

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

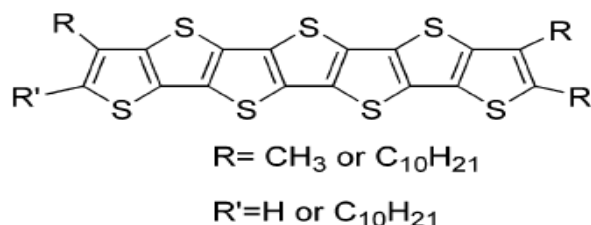
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Abstract

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 , -C₁₀H₂₁] 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 [U⁰,H⁰,S⁰,G⁰,A⁰]for all molecules . These compounds are compared with 28 the corresponding hydrocarbon compound.

الخلاصة:

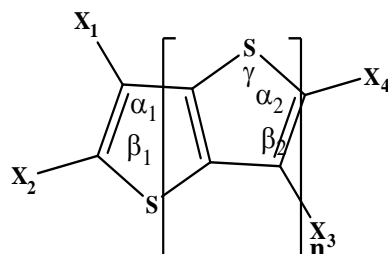
باستخدام إحدى طرق ميكانيك الكم الشبه تجريبية (PM3) تم حساب 28 مركب من مركبات الثيايوفين والمؤلفة من حلقة واحدة إلى سبع حلقات مدمجة , معوضة بمجاميع الكيلية [-CH₃, -C₁₀H₂₁] عند مواقع مختلفة ؛حيث منها تتضمن مجموعة المثلث فقط (-CH₃) ومنها تحتوي على مجموعة (-C₁₀H₂₁) فقط ومنها ما تحتوي على كلا المعوضين. تضمنت 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 التأين , الشحنات و الكثافات الاليكترونية و الدوال الترموداينميكية (U⁰,H⁰,S⁰,G⁰,A⁰) لجميع الجزيئات وتم مقارنة المركبات المذكورة مع 28 مركب من مركبات الهيدروكاربون المناظرة .



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 η⁵-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

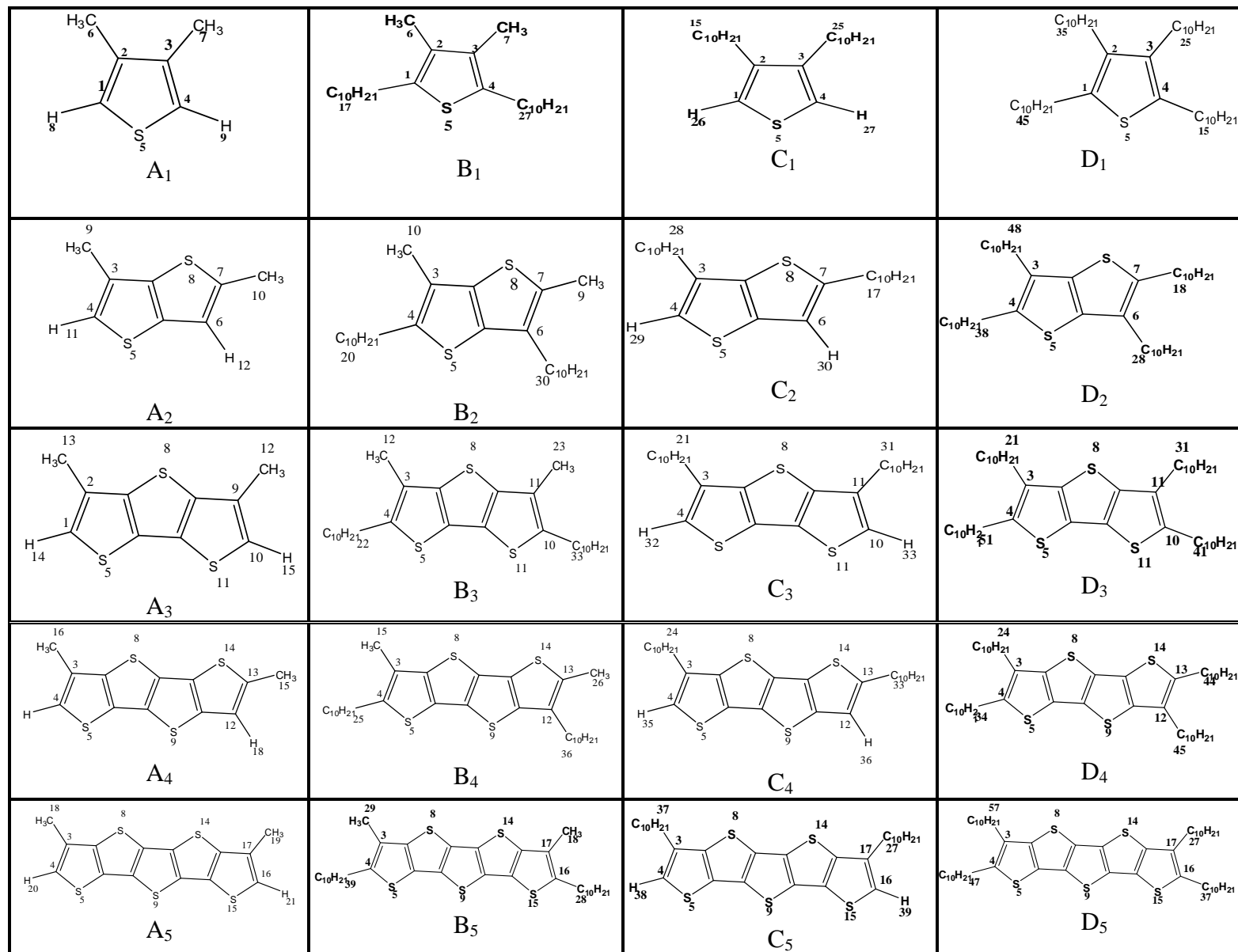
rings up to seven rings, therefore, we are used PM3 Semiempirical method⁽¹⁰⁾ to calculate the equilibrium geometries of thiophene fused rings⁽¹¹⁾ that substituted by Alkyl groups(Fig,1) and calculate some of physical properties along with the Hydrocarbon compounds that have the same substituted(Fig,2) 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

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



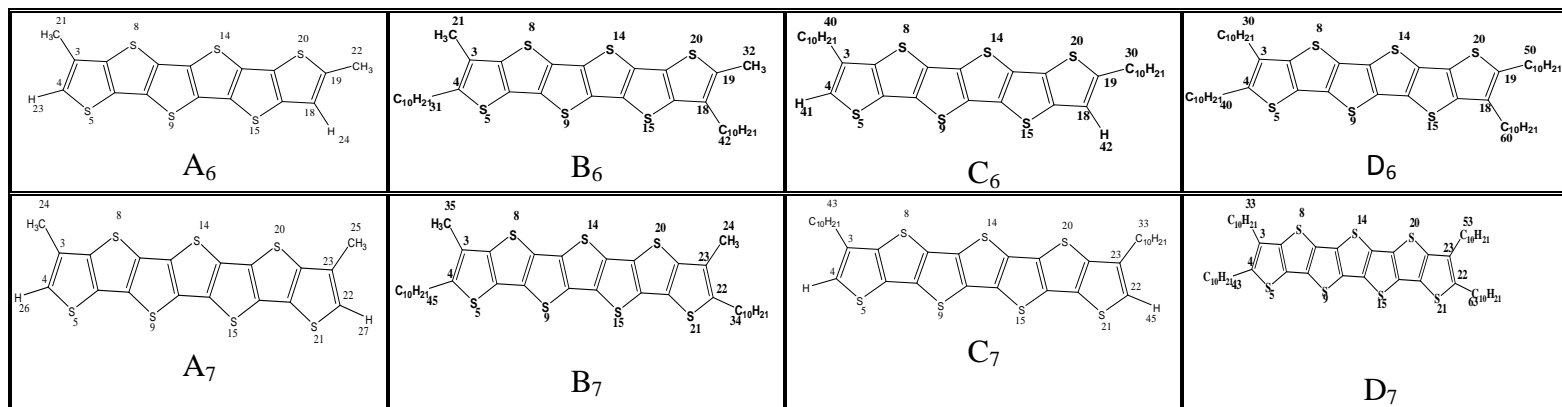
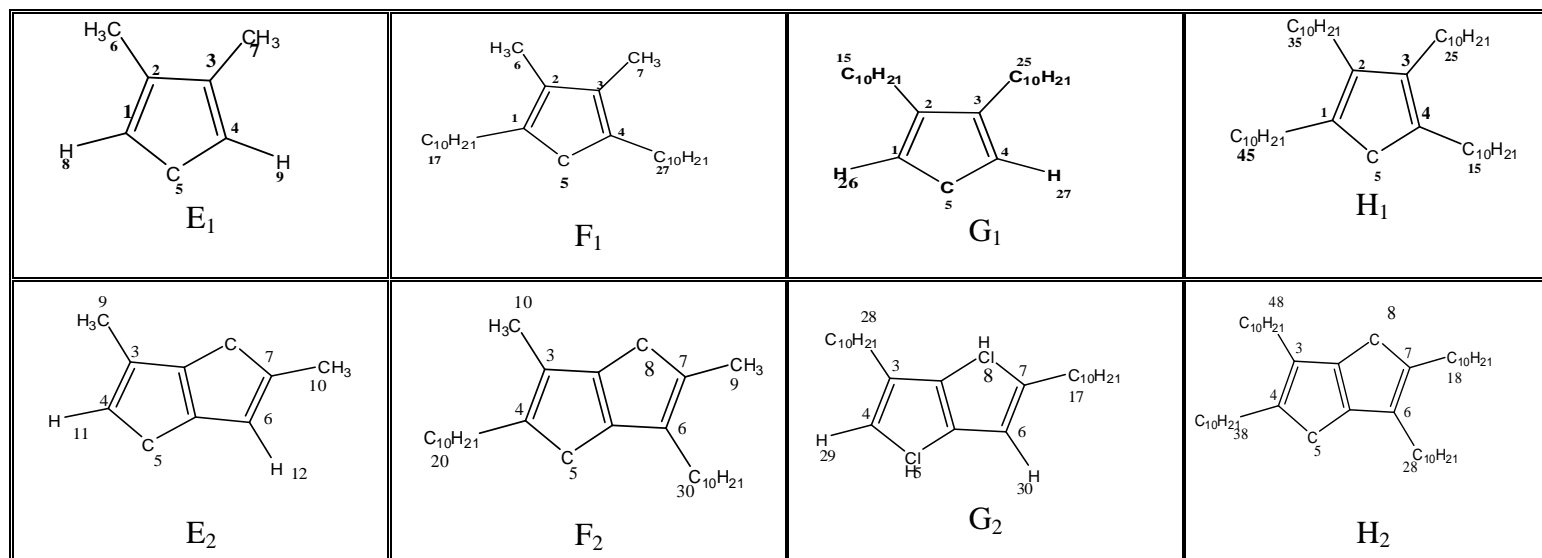


Fig.1 The thiophene fused rings that substituted by Alkyl groups molecules



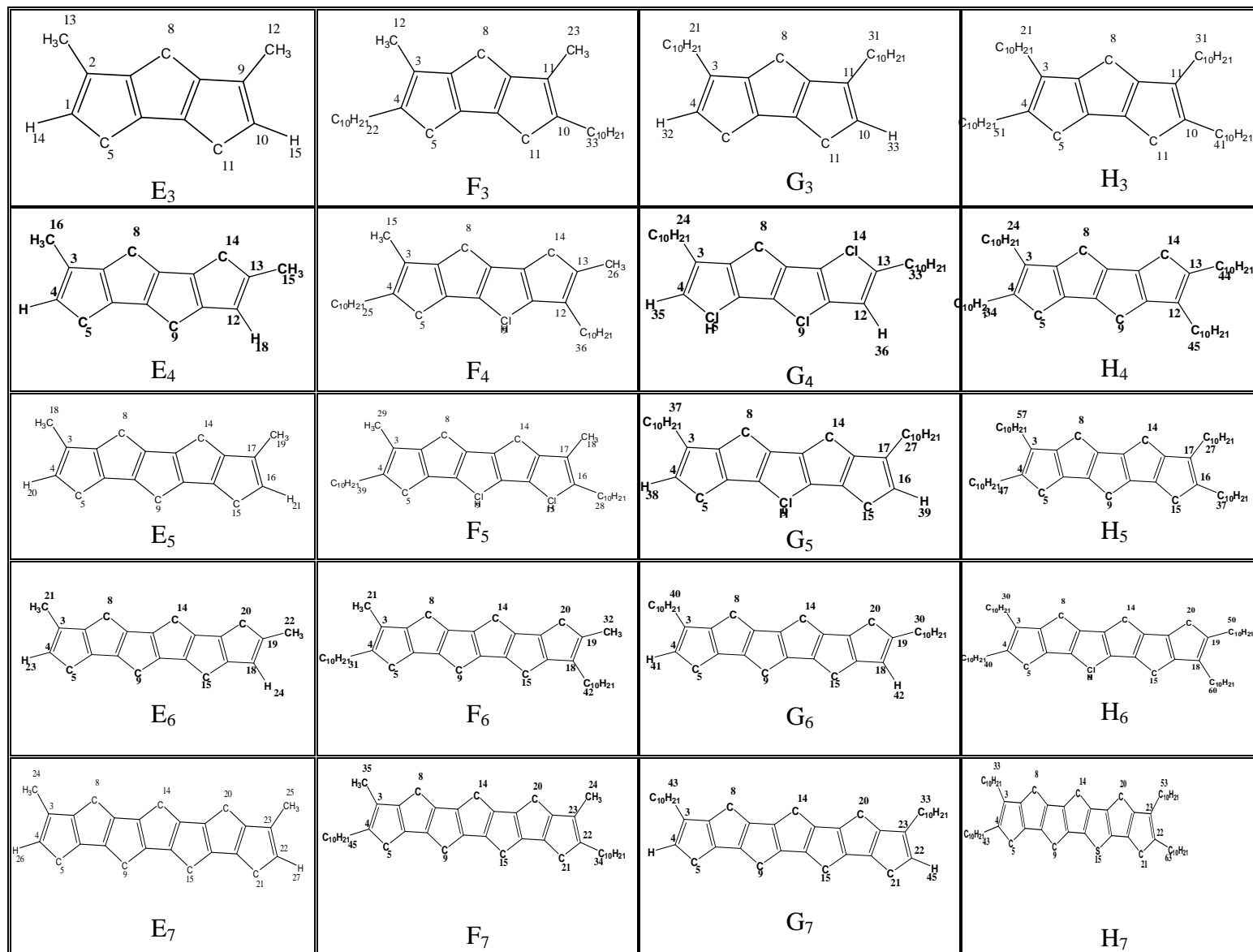
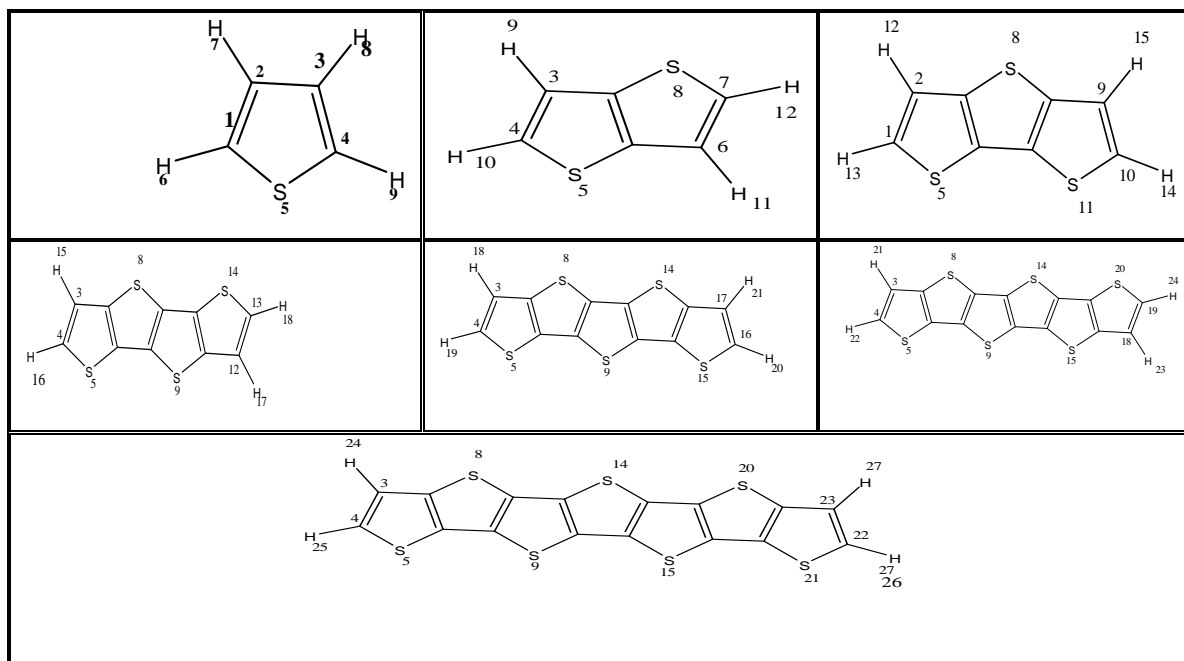


Fig.2 The hydrocarbon fused rings that substituted by Alkyl groups molecules



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 \cong 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 potential 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, A⁰ ,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 ₆ H ₈ S (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 ₈ H ₈ S 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 ₈ S 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 ₈ S 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 ₈ S 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 ₈ S 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 ₈ S 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	(H₂)	Geometric parameter	(G₂)	Geometric parameter	(F₂)	Geometric parameter	(E₂)
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	(H₃)	Geometric parameter	(G₃)	Geometric parameter	(F₃)	Geometric parameter	(E₃)
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

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