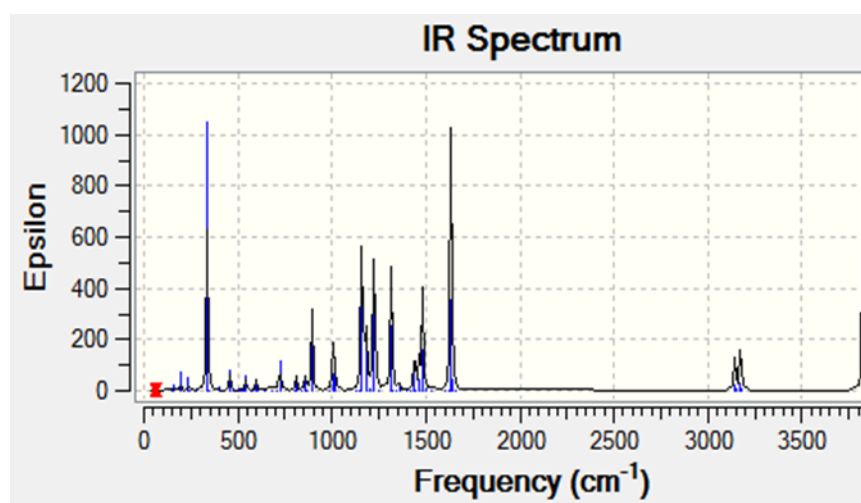




4



5



6

**Fig. (8):** Shows the calculated IR spectral frequencies for molecules under study.

### Conclusions:

We have used DFT in this study to obtain the geometry optimization and calculate some electronic properties of pyrene and hydroxyl pyrene molecules group using B3LYP hybrid functional. The calculated electronic properties such as ionization potential, electron affinity, electro negativity, hardness, softness and electrophilic index by using orbital-vertical method, the important conclusions are:

- 1- Geometry optimization for molecule 1 has been found in a good agreement with experimental data, while for other studied molecules (2 – 6) it has not been found a reference data.
  - 2- The total energies for di-hydroxyl pyrene found independent on the position of the hydroxyl sub group in the ring and substitution hydroxyl group causes decreasing energy and more stability.
  - 3- The presence of the substituent decreases the energy gap of the studied molecules, this is one of the important properties obtained in this work, and a small energy gap means small excitation energies of manifold of the excited states.
  - 4- The electronic properties (IP, EA,  $\chi$ ,  $\eta$ , S,  $\omega$ ) was calculated by using orbital-vertical method are a good agreement with experimental result.
  - 5- The results showed that all substitution groups leads to increase the average polarizability **and make** these compounds are more reactive than the original molecule.
  - 6- Calculation of IR-spectra showed a good agreement with experimental data for pyrene (molecules 1), adding the hydroxyl groups leads to increasing the vibration mode, and highest stretching vibration wave numbers and its gave suitable positions for hydroxyl with carbon atoms in phenyl ring.
- Molecule 2 is the best option for n-type organic semiconductors because of its better LUMO – HOMO ratio and other electronic properties.

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