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QUANTUM CHEMICAL STUDY OF THE EFFECT OF ALKYL GROUPS AND THEIR POSTION IN THIOPHENE FUSED RINGS ON GEOMETRY AND SOME PHYSICAL PROPERTIES

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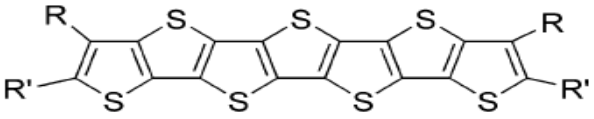
Abstract

The quantum mechanical calculations method by using the PM3 method were carried out for 28 compounds of thiophene fused ring containing from one to seven rings including Alkyl-groups[- CH3 , -$C_{10}H_{21}$] in addition to the unsubstituted group for four position of ring.
This study includes the equilibrium geometries[Bonds length and the bond Angles] and some of physical properties[total energy, dipole moments , energies of HOMO and LUMO and the difference between them, ionization energy ,charges and the electron densities and finally the standard thermodynamics functions [U^0,H^0,S^0,G^0,A^0]for all molecules . These compounds are compared with 28 the corresponding hydrocarbon compound.

الخلاصة:

باستخدام إحدى طرق ميكانيك الكم الشبه تجريبية(PM3) تم حساب 28مركب من مركبات الثايوفين والمؤلفة من حلقة واحدة إلى سبع حلقات مدمجة , معوضة بمجاميع الكيلية [-CH_3,-$C_{10}H_{21}$] عند مواقع مختلفة ؛حيث منها تتضمن مجموعة المثيل فقط(-CH_3) ومنها تحتوي على مجموعة (-$C_{10}H_{21}$) فقط ومنها ما تحتوي على كلا المعوضين.تضمنت هذه الدراسة حساب كل من الشكل الهندسي [الأواصر والزوايا]والخصائص الفيزيائية [الطاقة الكلية , عزم ثنائي القطب , طاقة أعلى مدار جزيئي مشغول , طاقة أوطأ مدار جزيئي فارغ , فرق الطاقة بينهما , طاقة التـأين , الشحنات و الكثافات الاليكترونية و الدوال الثرموداينميكية(U^0,H^0,S^0,G^0,A^0) لجميع الجزيئات وتم مقارنة المركبات المذكورة مع 28مركب من مركبات الهايدروكاربون المناظرة .



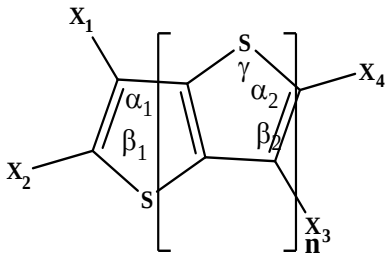
R= CH_3 or $C_{10}H_{21}$

R'=H or $C_{10}H_{21}$

Introduction.

In recent years, there has been growing interest in conjugated organic materials due to their interesting electronic Properties[(1)]. Heterocyclic compounds are widely distributed in nature and are essential for life. There are vast numbers of pharmacologically active heterocyclic compounds many of which are in regular clinical use[(2)]. Many studies on small molecules have been focused on pentacene, which has been used as an effective p-type semiconductor for organic field-effect transistors (OFETs)[(3-5)].On the other hand, devices based on oligothiophenes have poor air stability and show rapid device-performance degradation due to their low band gap and high-energy of the highest occupied molecular orbital (HOMO) level Therefore, high stability as well as high charge carrier mobility of the OFET is desirable[(6-8)]. the corresponding hydrocarbon compounds The η^5-cyclopentadienyl and related early transition metal derivatives have played an important role in structural, synthetic and catalytic organometallic chemistry. They are useful compounds which have found applications as reagents in organic chemistry[(9)]. To the best of our knowledge, there are no reported experimental and or advanced theoretical studies on the quantum study for thiophene fused

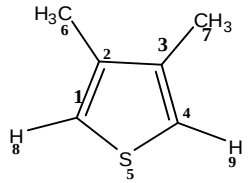
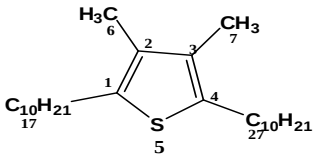
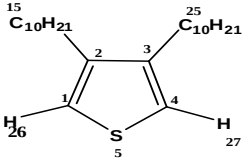
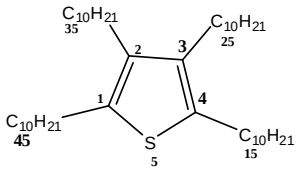
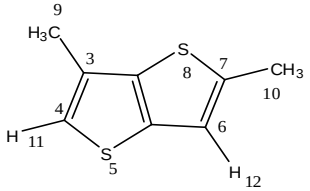
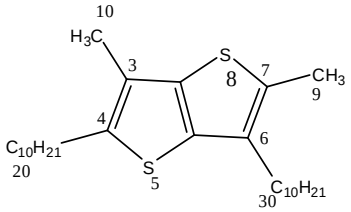
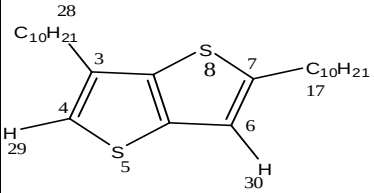
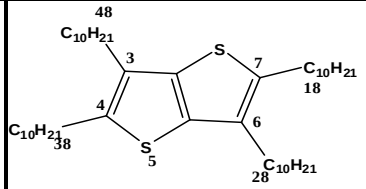
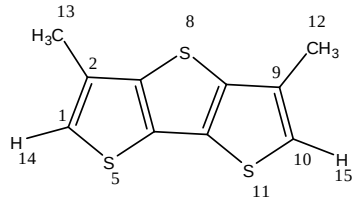
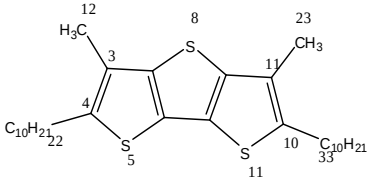
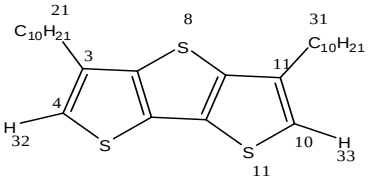
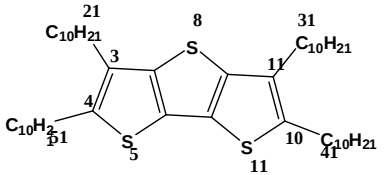
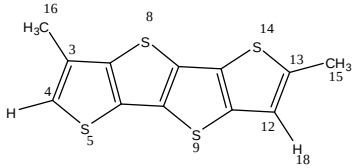
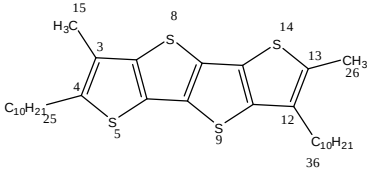
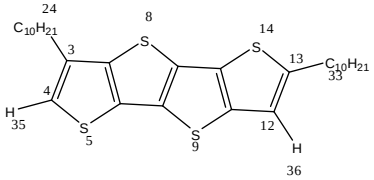
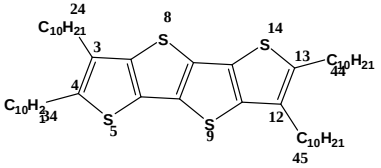
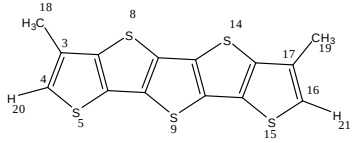
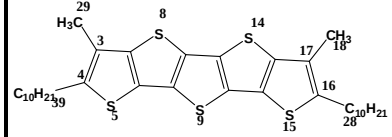
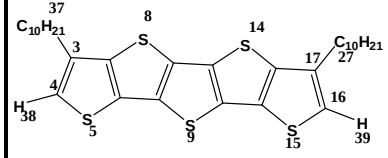
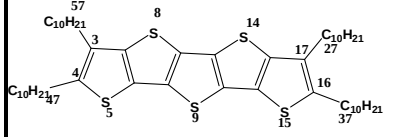
rings up to seven rings, therefore, we are used PM3 Semiemperical method[10] to calculate the equilibrium geometries of thiophene fused rings [11]that substituted by Alkyl groups(Fig,1) and calculate some of physical properties along with the Hydrocarbon compounds that have the same substituted(Fig,2) and unsubstituted thiophene and hydrocarbon .This study was investigated in four points every point reported the rings from one to seven rings with four type of substituted. Having this mainly structure.

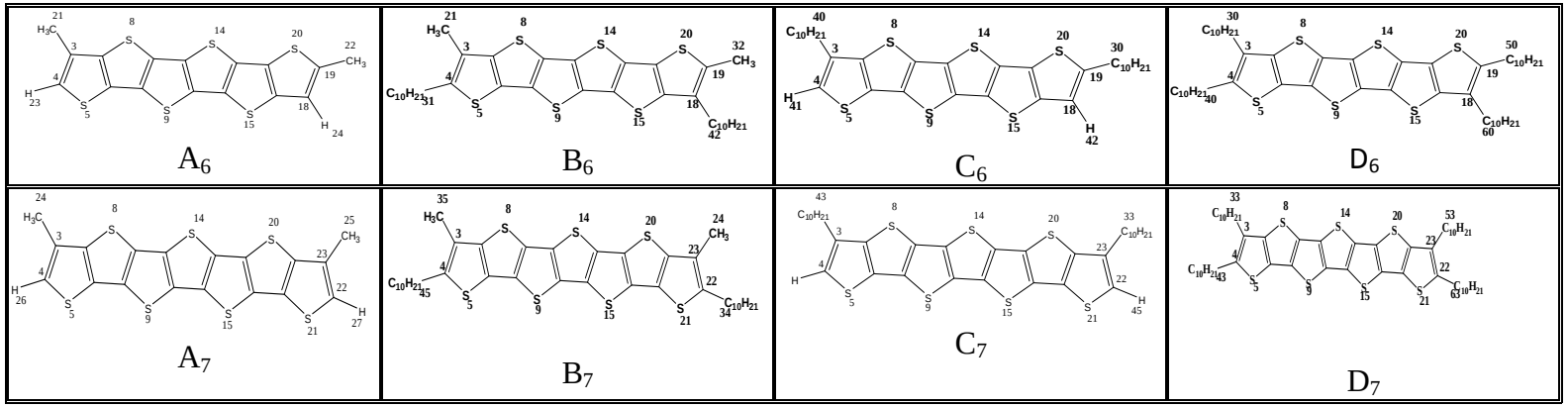


n=0,1,2,3,4,5,6,7

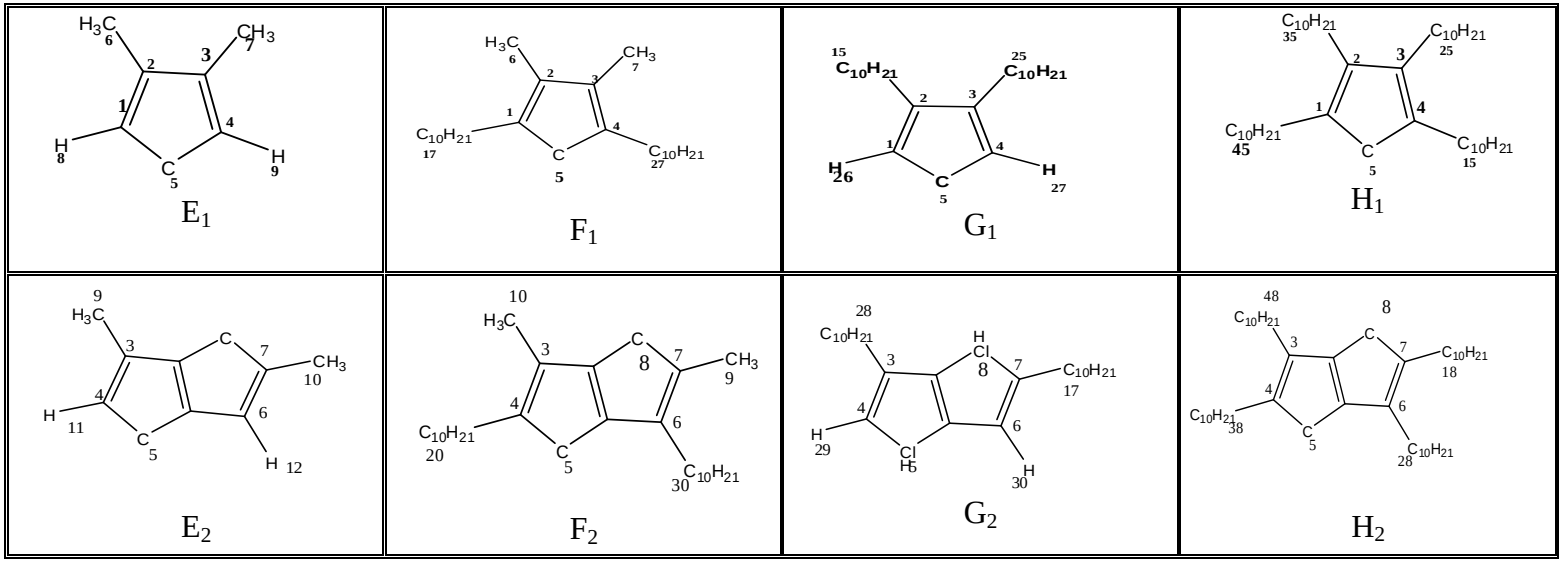
n=Number of the rings

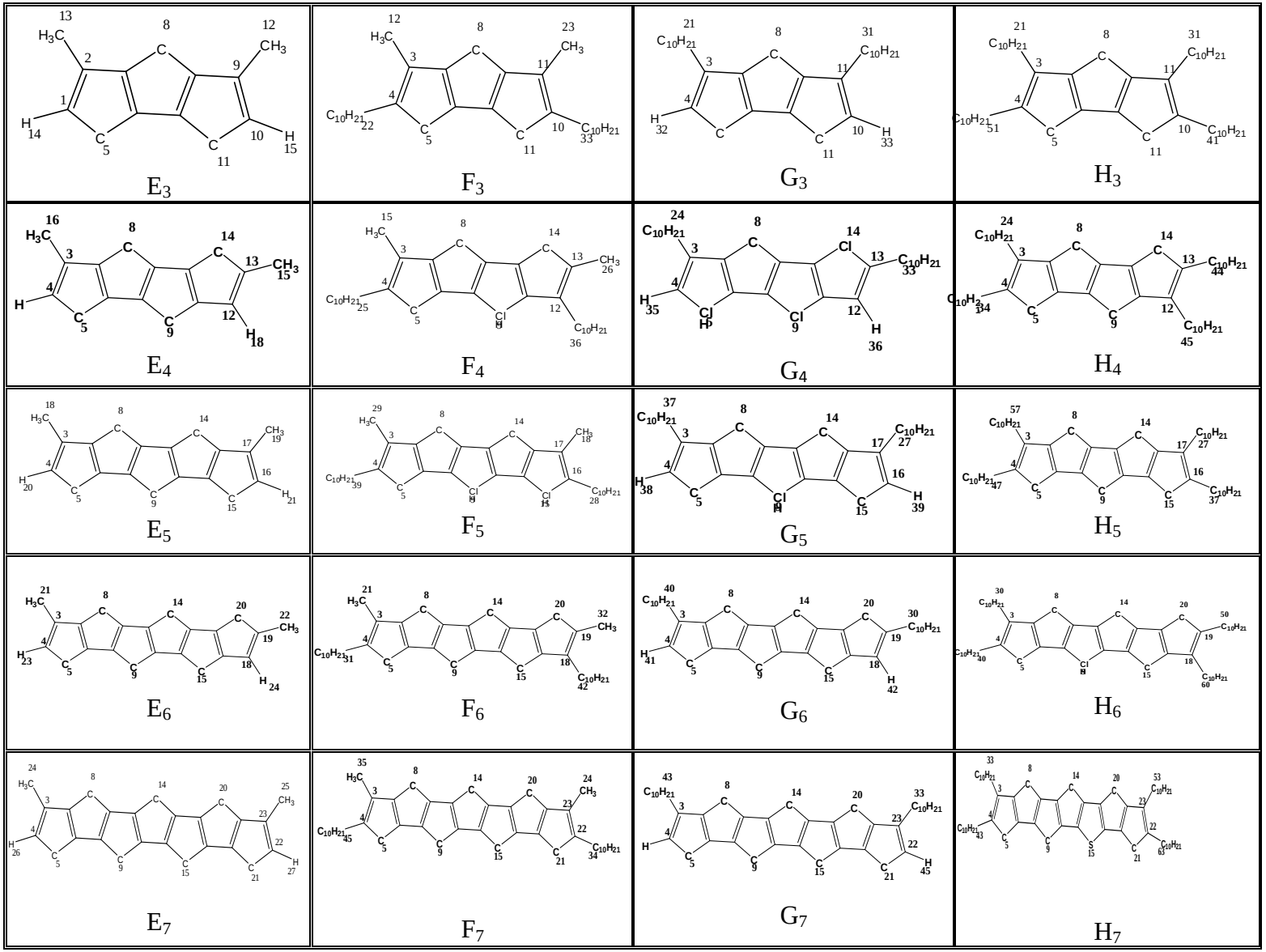
$X_1 = X_4 \ (A_n, B_n) = -CH_3.$
$X_1 = X_4 \ (C_n, D_n) = -C_{10}H_{21}.$
$X_2 = X_3 \ (A_n, C_n) = -H$
$X_2 = X_3 \ (B_n, D_n) = -C_{10}H_{21}$

 A_1	 B_1	 C_1	 D_1
 A_2	 B_2	 C_2	 D_2
 A_3	 B_3	 C_3	 D_3
 A_4	 B_4	 C_4	 D_4
 A_5	 B_5	 C_5	 D_5

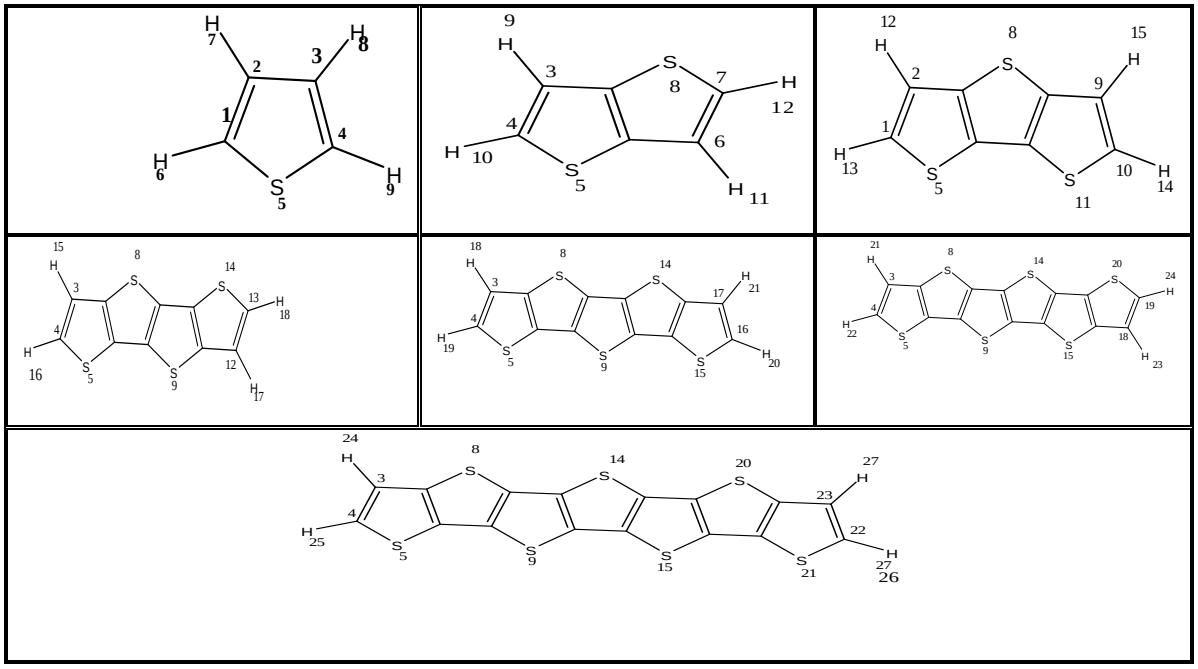


Fig,1 The thiophene fused rings that substituted by Alkyl groups molecules





Fig,2 The hydrocarbon fused rings that substituted by Alkyl groups molecules



Fig,3 The unsubstituted thiophene rings.

Results and Discussion

We investigated the equilibrium geometries and physical properties in four points: The first one: Is the study the effect of substituent group and it's position on thiophene compounds, the second point :Is the comparison study for hydrocarbon compounds that corresponding to thiophene compounds for the effect of the substituted group and its position, the third point :Is the study the effect of the increasment of the number of the rings on the substituted thiophene fused rings and the fourth point :Is the comparison study for the effect of the increasment of the number of the rings on the substituted thiophene fused rings and the increasment of the number of the rings on the substituted hydrocarbon their corresponding.

1st: The equilibrium geometries:

In first point; The bonds that carry substituted the electron denoting groups longer than the compounds that not substituted, the adjacent double bonds length are shorter than the compounds that not substituted due to the increasment of bond order and the bond angle attach to the substitute group is greater un substituted compound. In the second point; The bonds that carry substituted the electron denoting groups in thiophene longer than the hydrocarbon their corresponding compounds, the adjacent double bonds length in thiophene have high value than the hydrocarbon their corresponding compounds, the bond angle attach to the substitute group in thiophene compound have low value than the hydrocarbon their corresponding compounds. In the third point : Which study the length of sulfur bonds and sulfur angle bonds of thiophene fused rings; The bonds that contain sulfur atom longer than the other bonds in the ring which not containing sulfur atom but contain carbon atom due to ion pair on the sulfur atom. The bond angle that's formed from sulfur atom less than other angle in the ring. In the fourth point; The bonds atom that instead sulfur atom in hydrocarbon compound shorter than the bonds in the thiophene rings (i ,e)C-S >C-C. The bond angle for hydrocarbon compound has less value than other angle in the thiophene ring. Table (1-7)and(28-34).

2nd:Physical properties:

1- **Total energy :** In first point**;** for thiophene fused ring substituted compounds have low value compare with unsubstituted compound. In the second point; for hydrocarbon have high value compared with thiophene compounds. In the third point **;** for the compound formed from one ring has low value compare with the compound formed from two ring to seven ring. In the fourth point; for the hydrocarbon compound for all substituted have low value compare with thiophene their corresponding rings. Table 8 and 35.

2- **Dipole moment(12):** In first point; for substituted compounds having high value compare with unsubstituted compound. In the second point; for hydrocarbon compounds have low value

3- compare with thiophene compounds. In the third point ; for the compound formed from one ring has high value compare with the compound formed from two ring to seven ring in the first substituted but the other substituted was arranged according to the high value D_7,C_2,B_3 . In the fourth point; for the hydrocarbon compounds differ than thiophene compounds Table 9 and 36.

4- **Orbital Energies:** According to Koopmans' theorem (the negative HOMO is ≅ equal to the ionization potential) (13). In first point; the HOMO for thiophene fused ring substituted compounds have high value compare with unsubstituted compound, the LUMO for thiophene fused ring substituted compounds have high value compare with unsubstituted compound. In the second point; where in the hydrocarbon compounds have high value compare with thiophene compounds, the LUMO for hydrocarbon compounds have high value compare with thiophene compounds. In the third point ; the HOMO for thiophene formed from one ring has high value compare with other compounds but the other substituted was arranged according to the high value D_5,C_6,B_6 The LUMO for thiophene formed from one ring has low value compare with other compounds . In the fourth point; the HOMO in this point differ according to the substituted for thiophene and hydrocarbon compounds , the LUMO for the hydrocarbon compounds longer than thiophene compounds, Table (10 ,11)and (37,38).

5- **The difference energy between Orbital energies:** In first point; thiophene substituted has low value compare with unsubstituted compound. In the second point; hydrocarbon substituted compound has high value compare with thiophene compounds. In the third point; the compound formed from one ring has high value compare with other compounds. In the fourth point; in this point differ according to the substituted for thiophene and hydrocarbon compounds and increase the rings. table 12 and 39.

6- **Ionization potantial IP:** In first point; for thiophene fused ring substituted compounds have low value compare with unsubstituted compound. . In the second point; for hydrocarbon compounds have low value compare with thiophene compounds. In the third point; for thiophene formed from seven ring has high value compare with other compounds. In the fourth point; for hydrocarbon compounds has high value than thiophene compounds.table 13and 40.

7- **Thermodynamic functions:** In first point; functions for all substituted compounds longer than unsubstituted compound. In the second point; [U^0,H^0, G^0,A^0]for all hydrocarbon compounds have low than thiophene compounds but the entropy has high value than thiophene compounds. In the third point; for all substituted compounds for the compound formed from seven ring has high value than other compounds. In the fourth point; in this point differ according to the substituted for thiophene and hydrocarbon compounds and increase the rings. table (14-20) and(41-47).

8- **Charge and electron densities:** In first point; for carbon atom in thiophene fused ring substituted compounds are difference according to their near to the sulfur atom in the ring and according to the size of group substitute. In the second point; densities for hydrocarbon compounds have low electron densities than thiophene compounds . In the third point; for sulfur atom in the terminal ring that near to the substituted group differ than the electron density of the other ring . In the fourth point; for sulfur atoms in thiophene compounds have high value than hydrocarbon compounds. table (21-26)and(48-54).

Table 1– parameter for thiophene. [R : bond length, A^0 ,Angstrom ; A : bond angle, degree.]

Geometric parameter	$C_{44}H_{84}S$ (D_1)	Geometric parameter	$C_{24}H_{44}S$ (C_1)	Geometric parameter	$C_{26}H_{84}S$ (B_1)	Geometric parameter	C_6H_8S (A_1)
R(1-2)	1.374	**R(1-2)**	1.369	**R(1-2)**	1.374	**R(1-2)**	1.370
R(1-5)	1.739	**R(1-5)**	1.723	**R(1-5)**	1.742	**R(1-5)**	1.722
R(1-45)	1.484	**R(1-26)**	1.089	**R(1-17)**	1.485	**R(1-8)**	1.089
R(2-35)	1.486	**R(2-15)**	1.485	**R(2-6)**	1.478	**R(2-6)**	1.476
R(3-4)	1.374	**R(3-4)**	1.369	**R(3-4)**	1.375	**R(3-4)**	1.369
R(3-25)	1.487	**R(3-25)**	1.485	**R(3-7)**	1.477	**R(3-7)**	1.476
R(4-5)	1.737	**R(4-5)**	1.722	**R(4-5)**	1.739	**R(4-5)**	1.723
R(4-15)	1.484	**R(4-27)**	1.089	**R(4-27)**	1.484	**R(4-9**)	1.089
A(2-1-5)	111.9	**A(2-1-5)**	112.5	**A(2-1-5)**	111.6	**A(2-1-5)**	112.5
A(1-2-3)	112.3	**A(1-2-3)**	111.8	**A(1-2-3)**	112.5	**A(1-2-3)**	111.8
A(1-5-4)	91.4	**A(1-5-4)**	91.4	**A(1-5-4)**	91.7	**A(1-5-4)**	91.4
A(2-3-4)	112.3	**A(3-4-5)**	112.5	**A(2-3-4)**	112.6	**A(2-3-4)**	111.8
A(3-4-5)	112	**A(4-3-25)**	124	**A(3-4-5)**	111.6	**A(3-4-5)**	112.5

Table 2 parameter for thiophene

Geometric parameter	$C_{46}H_{84}S_2$ (D_2)	Geometric parameter	$C_{26}H_{44}S_2$ (C_2)	Geometric parameter	$C_{28}H_{48}S_2$ (B_2)	Geometric parameter	$C_8H_8S_2$ (A_2)
R(1-5)	1.723	**R(1-5)**	1.828	**R(1-5)**	1.721	**R(1-5)**	1.72
R(2-8)	1.717	**R(2-8)**	1.584	**R(2-8)**	1.721	**R(2-8)**	1.722
R(3-4)	1.376	**R(3-4)**	1.356	**R(3-4)**	1.377	**R(3-4)**	1.37
R(3-48)	1.486	**R(3-28)**	1.489	**R(3-10)**	1.476	**R(3-9)**	1.475
R(4-5)	1.751	**R(4-5)**	1.721	**R(4-5)**	1.756	**R(4-5)**	1.734
R(4-38)	1.484	**R(4-29)**	1.093	**R(4-20)**	1.484	**R(4-11)**	1.09
R(6-7)	1.376	**R(6-7)**	1.314	**R(6-7)**	1.375	**R(6-7)**	1.37
R(6-28)	1.49	**R(6-30)**	1.075	**R(6-30)**	1.486	**R(6-12)**	1.091
R(7-8)	1.76	**R(7-8)**	3.289	**R(7-8)**	1.752	**R(7-8)**	1.756
R(7-18)	1.486	**R(7-18)**	1.453	**R(7-9)**	1.475	**R(7-10)**	1.475
A(1-5-4)	91	**A(1-5-4)**	91.6	**A(1-5-4)**	91	**A(1-5-4)**	90.8
A(1-6-7)	110.7	**A(1-6-7)**	63.9	**A(1-6-7)**	111.1	**A(1-6-7)**	111.6
A(2-3-4)	111.2	**A(2-3-4)**	114.8	**A(2-3-4)**	111.4	**A(2-3-4)**	110.9
A(2-8-7)	91.1	**A(2-8-7)**	75.74	**A(2-8-7)**	90.9	**A(2-8-7)**	90.8

Table 3 parameter for thiophene

Geometric parameter	$C_{48}H_{84}S_3$ (D_3)	Geometric parameter	$C_{28}H_{44}S_3$ (C_3)	Geometric parameter	$C_{30}H_{48}S_3$ (B_3)	Geometric parameter	$C_{10}H_8S_3$ (A_3)
R(3-4)	1.403	R(3-4)	1.405	R(3-4)	1.403	R(1-2)	1.405
R(4-5)	1.716	R(4-5)	1.719	R(4-5)	1.716	R(1-5)	1.719
R(2-8)	1.736	R(2-8)	1.734	R(2-8)	1.735	R(3-6)	1.733
R(3-4)	1.376	R(3-4)	1.371	R(3-4)	1.376	R(1-2)	1.371
R(3-21)	1.487	R(3-21)	1.485	R(3-12)	1.476	R(2-13)	1.475
R(4-5)	1.754	R(4-5)	1.732	R(4-5)	1.753	R(1-5)	1.733
R(4-51)	1.484	R(4-32)	1.09	R(4-22)	1.483	R(1-14)	1.09
R(6-9)	1.717	R(6-9)	1.719	R(6-9)	1.716	R(8-11)	1.719
R(7-8)	1.735	R(7-8)	1.734	R(7-8)	1.735	R(6-7)	1.733
R(9-10)	1.751	R(9-10)	1.732	R(9-10)	1.752	R(10-11)	1.733
R(10-11)	1.377	R(10-11)	1.371	R(10-11)	1.376	R(9-10)	1.371
R(10-41)	1.484	R(10-33)	1.09	R(10-33)	1.484	R(10-15)	1.09
R(11-31)	1.486	R(11-31)	1.485	R(11-23)	1.476	R(9-12)	1.475
A(2-3-4)	111.2	A(2-3-4)	110.9	A(2-3-4)	111.2	A(1-2-3)	110.9
A(3-4-5)	113	A(3-4-5)	113.9	A(3-4-5)	113	A(2-1-5)	113.9
A(1-5-4)	90.9	A(1-5-4)	90.8	A(1-5-4)	90.9	A(1-5-4)	90.8
A(7-11-10)	111.2	A(7-11-10)	110.9	A(7-11-10)	111.2	A(7-9-10)	110.9
A(9-10-11)	113.1	A(9-10-11)	113.9	A(9-10-11)	113	A(9-10-11)	113.9
A(6-9-10)	90.9	A(6-9-10)	90.8	A(6-9-10)	90.9	A(8-11-10)	90.8

Table 4 parameter for thiophene

Geometric parameter	$C_{50}H_{84}S_4$ (D_4)	Geometric parameter	$C_{30}H_{44}S_4$ (C_4)	Geometric parameter	$C_{32}H_{48}S_4$ (B_4)	Geometric parameter	$C_{12}H_8S_4$ (A_4)
R(1-5)	1.718	**R(1-5)**	1.719	**R(1-5)**	1.716	**R(1-5)**	1.719
R(2-8)	1.734	**R(2-8)**	1.734	**R(2-8)**	1.735	**R(2-8)**	1.733
R(3-4)	1.377	**R(3-4)**	1.371	**R(3-4)**	1.376	**R(3-4)**	1.371
R(3-24)	1.484	**R(3-24)**	1.484	**R(3-15)**	1.477	**R(3-16)**	1.475
R(4-5)	1.75	**R(4-5)**	1.732	**R(4-5)**	1.756	**R(4-5)**	1.733
R(4-34)	1.484	**R(4-35)**	1.09	**R(4-25)**	1.485	**R(4-17)**	1.09
R(6-9)	1.73	**R(6-9)**	1.731	**R(6-9)**	1.731	**R(6-9)**	1.731
R(7-8)	1.731	**R(7-8)**	1.731	**R(7-8)**	1.731	**R(7-8)**	1.731
R(9-10)	1.736	**R(9-10)**	1.731	**R(9-10)**	1.735	**R(9-10)**	1.73
R(11-14)	1.717	**R(11-14)**	1.718	**R(11-14)**	1.717	**R(11-14)**	1.719
R(12-13)	**1.377**	**R(12-13)**	**1.371**	**R(12-13)**	**1.376**	**R(12-13)**	**1.371**
R(12-54)	1.486	**R(12-36)**	1.092	**R(12-36)**	1.485	**R(12-18)**	1.092
R(13-14)	1.754	**R(13-14)**	1.755	**R(13-14)**	1.752	**R(13-14)**	1.755
R(13-44)	1.485	**R(13-34)**	1.484	**R(13-26)**	1.475	**R(13-15)**	1.475
A(2-3-4)	111.4	**A(2-3-4)**	110.9	**A(2-3-4)**	111.3	**A(2-3-4)**	110.9
A(3-4-5)	113.1	**A(3-4-5)**	114	**A(3-4-5)**	112.9	**A(3-4-5)**	113.9
A(1-5-4)	90.8	**A(1-5-4)**	90.8	**A(1-5-4)**	90.9	**A(1-5-4)**	90.8
A(10-12-13)	111.3	**A(10-12-13)**	111.7	**A(10-12-13)**	111.2	**A(10-12-13)**	111.6
A(11-14-13)	90.8	**A(11-14-13)**	90.8	**A(11-14-13)**	90.9	**A(11-14-13)**	90.8
A(12-13-14)	113.1	**A(12-13-34)**	125	**A(12-13-14)**	113.1	**A(12-13-14)**	112.9

Table 5 parameter for thiophene

Geometric parameter	$C_{52}H_{84}S_5$ (D_5)	Geometric parameter	$C_{52}H_{84}S_5$ (C_5)	Geometric parameter	$C_{34}H_{48}S_5$ (B_5)	Geometric parameter	$C_{14}H_8S_5$ (A_5)
R(1-5)	1.717	**R(1-5)**	1.719	**R(1-5)**	1.717	**R(1-5)**	1.719
R(2-8)	1.735	**R(2-8)**	1.734	**R(2-8)**	1.733	**R(2-8)**	1.733
R(3-4)	1.378	**R(3-4)**	1.372	**R(3-4)**	1.376	**R(3-4)**	1.371
R(3-47)	1.487	**R(3-37)**	1.488	**R(3-29)**	1.476	**R(3-18)**	1.475
R(4-5)	1.754	**R(4-5)**	1.733	**R(4-5)**	1.753	**R(4-5)**	1.732
R(4-57)	1.485	**R(4-38)**	1.09	**R(4-39)**	1.484	**R(4-20)**	1.09
R(16-17)	1.38	**R(16-17)**	1.371	**R(16-17)**	1.377	**R(16-17)**	1.371
R(16-37)	1.485	**R(16-39)**	1.09	**R(16-28)**	1.484	**R(16-21)**	1.09
R(17-27)	1.488	**R(17-27)**	1.487	**R(17-18)**	1.476	**R(17-19)**	1.475
A(2-3-4)	111.3	**A(2-3-4)**	110.6	**A(2-3-4)**	111.4	**A(2-3-4)**	110.9
A(3-4-5)	113	**A(3-4-5)**	114.1	**A(3-4-5)**	113	**A(3-4-5)**	113.9
A(1-5-4)	90.8	**A(1-5-4)**	90.8	**A(1-5-4)**	90.8	**A(1-5-4)**	90.8
A(12-15-16)	90.7	**A(12-15-16)**	90.8	**A(12-15-16)**	90.9	**A(12-15-16)**	90.8
A(13-17-16)	110.7	**A(13-17-16)**	110.7	**A(13-17-16)**	111.2	**A(13-17-16)**	110.9

Table 6 parameter for thiophene

Geometric parameter	$C_{54}H_{84}S_6$ (D_6)	Geometric parameter	$C_{34}H_{44}S_6$ (C_6)	Geometric parameter	$C_{36}H_{48}S_6$ (B_6)	Geometric parameter	$C_{16}H_8S_6$ (A_6)
R(1-5)	1.716	R(1-5)	1.719	R(1-5)	1.717	R(1-5)	1.719
R(3-4)	1.377	R(3-4)	1.371	R(3-4)	1.376	R(3-4)	1.371
R(3-30)	1.484	R(3-40)	1.484	R(3-21)	1.476	R(3-21)	1.475
R(4-5)	1.754	R(4-5)	1.732	R(4-5)	1.752	R(4-5)	1.732
R(4-40)	1.485	R(4-41)	1.09	R(4-31)	1.484	R(4-23)	1.09
R(17-20)	1.718	R(17-20)	1.718	R(17-20)	1.718	R(17-20)	1.719
R(18-19)	1.377	R(18-19)	1.371	R(18-19)	1.376	R(18-19)	1.371
R(18-60)	1.485	R(18-42)	1.092	R(18-42)	1.485	R(18-24)	1.092
R(19-20)	1.75	R(19-20)	1.752	R(19-20)	1.751	R(19-20)	1.755
R(19-50)	1.484	R(19-30)	1.484	R(19-32)	1.476	R(19-22)	1.475
A(2-3-4)	111.3	A(2-3-4)	110.9	A(2-3-4)	111.4	A(2-3-4)	110.9
A(3-4-5)	113	A(3-4-5)	114	A(3-4-5)	113	A(3-4-5)	114
A(1-5-4)	90.8	A(1-5-4)	90.8	A(1-5-4)	90.8	A(1-5-4)	90.8
A(18-19-20)	113.1	A(18-19-20)	113	A(18-19-20)	113.2	A(18-19-20)	112.9
A(16-18-19)	111.3	A(16-18-19)	111.6	A(16-18-19)	111.3	A(16-18-19)	111.6
A(17-20-19)	90.8	A(17-20-19)	90.8	A(17-20-19)	90.8	A(17-20-19)	90.8

Table 7 parameter for thiophene

Geometric parameter	$C_{56}H_{84}S_7$ (D_7)	Geometric parameter	$C_{36}H_{44}S_7$ (C_7)	Geometric parameter	$C_{38}H_{48}S_7$ (B_7)	Geometric parameter	$C_{18}H_8S_7$ (A_7)
R(1-5)	1.717	R(1-5)	1.718	R(1-5)	1.716	R(1-5)	1.719
R(3-4)	1.375	R(3-4)	1.371	R(3-4)	1.376	R(3-4)	1.371
R(3-33)	1.486	R(3-43)	1.486	R(3-35)	1.476	R(3-24)	1.475
R(4-5)	1.755	R(4-5)	1.732	R(4-5)	1.753	R(4-5)	1.732
R(4-43)	1.484	R(4-44)	1.09	R(4-45)	1.484	R(4-26)	1.09
R(21-22)	1.749	R(21-22)	1.732	R(21-22)	1.752	R(21-22)	1.732
R(22-23)	1.381	R(22-23)	1.371	R(22-23)	1.377	R(22-23)	1.371
R(22-63)	1.485	R(22-45)	1.09	R(22-34)	1.484	R(22-27)	1.09
A(1-5-4)	91.1	A(1-5-4)	90.8	A(1-5-4)	90.9	A(1-5-4)	90.8
A(2-3-4)	111.1	A(2-3-4)	110.8	A(2-3-4)	111.2	A(2-3-4)	110.9
A(3-4-5)	113	A(3-4-5)	114	A(3-4-5)	113	A(3-4-5)	114
A(18-21-22)	90.8	A(18-21-22)	90.8	A(18-21-22)	90.9	A(18-21-22)	90.8
A(21-22-23)	113.5	A(21-22-23)	114	A(21-22-23)	113	A(21-22-23)	114
A(19-23-22)	110.6	A(19-23-22)	110.8	A(19-23-22)	111.2	A(19-23-22)	110.9

Table 8-- total energy for thiophene.

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	-8.5343	-3.6961	-4.1258	0.5254	1.3287
2.	-7.6677	0.7875	-3.1808	1.6217	5.7558
3.	-6.4222	-1.5409	-2.2035	2.6014	3.3751
4.	-5.3000	-0.4098	-1.0947	3.7046	4.4194
5.	-4.1652	0.6102	-0.1201	4.6909	5.4657
6.	7.5599	-3.2873	1.6520	0.9516	5.7967
7.	-1.9936	2.7010	1.9772	6.7846	7.5599

Table 9- (μ in deby).

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	1.0521	1.1427	0.8142	1.1638	0.6745
2.	0.1831	1.8882	0.1662	0.3979	2.0677
3.	0.9780	1.0831	0.9916	1.1136	0.5526
4.	0.2162	0.4482	0.0842	0.4201	0.0008
5.	0.8587	1.2336	0.9394	1.0850	0.5242
6.	0.1744	0.5051	0.0552	0.4308	0.0003
7.	1.0896	0.9798	0.9630	1.0724	0.5103

Table 10-HOMO for thiophene

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	-9.1747	-9.2378	-9.0242	-9.1564	-9.5434
2.	-8.6215	-8.8332	-8.5687	-8.7260	-9.5434
3.	-8.5507	-8.5991	-8.5347	-8.5913	-8.6846
4.	-8.4783	-8.5270	-8.4639	-8.5273	-8.5872
5.	-8.4593	-8.5110	-8.4702	-8.5134	-8.5624
6.	-8.4664	-8.4995	-8.4634	-8.5006	-8.5423
7.	-8.4653	-8.5085	-8.4710	-8.5083	-8.5425

Table 11-LUMO for thiophene

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	-0.1663	-0.1363	-0.0811	-0.1124	-0.1921
2.	-0.7568	-1.8406	-0.7214	-0.7905	-0.1921
3.	-1.1399	-1.1745	-1.1304	-1.1622	-1.2335
4.	-1.4063	-1.4452	-1.3943	-1.4414	-1.4912
5.	-1.5832	-1.6352	-1.5886	-1.6251	-1.6743
6.	-1.7380	-1.7698	-1.7342	-1.7690	-1.8096
7.	-1.8395	-1.8792	-1.8420	-1.8779	-1.9135

Table 12-ΔE for thiophene.

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	9.0084	9.1015	8.9431	9.0441	9.3513
2.	7.8647	6.9926	7.8473	7.9355	9.3513
3.	7.4108	7.4247	7.4043	7.4290	7.4511
4.	7.07202	7.0818	7.0696	7.0859	7.0960
5.	6.8761	6.8758	6.8815	6.8883	6.8881
6.	6.7283	6.7297	6.7292	6.7316	6.7327
7.	6.6258	6.62929	6.6290	6.6304	6.6290

Table 13-IP for thiophene.

NO . of ring(n)	D_n	C_n	B_n	A_n	Ref. thiophene
1.	9.1747	9.2378	9.0242	9.1564	9.5434
2.	8.6215	8.8332	8.5687	8.7259	9.5434
3.	8.5507	8.5992	8.5347	8.5913	8.6846
4.	8.4783	8.5271	8.4639	8.5280	8.5872
5.	8.4593	8.5110	8.4702	8.5134	8.5624
6.	8.4664	8.4995	8.4634	8.5006	8.5423
7.	8.4653	8.5085	8.4710	8.5083	8.5426

Table 14- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_1	3261.9007	3264.3795	1.5595	2799.4002	2334.4208
C_1	1722.720	1725.1988	0.93223	1447.2524	1169.3059
B_1	1870.9676	1873.4463	0.9667	1585.2220	1296.9977
A_1	337.3559	339.8346	0.3393	238.6650	137.5360
T_1	184.3763	186.8549	0.2855	101.7084	16.5618

Table 15- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_2	3309.5820	3312.0603	1.5298	2855.9391	2399.8180
C_2	1761.7694	1764.2481	1.0273	1457.9510	1151.6531
B_2	1918.6903	1921.1690	1.0290	1614.4399	1307.7110
A_2	381.6184	384.0971	0.39762	265.5180	146.9950
T_2	225.3042	225.8966	0.3534	120.5303	15.1642

Table 16- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_3	3350.0702	3352.5489	1.6775	2852.4724	2352.3122
C_3	1805.4420	1807.9207	0.9896	1512.8853	1217.8498
B_3	1966.3293	1968.8080	1.1130	1636.9601	1305.1121
A_3	428.6800	431.1590	0.4659	292.2217	153.2846
T_3	273.5541	274.1465	0.3872	158.7028	43.2591

Table 17- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_4	3390.7638	3393.2425	1.6834	2891.3508	2389.4592
C_4	1852.8509	1855.3296	1.0576	1539.9955	889.9415
B_4	2010.1191	2012.5978	1.1637	1665.6356	1318.6734
A_4	470.8924	473.3712	0.4993	324.5192	175.6674
T_4	318.2058	318.7982	0.4379	188.2383	57.6784

Table 18- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_5	3435.8715	3438.3502	1.6799	2937.4998	2436.6501
C_5	1901.4523	1903.9309	1.0198	1599.8864	1295.8418
B_5	2056.5573	2059.0360	1.2026	1700.4912	1341.9464
A_5	517.9959	520.4746	0.5675	351.2866	182.0987
T_5	362.8699	363.4623	0.4886	217.7862	72.1101

Table 19- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_6	3483.6402	3486.1189	1.8136	2945.3826	2404.6463
C_6	1942.3802	1944.8589	1.1622	1598.3607	1251.8626
B_6	2100.9370	2103.4157	1.2819	1721.2053	1338.9949
A_6	560.2250	562.7037	0.6006	383.6247	204.5456
T_6	407.5425	408.1349	0.5393	247.3420	86.5504

Table 20- thermodynamic function for thiophene.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
D_7	3527.7103	3530.1889	1.7885	2996.9337	2463.6784
C_7	1988.7974	1991.2761	1.2646	1612.7470	1234.2179
B_7	2144.9736	2147.4557	1.3091	1757.1534	1366.8544
A_7	607.3285	609.8071	0.6689	410.3708	210.9345
T_7	452.2109	452.8033	0.5899	276.9246	101.0459

Table 21-charge and electron density for thiophene.

Symbol	D_1		C_1		B_1		A_1	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.2682	4.2682	-0.3066	4.3066	-0.2655	4.2655	-0.3126	4.3126
C_2	-0.0856	4.0856	-0.0861	4.0861	-0.0920	4.092	-0.0868	4.0868
C_3	-0.0862	4.0862	-0.0862	4.0862	-0.0981	4.0981	-0.0863	4.0863
C_4	-0.2667	4.2667	-0.30602	4.3060	-0.2703	4.2703	-0.3102	4.3102
S_5	0.2975	5.7024	0.3081	5.6918	0.2992	5.7008	0.3093	5.6907

Table 22-charge and electron density for thiophene.

Symbol	D_2		C_2		B_2		A_2	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.2688	4.2688	-0.1707	4.1707	-0.25560	4.2560	-0.2647	4.2647
C_2	-0.2505	4.2505	-0.0239	4.0239	-0.2546	4.2546	-0.2633	4.2633
C_3	-0.0378	4.0378	-0.1492	4.1492	-0.0470	4.0470	-0.0285	4.0285
C_4	-0.2540	4.2540	-0.1799	4.1799	-0.2561	4.2561	-0.2998	4.2998
S_5	0.3279	5.6721	0.1486	5.8514	0.3326	5.6674	0.3393	5.6607
C_6	-0.0254	4.0254	-0.0871	4.0871	-0.0415	4.0415	-0.0661	4.0661
C_7	-0.2466	4.2466	-0.0618	4.0618	-0.2521	4.2521	-0.2476	4.2476
S_8	0.3178	5.6822	-0.0846	6.0846	0.3273	5.6727	0.3263	5.6737
C_9	-0.1247	4.1247	-0.1094	4.1094	-0.0458	4.0458	-0.0520	4.0520

Table 23-charge and electron density for thiophene.

Symbol	D_3		C_3		B_3		A_3	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.2098	4.2098	-0.2127	4.2127	-0.2090	4.2090	-0.3007	4.3007
C_2	-0.2476	4.2476	-0.24955	4.2496	-0.2501	4.2501	-0.0306	4.0306
C_3	-0.0362	4.0362	-0.0334	4.0334	-0.0335	4.0335	-0.2544	4.2544
C_4	-0.2527	4.2527	-0.2981	4.2981	-0.2596	4.2596	-0.2109	4.2109
S_5	0.3457	5.6543	0.3586	5.6414	0.3462	5.6538	0.3566	5.6434
C_6 (S)	-0.2118	4.2118	-0.2127	4.2127	-0.2101	4.2101	0.3676	5.6324
S_8 (C)	0.3611	5.6389	0.3663	5.6337	0.3618	5.6382	-0.2110	4.2110
S_9 (C)	0.3501	5.6499	0.3586	5.6414	0.3483	5.6517	-0.0306	4.0306
C_{10}	-0.2566	4.2566	-0.2981	4.2981	-0.2620	4.2620	-0.3007	4.3007
C_{11}(S)	-0.0394	4.0394	-0.0334	4.0334	-0.0343	4.0343	0.3567	5.6433
C_{12}	-0.1094	4.1094	-0.1093	4.1093	-0.0549	4.0549	-0.0524	4.0524

Table 24-charge and electron density for thiophene.

Symbol	D_4		C_4		B_4		A_4	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0374	4.0374	-0.0292	4.0292	-0.0330	4.0330	-0.0296	4.0296
C_4	-0.2577	4.2577	-0.2976	4.2976	-0.2553	4.2553	-0.2996	4.2996
S_5	0.3529	5.6471	0.3598	5.6402	0.3445	5.6555	0.3579	5.6421
S_8	0.3798	5.6202	0.3813	5.6187	0.3800	5.6200	0.3836	5.6160
S_9	0.3802	5.6198	0.3843	5.6157	0.3806	5.6194	0.3855	5.6145
C_{10}	-0.2461	4.2461	-0.2575	4.2575	-0.2448	4.2448	-0.2569	4.2569
C_{11}	-0.2121	4.2121	-0.2135	4.2135	-0.2165	4.2165	-0.2134	4.2134
S_{14}	0.3472	5.6528	0.3478	5.6522	0.3485	5.6515	0.3457	5.6543

Table 25-charge and electron density for thiophene.

Symbol	D_5		C_5		B_5		A_5	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0417	4.0417	-0.0315	4.0315	-0.0360	4.0360	-0.0301	4.0301
C_4	-0.2522	4.2522	-0.2964	4.2964	-0.2580	4.2580	-0.2984	4.2984
S_5	0.3524	5.6476	0.3605	5.6395	0.3521	5.6479	0.3606	5.6394
S_8	0.3808	5.6192	0.3872	5.6128	0.3827	5.6173	0.3852	5.6148
S_9	0.3974	5.6026	0.3970	5.6030	0.3990	5.6010	0.4009	5.5991
S_{14}	0.3809	5.6191	0.3861	5.6139	0.3816	5.6184	0.3851	5.6149
S_{15}	0.3556	5.6444	0.3601	5.6399	0.3523	5.6477	0.3607	5.6393
C_{16}	-0.2710	4.2710	-0.2957	4.2957	-0.2588	4.2588	-0.2984	4.2984
C_{17}	-0.0264	4.0264	-0.03258	4.0326	-0.0346	4.0346	-0.0301	4.0301

Table 26-charge and electron density for thiophene.

Symbol	D_6		C_6		B_6		A_6	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0362	4.0362	-0.0297	4.0297	-0.0362	4.0362	-0.0300	4.0301
C_4	-0.2497	4.2497	-0.2960	4.2960	-0.2571	4.2571	-0.2978	4.2978
S_5	0.3496	5.6504	0.3630	5.6370	0.3530	5.6470	0.3611	5.6389
S_8	0.3827	5.6173	0.3847	5.6153	0.3851	5.6149	0.3870	5.6130
S_9	0.4000	5.6000	0.4013	5.5987	0.3999	5.6001	0.4015	5.5985
S_{14}	0.3994	5.6006	0.4002	5.5998	0.3997	5.6003	0.4007	5.5993
S_{15}	0.3847	5.6153	0.3872	5.6128	0.3846	5.6154	0.3885	5.6115
C_{18}	-0.0416	4.0416	-0.0674	4.0674	-0.0431	4.0431	-0.0682	4.0682
C_{19}	-0.2549	4.2549	-0.2484	4.2484	-0.2496	4.2496	-0.2454	4.2454
S_{20}	0.3564	5.6436	0.3543	5.6457	0.3504	5.6496	0.3484	5.6516

Table 27-charge and electron density for thiophene.

Symbol	D_7		C_7		B_7		A_7	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0378	4.0378	-0.0306	4.0306	-0.0345	4.0345	-0.0304	4.0304
C_4	-0.246	4.2460	-0.2955	4.2955	-0.2549	4.2549	-0.2973	4.2973
S_5	0.3496	5.6504	0.3636	5.6364	0.3524	5.6476	0.3624	5.6376
S_8	0.3876	5.6124	0.3853	5.6147	0.3846	5.6154	0.3878	5.6122
S_9	0.3986	5.6011	0.4033	5.5967	0.4021	5.5979	0.4034	5.5966
S_{14}	0.40227	5.5790	0.4016	5.5984	0.4006	5.5994	0.4018	5.5982
S_{15}	0.3980	5.6020	0.4033	5.5967	0.4019	5.5981	0.4035	5.5965
S_{20}	0.3874	5.6126	0.3853	5.6147	0.3845	5.6155	0.3877	5.6123
S_{21}	0.3556	5.6444	0.3636	5.6459	0.3540	5.6459	0.3624	5.6376
C_{22}	-0.2685	4.2685	-0.2955	4.2955	-0.2572	4.2572	-0.2973	4.2973
C_{23}	-0.0292	4.0292	-0.0306	4.0306	-0.0353	4.0353	-0.0304	4.0304

Table 28– parameter for hydrocarbon .

Geometric parameter	(H_1)	Geometric parameter	(G_1)	Geometric parameter	(F_1)	Geometric parameter	(E_1)
R(1-2)	1.366	R(1-2)	1.359	R(1-2)	1.362	R(1-2)	1.355
R(1-5)	1.498	R(1-5)	1.497	R(1-5)	1.505	R(1-5)	1.501
R(1-35)	1.48	R(1-26)	1.088	R(1-17)	1.48	R(1-8)	1.088
R(2-15)	1.486	R(2-25)	1.486	R(2-6)	1.473	R(2-6)	1.473
R(3-4)	1.364	R(3-4)	1.357	R(3-4)	1.362	R(3-4)	1.355
R(3-25)	1.484	R(3-15)	1.481	R(3-7)	1.473	R(3-7)	1.473
R(4-5)	1.503	R(4-5)	1.498	R(4-5)	1.503	R(4-5)	1.501
R(4-45)	1.481	R(4-27)	1.089	R(4-27)	1.479	R(4-9)	1.088
A(2-1-5)	109.7	A(2-1-5)	110.2	A(2-1-5)	109.3	A(2-1-5)	109.6
A(1-2-3)	108.7	A(1-2-3)	108.3	A(1-2-3)	109	A(1-2-3)	108.9
A(1-5-4)	103.2	A(1-5-4)	102.7	A(1-5-4)	103.3	A(1-5-4)	103.1
A(2-3-4)	108.7	A(2-3-4)	108.7	A(2-3-4)	109	A(2-3-4)	108.9

Table 29– parameter for hydrocarbon.

Geometric parameter	(H_2)	Geometric parameter	(G_2)	Geometric parameter	(F_2)	Geometric parameter	(E_2)
R(1-5)	1.501	R(1-5)	1.502	R(1-5)	1.502	R(1-5)	1.507
R(3-4)	1.354	R(3-4)	1.349	R(3-4)	1.354	R(3-4)	1.348
R(3-48)	1.483	R(3-28)	1.481	R(3-20)	1.474	R(3-9)	1.474
R(4-5)	1.505	R(4-5)	1.502	R(4-5)	1.505	R(4-5)	1.5
R(5-50)	1.108	R(5-31)	1.107	R(5-32)	1.108	R(5-13)	1.106
R(6-7)	1.414	R(6-7)	1.407	R(6-7)	1.416	R(6-7)	1.415
R(6-28)	1.499	R(6-32)	1.099	R(6-19)	1.499	R(6-14)	1.101
R(7-18)	1.468	R(7-18)	1.449	R(7-9)	1.449	R(7-10)	1.449
A(2-3-4)	109.7	A(2-3-4)	109.7	A(2-3-4)	109.7	A(2-3-4)	110.1
A(3-4-5)	111.1	A(3-4-5)	111.5	A(3-4-5)	111.2	A(3-4-5)	111.1
A(1-6-7)	116.9	A(1-6-7)	118.2	A(1-6-7)	117	A(1-6-7)	120.3

Table 30– parameter for hydrocarbon.

Geometric parameter	(H_3)	Geometric parameter	(G_3)	Geometric parameter	(F_3)	Geometric parameter	(E_3)
R(1-5)	1.487	R(1-5)	1.488	R(1-5)	1.487	R(1-5)	1.488
R(2-8)	1.499	R(2-8)	1.499	R(2-8)	1.499	R(2-8)	1.499
R(3-4)	1.368	R(3-4)	1.362	R(3-4)	1.367	R(3-4)	1.363
R(3-41)	1.482	R(3-31)	1.48	R(3-12)	1.472	R(3-12)	1.472
R(4-5)	1.517	R(4-5)	1.512	R(4-5)	1.518	R(4-5)	1.512
R(4-51)	1.48	R(4-32)	1.088	R(4-22)	1.48	R(4-14)	1.088
R(7-8)	1.5	R(7-8)	1.498	R(7-8)	1.499	R(7-8)	1.499
R(9-10)	1.516	R(9-10)	1.513	R(9-10)	1.518	R(9-10)	1.512
R(10-31)	1.479	R(10-39)	1.088	R(10-33)	1.48	R(10-21)	1.088
R(10-11)	1.368	R(10-11)	1.362	R(10-11)	1.368	R(10-11)	1.363
R(11-21)	1.481	R(11-21)	1.48	R(11-23)	1.472	R(11-13)	1.472
A(1-5-4)	101.7	A(1-5-4)	101.7	A(1-5-4)	101.7	A(1-5-4)	101.7
A(2-3-4)	107.7	A(2-3-4)	107.9	A(2-3-4)	107.8	A(2-3-4)	107.9
A(3-4-5)	111	A(3-4-5)	111.2	A(3-4-5)	111	A(3-4-5)	111.2
A(9-10-11)	111	A(9-10-11)	111.1	A(9-10-11)	110.9	A(9-10-11)	111.2

Table 31– parameter for hydrocarbon.

Geometric parameter	(H_4)	Geometric parameter	(G_4)	Geometric parameter	(F_4)	Geometric parameter	(E_4)
R(1-5)	1.487	R(1-5)	1.489	R(1-5)	1.487	R(1-5)	1.488
R(3-4)	1.368	R(3-4)	1.362	R(3-4)	1.368	R(3-4)	1.363
R(3-24)	1.481	R(3-24)	1.48	R(3-15)	1.472	R(3-16)	1.472
R(4-5)	1.516	R(4-5)	1.513	R(4-5)	1.517	R(4-5)	1.512
R(4-34)	1.479	R(4-35)	1.088	R(4-25)	1.479	R(4-17)	1.088
R(7-8)	1.498	R(7-8)	1.498	R(7-8)	1.498	R(7-8)	1.498
R(8-57)	1.105	R(8-38)	1.109	R(8-39)	1.105	R(8-20)	1.105
R(11-14)	1.487	R(11-14)	1.487	R(11-14)	1.488	R(11-14)	1.488
R(12-13)	1.368	R(12-13)	1.363	R(12-13)	1.368	R(12-13)	1.363
R(12-54)	1.481	R(12-42)	1.088	R(12-36)	1.48	R(12-24)	1.088
R(13-14)	1.517	R(13-14)	1.518	R(13-14)	1.516	R(13-14)	1.518
R(13-44)	1.48	R(13-34)	1.479	R(13-26)	1.47	R(13-15)	1.47
A(1-5-4)	101.6	A(1-5-4)	101.8	A(1-5-4)	101.7	A(1-5-4)	101.7
A(2-3-4)	107.9	A(1-6-9)	140.4	A(2-3-4)	107.8	A(2-3-4)	107.9
A(3-4-5)	111	A(2-8-39)	112.2	A(3-4-5)	111	A(3-4-5)	111.2
A(10-12-13)	107.9	A(10-12-13)	108	A(10-12-13)	107.9	A(10-12-13)	108
A(12-13-14)	111	A(12-13-14)	111	A(12-13-14)	111.1	A(12-13-14)	111.1

Table 32 – parameter for hydrocarbon.

Geometric parameter	(H_5)	Geometric parameter	(G_5)	Geometric parameter	(F_5)	Geometric parameter	(E_5)
R(1-5)	1.488	R(1-5)	1.488	R(1-5)	1.487	R(1-5)	1.488
R(3-4)	1.368	R(3-4)	1.363	R(3-4)	1.368	R(3-4)	1.363
R(3-47)	1.48	R(3-27)	1.48	R(3-18)	1.472	R(3-19)	1.472
R(4-5)	1.516	R(4-5)	1.512	R(4-5)	1.517	R(4-5)	1.512
R(4-57)	1.479	R(4-38)	1.088	R(4-28)	1.479	R(4-20)	1.088
R(16-17)	1.368	R(16-17)	1.363	R(16-17)	1.368	R(16-17)	1.363
R(16-37)	1.48	R(16-49)	1.088	R(16-39)	1.48	R(16-31)	1.088
R(17-27)	1.481	R(17-37)	1.48	R(17-29)	1.472	R(17-18)	1.472
A(1-5-4)	101.6	A(1-5-4)	101.7	A(1-5-4)	101.7	A(1-5-4)	101.7
A(2-3-4)	107.9	A(2-3-4)	107.9	A(2-3-4)	107.8	A(2-3-4)	107.9
A(3-4-5)	111.1	A(3-4-5)	111.2	A(3-4-5)	111	A(3-4-5)	111.2
A(12-15-16)	101.8	A(12-15-16)	101.7	A(12-15-16)	101.8	A(12-15-16)	101.7
A(15-16-17)	110.9	A(15-16-17)	111.2	A(15-16-17)	110.9	A(15-16-17)	111.2
A(13-17-16)	107.9	A(13-17-16)	107.9	A(13-17-16)	107.8	A(13-17-16)	107.9

Table 33 – parameter for hydrocarbon.

Geometric parameter	(H_6)	Geometric parameter	(G_6)	Geometric parameter	(F_6)	Geometric parameter	(E_6)
R(1-5)	1.487	R(1-5)	1.488	R(1-5)	1.488	R(1-5)	1.488
R(3-4)	1.368	R(3-4)	1.363	R(3-4)	1.368	R(3-4)	1.363
R(4-5)	1.516	R(4-5)	1.512	R(4-5)	1.516	R(4-5)	1.512
R(4-40)	1.479	R(4-41)	1.088	R(4-31)	1.479	R(4-23)	1.088
R(3-30)	1.481	R(3-30)	1.48	R(3-21)	1.472	R(3-21)	1.472
R(17-20)	1.488	R(17-20)	1.488	R(17-20)	1.488	R(17-20)	1.488
R(19-20)	1.516	R(19-20)	1.518	R(19-20)	1.516	R(19-20)	1.518
R(18-19)	1.368	R(18-19)	1.363	R(18-19)	1.368	R(18-19)	1.363
A(1-5-4)	101.6	A(1-5-4)	101.7	A(1-5-4)	101.6	A(1-5-4)	101.7
A(3-4-5)	111	A(3-4-5)	111.2	A(3-4-5)	111	A(3-4-5)	111.2
A(17-20-19)	101.6	A(16-18-52)	124.8	A(17-20-19)	101.6	A(17-20-19)	101.5
A(18-19-20)	111.1	A(18-19-20)	111	A(18-19-20)	111.1	A(18-19-20)	111.1
A(16-18-19)	107.9	A(16-17-20)	110	A(16-18-19)	107.9	A(16-18-19)	108

Table 34 – parameter for hydrocarbon.

Geometric parameter	(H_7)	Geometric parameter	(G_7)	Geometric parameter	(F_7)	Geometric parameter	(E_7)
R(1-5)	1.486	R(1-5)	1.488	R(1-5)	1.487	R(1-5)	1.488
R(3-4)	1.37	R(3-4)	1.363	R(3-4)	1.367	R(3-4)	1.363
R(3-63)	1.482	R(3-43)	1.48	R(3-24)	1.472	R(3-24)	1.472
R(4-5)	1.518	R(4-5)	1.512	R(4-5)	1.518	R(4-5)	1.512
R(4-53)	1.48	R(4-44)	1.088	R(4-34)	1.479	R(4-26)	1.088
R(17-20)	1.498	R(17-20)	1.498	R(17-20)	1.498	R(17-20)	1.499
R(23-33)	1.483	R(23-33)	1.48	R(23-35)	1.472	R(23-25)	1.472
R(22-23)	1.368	R(22-23)	1.363	R(22-23)	1.368	R(22-23)	1.363
R(22-43)	1.481	R(22-59)	1.088	R(22-45)	1.48	R(22-41)	1.088
A(1-5-4)	101.9	A(1-5-4)	101.7	A(1-5-4)	101.7	A(1-5-4)	101.7
A(2-3-4)	107.8	A(2-3-4)	107.9	A(2-3-4)	107.8	A(2-3-4)	107.9
A(19-23-22)	107.6	A(19-23-22)	107.9	A(19-23-22)	107.8	A(19-23-22)	107.9
A(21-22-23)	110.8	A(21-22-23)	111.2	A(21-22-23)	110.9	A(21-22-23)	111.2

Table 35- total energy for hy

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	-8.3939	-3.5089	-4.4323	0.5304	1.3731
2	-4.8035	0.4820	-0.2993	4.6909	5.9693
3	-6.6531	-1.5694	-2.4436	2.6057	3.4517
4	-5.5956	-0.5693	-1.4211	3.6054	4.4709
5	-4.6166	0.4583	-0.4055	4.6461	5.4906
6	-3.5850	1.4601	0.6089	5.6448	6.5117
7	-2.4545	2.4977	1.6353	6.6858	7.5290

Table 36-(μ in Debye) for hy.

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	0.3016	0.0185	0.3403	0.0730	0.5338
2	1.8332	1.3751	1.5988	1.6753	2.3309
3	0.2739	0.1604	0.1299	0.0413	0.4860
4	0.0447	0.2940	0.1431	0.3716	0.0003
5	0.2863	0.1818	0.1769	0.0404	0.4803
6	0.1020	0.2809	0.1209	0.3787	0.0003
7	0.3952	0.1593	0.1628	0.0403	0.4784

Table 37- HOMO in e V for hy.

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	-8.4911	-8.9578	-8.5023	-8.9591	-9.2326
2	-7.9814	-7.9719	-7.9401	-8.0486	-7.9739
3	-7.9039	-8.0601	-7.8873	-8.0380	-8.0829
4	-7.6783	-7.7531	-7.6598	-7.7210	-7.8092
5	-7.5267	-7.6116	-7.5164	-7.5999	-7.6214
6	-7.4146	-7.4535	-7.3956	-7.4326	-7.4865
7	-7.3167	-7.3806	-7.3210	-7.3721	-7.3869

Table 38- LUMO in e V for hy.

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	0.3425	0.3619	0.3418	0.3679	0.3244
2	-1.3004	-1.2272	-1.1603	-1.1499	-1.4439
3	-0.4452	-0.4286	-0.4225	-0.4065	-0.4525
4	-0.6378	-0.6523	-0.6251	-0.6299	-0.6585
5	-0.7839	-0.7861	-0.7704	-0.7725	-0.8044
6	-0.8909	-0.9015	-0.8759	-0.8851	-0.9108
7	-0.9568	-0.9774	-0.9595	-0.9679	-0.9905

Table 39- ΔE in e V for hy.

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	8.8337	9.3197	8.8440	9.3270	9.5570
2	6.6809	6.7446	6.7798	6.8987	6.5299
3	7.4587	7.6315	7.4647	7.6315	7.6304
4	7.0405	7.1009	7.0347	7.0911	7.1507
5	6.7428	6.8255	6.7460	6.8274	6.8171
6	6.5237	6.5520	6.5196	6.5474	6.5757
7	6.3599	6.4032	6.3615	6.4043	6.3964

Table 40- IP in (eV)for hy.

NO . of ring(n)	H_n	G_n	F_n	E_n	Ref. Hydrocarbon
1	8.4911	8.9578	8.5023	8.9591	9.2326
2	7.9814	7.9719	7.9401	8.0486	7.9739
3	7.9039	8.0601	7.8873	8.0380	8.0829
4	7.6783	7.7531	7.6598	7.7210	7.8092
5	7.5267	7.6116	7.5164	7.5999	7.6214
6	7.4146	7.4535	7.3956	7.4326	7.4865
7	7.3167	7.3806	7.3210	7.3721	7.3869

Table 41- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_1	3326.5645	3329.0431	1.5309	2872.5838	2416.1248
G_1	1789.1955	1791.6742	0.8885	1526.7537	1261.8333
F_1	1940.5015	1942.9801	0.9633	1655.7651	1368.5500
E_1	407.3208	409.7994	0.3312	311.0655	212.3315
I_1	254.2575	254.8499	0.2790	171.6660	88.4823

Table 42- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_2	3434.2188	3436.6974	1.5585	2972.0061	2507.3151
G_2	1885.9506	1888.4292	0.9361	1888.4275	1609.3220
F_2	2047.8881	2050.3668	1.0725	1730.5928	1410.8192
E_2	510.1342	512.6128	0.16774	462.5997	412.5866
I_2	351.8200	352.4124	0.3488	248.4177	144.4229

Table 43- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_3	3555.9230	3558.4016	1.6677	3061.1282	2563.8544
G_3	2017.3030	2019.7816	0.5562	1716.0029	1412.2238
F_3	2173.4834	2175.9620	1.1070	1845.9101	1515.8586
E_3	635.5454	638.0241	0.1909	581.1024	524.1810
I_3	480.8295	481.4219	0.3682	371.6431	261.8643

Table 44- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_4	3665.6609	3668.1396	1.6882	3164.7550	2661.3700
G_4	2130.4886	2132.9672	1.0805	1810.8130	1488.6593
F_4	2285.5141	2287.9930	1.1498	1945.1659	1602.3381
E_4	748.8063	751.2850	0.4918	604.6661	458.0472
I_4	594.1113	594.70372	0.4126	471.6870	348.67041

Table 45- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_5	3781.6289	3784.1075	1.7682	3256.8900	2729.6726
G_5	2244.4733	2242.7679	1.11324	1910.8504	1578.9324
F_5	2399.9633	2402.4419	1.1832	2049.6629	1696.8835
E_5	862.1132	864.5919	0.2675	784.8468	705.1017
I_5	707.3889	707.9813	0.4570	571.7268	435.4723

Table 46- Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_6	3894.3249	3896.8035	1.8129	3356.2454	2815.6876
G_6	2357.8137	2360.2906	1.1604	2014.3157	1668.3390
F_6	2512.0192	2514.4978	1.2318	2147.1957	1779.8941
E_6	975.3490	977.8277	0.3057	886.6721	795.5165
I_6	820.6623	821.2547	0.5015	671.7325	522.2103

Table 47 -Thermodynamic function for hy.

The molecule	U^0 (kJ mol^{-1})	H^0 (kJ mol^{-1})	S^0 (kJ mol^{-1} deg^{-1})	G^0 (kJ mol^{-1})	A^0 (kJ mol^{-1})
H_7	4009.1673	4011.6459	1.8510	3459.7349	3744.6239
G_7	2470.7858	2473.2645	1.2121	2111.8619	1750.4588
F_7	2626.6315	2629.1101	1.2760	2248.6686	1868.2271
E_7	1088.6600	1091.1388	0.3440	988.5726	886.0065
I_7	933.9357	934.5281	0.5459	771.7680	609.0079

Table 48 – Charge and Electron density for hy.

Symbol	H_1		G_1		F_1		E_1	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.1603	4.1603	-0.1819	4.1819	-0.1482	4.1482	-0.1706	4.1706
C_2	-0.0922	4.0922	-0.0851	4.0851	-0.0914	4.0914	-0.0899	4.0899
C_3	-0.0750	4.0750	-0.0750	4.0750	-0.0958	4.0958	-0.0899	4.0899
C_4	-0.1454	4.1454	-0.1775	4.1775	-0.1510	4.1510	-0.1706	4.1706
C_5	-0.0236	4.0236	-0.0408	4.0408	-0.0187	4.0187	-0.0415	4.0415

Table 49 – Charge and Electron density for hy.

Symbol	H_2		G_2		F_2		E_2	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0629	4.0629	-0.0614	4.0614	-0.0627	4.0627	-0.0782	4.0782
C_4	-0.1509	4.1509	-0.1807	4.1807	-0.1573	4.1573	-0.1678	4.1678
C_5	-0.0673	4.0673	-0.0692	4.0692	-0.0556	4.0556	-0.0700	4.0700
C_6	-0.2597	4.2597	-0.2786	4.2786	-0.2426	4.2426	-0.2725	4.2725
C_7	-0.0880	4.088	-0.1255	4.1255	-0.0856	4.0856	-0.0977	4.0977
C_8	-0.1139	4.1139	-0.1125	4.1125	-0.1252	4.1252	-0.0533	4.0533

Table 50 – Charge and Electron density for hy.

Symbol	H_3		G_3		F_3		E_3	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.0950	4.0950	-0.0918	4.0918	-0.0931	4.0931	-0.0921	4.0921
C_2	-0.1365	4.1365	-0.1360	4.1360	-0.1391	4.1391	-0.1414	4.1414
C_3	-0.0514	4.0514	-0.0546	4.0546	-0.0483	4.0483	-0.0527	4.0527
C_4	-0.1520	4.1520	-0.1750	4.1750	-0.1589	4.1589	-0.1804	4.1804
C_5	0.0092	3.9908	-0.0002	4.0002	0.0099	3.9901	0.0013	3.9987
C_6	-0.0951	4.0951	-0.0924	4.0924	-0.0954	4.0954	-0.0921	4.0921
C_7	-0.1319	4.1319	-0.1413	4.1413	-0.1365	4.1365	-0.1413	4.1413
C_8	0.0416	3.9584	0.0362	3.9638	0.0441	3.9559	0.0451	3.9549
C_9	0.0105	3.9895	0.0018	3.9982	0.0111	3.9889	0.0013	3.9987
C_{10}	-0.1548	4.1548	-0.1753	4.1753	-0.1583	4.1583	-0.1804	4.1804
C_{11}	-0.0546	4.0546	-0.0550	4.0550	-0.0507	4.0507	-0.0527	4.0527
C_{12}	-0.1094	4.1094	-0.1094	4.1094	-0.0509	4.0509	-0.0484	4.0484

Table 51 – Charge and Electron density for hy.

Symbol	H_4		G_4		F_4		E_4	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.0959	4.0959	-0.0920	4.0920	-0.0943	4.0943	-0.0911	4.0911
C_2	-0.1339	4.1339	-0.1443	4.1443	-0.1393	4.1393	-0.1448	4.1448
C_3	-0.0544	4.0544	-0.0544	4.0544	-0.0491	4.0491	-0.0520	4.0520
C_4	-0.1548	4.1548	-0.1758	4.1758	-0.1605	4.1605	-0.1812	4.1812
C_5	0.0103	3.9897	0.0016	3.9984	0.0107	3.9893	0.0011	3.9989
C_6	-0.1010	4.1010	-0.0998	4.0998	-0.1014	4.1014	-0.1024	4.1024
C_7	-0.1003	4.1003	-0.0973	4.0973	-0.0995	4.0995	-0.0986	4.0986
C_8	0.0415	3.9585	0.0365	3.9635	0.0432	3.9568	0.0439	3.9561
C_9	0.0416	3.9584	0.0427	3.9573	0.0415	3.9585	0.0432	3.9568
C_{10}	-0.1335	4.1335	-0.1469	4.1469	-0.1312	4.1312	-0.1442	4.1442
C_{11}	-0.0965	4.0965	-0.0962	4.0962	-0.0985	4.0985	-0.0988	4.0988
C_{12}	-0.0573	4.0573	-0.0726	4.0726	-0.0592	4.0592	-0.0780	4.0780
C_{13}	-0.1519	4.1519	-0.1538	4.1538	-0.1535	4.1535	-0.1515	4.1515
C_{14}	0.0097	3.9903	0.0065	3.9935	0.0117	3.9883	0.0072	3.9928
C_{15}	-0.1094	4.1094	-0.1093	4.1093	-0.0489	4.0489	-0.0477	4.0477
C_{16}	-0.0978	4.0978	-0.0978	4.0978	-0.1093	4.1093	-0.0484	4.0484

Table 52 – Charge and Electron density for hy.

Symbol	H_5		G_5		F_5		E_5	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0550	4.0550	-0.0539	4.0539	-0.0491	4.0491	-0.0520	4.0520
C_4	-0.1555	4.1555	-0.1754	4.1754	-0.1602	4.1602	-0.1809	4.1809
C_5	0.0119	0.9881	4.6E-5	4.00004	0.0108	0.9892	0.0012	0.9988
C_8	0.0419	3.9581	0.0418	3.9582	0.0430	3.9570	0.0437	3.9563
C_9	0.0424	3.9576	0.0426	3.9574	0.0425	3.9575	0.0427	3.9573
C_{11}	-0.1012	4.1012	-0.1001	4.1001	-0.1015	4.1015	-0.1004	4.1004
C_{14}	0.0422	3.9578	0.0418	3.9582	0.0431	3.9569	0.0437	3.9563
C_{15}	0.0097	3.9903	4.30E-05	4.00004	0.0109	3.9891	0.0012	3.9988
C_{17}	-0.053	4.053	-0.0539	4.0539	-0.0504	4.0504	-0.0520	4.0520
C_{18}	-0.1094	4.1094	-0.1093	4.1093	-0.0489	4.0489	-0.0485	4.0485
C_{19}	-0.0978	4.0978	-0.0978	4.0978	-0.1093	4.1093	-0.0485	4.0485
C_{20}	-0.1032	4.1032	-0.1032	4.1032	-0.0978	4.0978	0.1168	3.8832
C_{21}	-0.1019	4.1019	-0.1018	4.1018	-0.1032	4.1032	0.0800	0.9200

Table 53 – Charge and Electron density for hy.

Symbol	H_6		G_6		F_6		E_6	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0544	4.0544	-0.0538	4.0538	-0.0530	4.0530	-0.0518	4.0518
C_4	-0.1546	4.1546	-0.1755	4.1755	-0.1600	4.1600	-0.1811	4.1811
C_5	0.0103	3.9897	2.60E-05	4.00003	0.0120	3.988	0.0012	3.9988
C_8	0.0414	3.9586	0.0419	3.9581	0.0435	3.9565	0.0437	3.9563
C_9	0.0423	3.9577	0.0424	3.9576	0.0423	3.9577	0.0425	3.9575
C_{10}	-0.1028	4.1028	-0.1020	4.1020	-0.1022	4.1022	-0.1015	4.1015
C_{11}	-0.1026	4.1026	-0.1032	4.1032	-0.1034	4.1034	-0.1040	4.1040
C_{14}	0.0422	3.9578	0.0424	3.9576	0.0424	3.9576	0.0425	3.9575
C_{15}	0.0419	3.9581	0.0430	3.9570	0.0414	3.9576	0.0430	3.9570
C_{18}	-0.0551	4.0551	-0.0723	4.0723	-0.0592	4.0592	-0.0778	4.0778
C_{19}	-0.1553	4.1553	-0.1540	4.1540	-0.1534	4.1534	-0.1516	4.1516
C_{20}	0.0118	3.9882	0.0065	3.9935	0.01167	3.9883	0.0072	3.9928
C_{21}	-0.1094	4.1094	-0.1093	4.1093	-0.0549	4.0549	-0.0485	4.0485

Table 54 – Charge and Electron density for hy.

Symbol	H_7		G_7		F_7		E_7	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0627	4.0627	-0.0538	4.0538	-0.0482	4.0482	-0.0519	4.0519
C_4	-0.1441	4.1441	-0.1754	4.1754	-0.1584	4.1584	-0.1809	4.1809
C_5	0.0099	3.9901	3.90E-05	4.00004	0.0097	3.9903	0.0012	3.9988
C_8	0.0418	3.9582	0.0418	3.9582	0.0432	3.9568	0.0437	3.9563
C_9	0.0422	3.9578	0.0424	3.9576	0.0424	3.9576	0.0425	3.9575
C_{14}	0.0421	3.9579	0.0421	3.9579	0.0422	3.9578	-0.0913	4.0913
C_{15}	0.0423	3.9577	0.0424	3.9576	0.0424	3.9576	0.0423	3.9577
C_{18}	-0.0952	4.0952	-0.0924	4.0924	-0.0960	4.0960	-0.0997	4.0997
C_{19}	-0.1435	4.1435	-0.1410	4.1410	-0.1379	4.1379	-0.0913	4.0913
C_{20}	0.0420	3.9580	0.0418	3.9582	0.0431	3.9569	-0.1442	4.1442
C_{21}	0.0059	3.9941	3.60E-05	4.00004	0.0110	3.9890	0.0437	3.9563
C_{22}	-0.1471	4.1471	-0.1754	4.1754	-0.1580	4.1580	0.0012	3.9988
C_{23}	-0.0472	4.0472	-0.0538	4.0538	-0.0505	4.0505	-0.1809	4.1809
C_{24}	-0.1094	4.1094	-0.1093	4.1093	-0.0509	4.0509	-0.0519	4.0519

Table 55 – parameter for unsubstituted thiophene.

Geo. Para.	T_7	T_6	T_5	T_4	T_3	T_2	T_1
R(1-2)	1.407	1.407	1.407	1.407	1.406	1.501	1.366
R(1-5)	1.719	1.719	1.72	1.719	1.72	1.829	1.725
R(1-6)	1.422	1.422	1.422	1.422	1.422	1.489	1.088
R(2-3)	1.429	1.429	1.429	1.43	1.429	1.489	1.436
R(2-8)	1.73	1.73	1.73	1.73	1.732	1.46	1.09
R(3-4)	1.367	1.367	1.367	1.367	1.367	1.579	1.366
R(3-24)	1.091	1.091	1.091	1.091	1.091	1.35	1.09
R(4-5)	1.735	1.735	1.735	1.736	1.735	1.095	1.725
R(4-25)	1.089	1.089	1.089	1.089	1.089	1.727	1.088
R(6-7)	1.409	1.409	1.409	1.408	1.406	1.092	---
R(6-9)	1.73	1.73	1.73	1.732	1.72	1.312	---
R(7-8)	1.731	1.731	1.731	1.731	1.731	1.075	---
R(7-11)	1.421	1.422	1.422	1.422	1.43	1.075	---
R(9-10)	1.73	1.73	1.73	1.73	1.735	---	---
R(10-11)	1.409	1.409	1.409	1.407	1.367	---	---
R(10-12)	1.421	1.422	1.422	1.43	1.089	---	---
R(11-14)	1.73	1.731	1.731	1.719	1.091	---	---
R(12-13)	1.409	1.409	1.407	1.367	---	---	---
R(12-15)	1.73	1.731	1.719	1.091	---	---	---
R(13-14)	1.73	1.73	1.73	1.735	---	---	---
R(15-16)	1.73	1.422	1.429	---	---	---	---
R(16-17)	1.409	1.73	1.735	---	---	---	---
R(16-18)	1.422	1.407	1.367	---	---	---	---
R(17-20)	1.731	1.429	1.089	---	---	---	---
R(18-19)	1.407	1.719	---	---	---	---	---
R(18-21)	1.719	1.367	---	---	---	---	---
R(19-20)	1.73	1.091	---	---	---	---	---
R(19-23)	1.429	1.735	---	---	---	---	---
R(21-22)	1.735	1.089	---	---	---	---	---
R(22-23)	1.367	---	---	---	---	---	---
R(22-26)	1.089	---	---	---	---	---	---
R(23-27)	1.091	---	---	---	---	---	---

Table 56 –charge and electron density for unsubstituted thiophene.

Symbol	T_7		T_6		T_5		T_4	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0573	4.0573	-0.0571	4.0571	-0.0570	4.0570	-0.0567	4.0567
C_4	-0.2867	4.2867	-0.2871	4.2871	-0.2879	4.2879	-0.2884	4.2884
S_5	0.3606	5.6394	0.3599	5.6401	0.3590	5.6410	0.3570	5.6430
S_8	0.3906	5.6094	0.3899	5.6101	0.3886	5.6114	0.3866	5.6134
S_9	0.4034	5.5966	0.4020	5.5980	0.4013	5.5987	0.3866	5.6134
C_{12}	-0.2059	4.2059	-0.2035	4.2035	-0.2152	4.2152	-0.0567	4.0567
C_{13}	-0.2045	4.2045	-0.2013	4.2013	-0.2634	4.2634	-0.2886	4.2886
S_{14}	0.4033	5.5967	0.4019	5.5981	0.3884	5.6116	0.3571	5.6429
S_{15}(C)	0.4036	5.5964	0.3899	5.6101	0.3589	5.6411	0.1321	4.1321
C_{16}(H)	-0.2005	4.2005	-0.2628	4.2628	-0.2878	4.2878	0.1486	0.8514
C_{17}(H)	-0.2043	4.2043	-0.2163	4.2163	-0.0570	4.0570	0.1321	0.8679
C_{18}(H)	-0.2168	4.2168	-0.0571	4.0571	0.1324	0.8676	0.1486	0.8514
C_{19}(H)	-0.2622	4.2622	-0.2871	4.2871	0.1489	0.8511	---	---
S_{20} (H)	0.3904	5.6096	0.3593	5.6407	0.1489	0.8511	---	---
S_{21}(H)	0.3605	5.6395	0.1326	0.8674	0.1324	0.8676	---	---
C_{22}(H)	-0.2866	4.2866	0.1490	0.8510	---	---	---	---
C_{23}(H)	-0.0573	4.0573	0.1326	0.8674	---	---	---	---

Symbol	**T_3**		**T_2**		**T_1**	
	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.2115	4.2115	-0.1829	4.1829	-0.3001	4.3001
C_2	-0.2614	4.2614	-0.0408	4.0408	-0.1216	4.1216
C_3	-0.0576	4.0576	-0.1812	4.1812	-0.1216	4.1216
C_4	-0.2902	4.2902	-0.1689	4.1689	-0.3	4.3
S_5	0.3552	5.6448	0.1463	5.8537	0.3042	5.6958
C_6(H)	-0.2115	4.2115	-0.0762	4.0762	0.1460	0.8540
C_7(H)	-0.2617	4.2617	-0.0763	4.0763	0.1235	0.8765
S_8(C)(H)	0.3722	5.6448	-0.0735	4.0735	0.1235	0.8765
S_9(C)(H)	0.3551	5.6449	0.1478	0.8522	0.1460	0.8540
C_{10}(H)	-0.2901	4.2901	0.1428	0.8572	---	---
C_{11}(H)	-0.0577	4.0577	0.1814	0.8186	---	---

Table 57 — parameter for unsubstituted hy.

Geo. Para.	**I_7**	**I_6**	**I_5**	**I_4**	**I_3**	**I_2**	**I_1**
R(1-2)	1.387	1.387	1.387	1.387	1.386	1.459	1.352
R(1-5)	1.488	1.488	1.488	1.488	1.488	1.5	1.502
R(3-4)	1.359	1.359	1.359	1.359	1.359	1.346	1.352
R(3-24)	1.088	1.088	1.088	1.088	1.088	1.089	1.088
R(4-5)	1.513	1.513	1.513	1.513	1.513	1.504	1.502
R(4-25)	1.088	1.088	1.088	1.088	1.088	1.089	1.087
R(7-8)	1.499	1.499	1.499	1.498	1.499	1.092	---
R(7-11)	1.43	1.431	1.431	1.432	1.448	1.084	---
R(9-10)	1.498	1.498	1.498	1.499	1.513	---	---
R(10-11)	1.396	1.395	1.395	1.387	1.359	---	---
R(10-12)	1.43	1.431	1.432	1.448	1.088	---	---
R(11-14)	1.498	1.498	1.499	1.488	1.088	---	---
R(13-14)	1.498	1.498	1.498	1.513	---	---	---
R(15-34)	1.105	1.105	1.105	---	---	---	---

Table 58 –charge and electron density for unsubstituted hy.

Symbol	I_7		I_6		I_5		I_4	
	Charge	Electron density	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_3	-0.0723	4.0723	-0.0724	4.0724	-0.0725	4.0725	-0.0728	4.0728
C_4	-0.1749	4.1749	-0.1748	4.1748	-0.1748	4.1748	-0.1744	4.1744
C_5	-0.0034	4.0034	-0.0034	4.0034	-0.0034	4.0034	-0.0035	4.0035
C_8	0.0432	3.9568	0.0433	3.9567	0.0432	3.9568	0.0435	3.9565
C_9	0.0425	3.9575	0.0425	3.9575	0.0427	3.9573	0.0435	3.9565
C_{11}	-0.1031	4.1031	-0.1026	4.1026	-0.0997	4.0997	-0.0932	4.0932
C_{14}	0.0423	3.9577	0.0425	3.9575	0.0433	3.9567	-0.0034	4.0034
C_{18}(H)	-0.0921	4.0921	-0.0724	4.0724	0.1139	0.8861	0.0814	0.9186
C_{20} (H)	0.0433	3.9567	-0.0034	4.0034	0.0812	0.9188	0.0809	0.9194
C_{21}(H)	-0.0034	4.0034	0.1139	0.8861	0.0813	0.9187	0.0809	0.9194
C_{22}(H)	-0.1749	4.1749	0.1142	0.8858	0.0810	0.9190	0.0809	0.9194

Symbol	I_3		I_2		I_1	
	Charge	Electron density	Charge	Electron density	Charge	Electron density
C_1	-0.0934	4.0934	0.1776	0.8224	-0.1626	4.1626
C_2	-0.1493	4.1493	-0.1709	4.1709	-0.1213	4.1213
C_3	-0.0734	4.0734	-0.0835	4.0835	-0.1213	4.1213
C_4	-0.1740	4.1740	-0.1694	4.1694	-0.1626	4.1626
C_5	-0.0033	4.0033	-0.0753	4.0753	-0.0525	4.0525
C_8(H)	0.0442	0.0442	-0.0915	4.0915	0.1135	0.8865
C_9(H)	-0.0033	4.0033	0.1181	0.8819	0.1150	0.885

References

1:- A. A. Patel, G. A. Mehta; J. of Der Pharma Chemica; vol. 2(1), p 215, (2010).

2:- J. A. Joule, G. F. Smith; **"Heterocyclic Chemistry**",**1**st ed. London; (1972).

3:- E.A. John ; J. of Chem. Rev., vol . 106 , p 5028–5048 , (2006).

4:- J.A. Merlo, C.R. Newman, C.P. Gerlach, T.W. Kelley, D.V Muyres, S.E. Fritz , M.F .Toney ; J . of Am. Chem. Soc, vol . 127, p 3997–4009, (2005).

5:- M.K. Young , L.Eunhee , L. Jaemin , W.K. Bon, D. Lee-Mi , S. Hong-Ku; J. of **Macromolecules** , vol . 39 , p 4081–4085, (2006).

6:- H.K. Tian, J.W. Shi, D.H .Yan, L.X. Wang, Y.H . Geng , F.S. Wang ; J. of **Adv. Mater**, vol . 18, p 2149–2152 ,(2006).

7:- H. Meng , J. Zheng , A . J. Lovinger , B. Wang, P.G. van Patten, Z. Bao , J. of **Chem. Mater**, vol . 15 , p 1778–1787 , (2003).

8:- G. Dennler, M.C. Scharber, C.J. Brabec. J. of Adv. Mater, vol . 21, p 1323, (2009).

9:- T.Cuenca, P. Royo ,J. of Coordination Chemistry Reviews, p 447–498 , (1999).

10: - H.Kaya, **"Parameterization of the AM1* semiempirical molecular orbital method for the first-row transition metals and other elements"** ,ph,thesis,Der Naturwissenschaftlichen Fakultät der, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germani, (2009).

11:- M. He and F. Zhang ; J. of **Org. Chem** , vol. 72 , p 442- 451 , (2007) .

12:- A. A. M. Al-Asser **" Introduction to Quantum Chemistry , Atoms and Molecules and Spectroscopy "** 1st. ed , California , (2001) **.**

13:- J.H. Ali, **National Journal of Chemistry**, vol. 45 ,p 30 - 44, (2012)**.**