

Investigation of The Thermodynamic Properties of Tetra Fluoro Tetra Cyanoquino Dimethane Molecule (F4-Tcnq) By Using Quantum Semi-Empirical Software

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Abstract

In The Current, the thermodynamic properties of a F₄-TCNQ molecule were studied using MNDO-PM3 semi-empirical quantum programs using HyperChem program to draw the engineering structure and the primary matrix containing (r, θ, φ) It was used to obtain the final matrix using WinMopac, where the thermal properties of the molecule were calculated and from these properties the entropy and the enthalpy, the formation temperature and the heat capacity in addition to the according to the values of the functions and the graphical relationship was drawn to them as a function of temperature and from the graphic relationship and at the temperature Standard 298 K The Heat of Formation (ΔH^of), enthalpy (H), Heat Capacity (C_p), Entropy (S) and Gibbs free energy (G), their values, respectively (ΔH^of=55.740 Kcal/mol), (H=11045.4722 cal/mol), (C_p=60.3194 Cal.mol/ K), (S=138.5499 cal/K/mol), (G =-30242.3980 cal.mol/K).

Keywords: thermodynamic, F₄-TCNQ, Gibbs, HyperChem, WinMopac, MNDO-PM3, OTFTs, OLEDs.

I. Introduction

The molecule 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano quinodimethane, are considered important organic compounds that are used in the manufacture of some types of semiconductors such as a semiconductor type of triple or pentagonal type [1]. Organic semiconductors have attracted significant attention recently due to a number of advantages they have over conventional inorganic materials. Which may include low cost, light weight, compatibility with flexible substrates, biocompatibility, little environment damage and chemical compatibility [2-3-4-5]. The F₄-TCNQ molecule is a non-linear complex molecule and it is a greenish yellow powder at room temperature and has a 20 atoms, consisting of carbon (12 atoms), fluorine (4 atoms) and nitrogen (4 atoms) and its chemical formula is C₁₂F₄N₄ and its molecular weight is 276.15 g / mol As well as the melting point range is 285-290 ° C [6]. Whereas, over time, it gained increasing importance in the fields of materials science [7-8]. The F₄-TCNQ is one of the most widely used and most effective types of compounds due to its ability to accept electron. It has a deep LUMO (5.2 eV) level which is near the (8.3 eV) HOMO level of many organic semiconductors. Grafting is accomplished by transferring the charge from the HOMO level of the host to the LUMO of the gifted molecule [9]. The organic compound has been widely studied due to its great applications in electronic and photoelectric devices, such as (OFETs) [10], organic thin film transistors (OTFTs) [11] organic light-emitting diodes (OLEDs) [12] Schottky diodes [13], organic solar cells [14], and organic photodetectors. Given the importance of the compound from the scientific and industrial point of view, which made scientists interested in studying its properties theoretically and practically, as well as studying thermodynamics to give a complete description of the composition of the molecules and their thermal properties [15].

II. Calculations

The rapid development of software and the high speed that electronic computers have reached had a greater impact on the development of the theoretical treatment of molecular spectra for the calculation of thermodynamic properties. The calculation of the balanced geometry (obtaining the best stable and balanced shape of the molecule) and the energy of the molecular levels of the compounds are taken from Schrödinger's equation and approximate solutions have the basis in the formulation of these methods and software. these methods adopted two directions, the first did not depend on quantum mechanics, and the other method was quantum mechanics, and these treatments are generally called semi-experimental methods [16].

To study the molecular spectra of any molecule, no matter how complex, there are two main methods: 1- Raman spectra, which depend on the scattering principle of electromagnetic radiation. 2- The infrared frequency, which depends on the interaction of electromagnetic radiation with the substance molecules, where the molecule absorbs infrared radiation and converts its energy into vibrational energy for the atoms that make up the molecule.



The vibrational motion of a diatomic molecule consisting of the two atoms is linked by a chemical bond, and for an approximation we can imagine that the masses of the two nuclei are (m_1, m_2) respectively. The joints between them represent a massless spiral spring vibrating harmonic any with respect to the center of mass [17]. According to Hooke's law, the force in which it is restored is:

$$F = -k(r - r_e) \dots\dots\dots (1)$$

Where (r_e) is the equilibrium distance (the length of the image at the point of stability). (k) Represents the force constant (r) the displacement from the center of mass. Both masses can move together as one effective mass, denoted by the symbol (μ) , where is the reduced mass as:

$$\dots\dots\dots (2) \mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$$

As the classical frequency of harmonic motion [18].

$$\dots\dots\dots (3) v_{vib} = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$$

From this equation, we note that the frequency increases with increasing k (the force constant) and decreases with the increase of the reduced mass (μ) The restoring force can be written in terms of potential energy as in the following equation

$$\dots\dots\dots (4) F = \frac{dV(r)}{dr} = -kr$$

Where $V(r)$ is the potential energy in terms of displacement, and by integrating both sides of the equation we get the equation

$$\dots\dots\dots (5) V_r = \frac{1}{2} k (r - r_e)^2$$

According to quantum mechanics, the total quantum mechanical Hamiltonian energy of the harmonic oscillator in one dimension is given by the following relationship [19-20].

$$\dots\dots\dots (6) \hat{H} = \frac{-\hbar^2}{2\mu} \nabla^2 + \frac{1}{2} k (r - r_e)^2$$

Inserting the Schrödinger equation $H\psi = E\psi$ gives

$$\dots\dots\dots (7) \frac{d^2\psi}{dx^2} + \left(\frac{2\mu E_v}{\hbar^2} - \frac{\mu k (r - r_e)^2}{\hbar^2} \right) \psi = 0$$

From a solution to the Schrödinger equation, we find that the energy of the vibrational energy.

$$E_v = h\nu \left(v + \frac{1}{2} \right) \dots\dots\dots (8)$$

Since the number of vibrational quantum v takes the values $(\dots, 0, 1, 2, 3, 4)$, or equation (8) can be written in terms of the wave number, as is the custom in studying spectra after division by the expression hc as in the equation (9).

$$G(V) = E_v / hc = \omega \left(V + \frac{1}{2} \right) \dots\dots\dots (9)$$

Where ω is the wavenumber in cm^{-1} ,

The main vibrational energy is $G_{(0)}$ and is called the zero point energy when the value of $(v=0)$ is as in the following equation:

$$\dots\dots\dots (10) G_{(0)} = \frac{1}{2} \omega$$

Which represents the lowest energy that the molecule can possess even at a temperature of absolute zero, $(-273.15^\circ C)$ and in this model the transition velocity was calculated for the nuclei of the molecule equal to zero and all the energy is in the form of potential energy, and this is contrary to reality, so there was a big difference between the theoretical and practical results [21].

Since the binary particles do not behave in exact harmonic behavior, when the value of $(r - r_e)$ is very small, the particles behave in harmonic behavior, and with increasing displacement, the particles begin to deviate from the harmonic behavior by acting as an harmonic oscillator until it reaches a specific value in which the molecule disintegrates. To its constituent atoms and the potential energy at this point is called the dissociation energy [22].

It suggested several potential functions that match the empirical curve better. Where equation (11) represents a Morse potential function [23-24].

$$\dots\dots\dots (11)U_{morse} = D_e(1 - e^{-\alpha(r-r_e)})^2$$

$$\dots\dots\dots (12)\alpha = \sqrt{\frac{8\pi^2\mu\omega_e x_e}{h}}$$

Where is (α) a special constant of the electronic energy levels of the molecule, The potential energy of the bond does not represent that the value of (Um) approaches (D_e) and when the value of (r) approaches infinity this matches the true behavior of the diatomic molecules. the energy treatment of a non-harmonic oscillator can be written using the Schrödinger equation in terms of the quantum vibration number (v = 0, 1,2,3,4 ...) [25].

$$G_{(v)}=(v+\frac{1}{2})-(v+\frac{1}{2})^2\omega_e x_e\dots\dots\dots(13)$$

So that G_(v) represents the energy of the vibrational plane, (ω_e) the vibrational frequency in the non-harmonic motion, (x_e) the incompatible constant

$$\omega_e x_e = \frac{\alpha^2 hc}{2\mu} \dots\dots\dots (14)$$

From the Morse potential equation we can extract the number of vibrational energy levels(v = 1, 2, 3 ... Vmax) [21].

$$\dots\dots\dots (15)V_{max} = \frac{\omega_e}{2\omega_e x_e} - \frac{1}{2}$$

To find the zero point energy G₍₀₎ from Morse's equation we use the equation (when 0 = v)to find the zero point energy G₍₀₎ from Morse's equation we use the equation (when v = 0)

$$\dots\dots\dots (16)G_{(0)} = \frac{1}{2}\omega_e(1 + \frac{1}{2}x_e)cm^{-1}$$

Inorder to obtain a frequency Lay pckage be any that

$$v_{0 \rightarrow v} = G_{(v)} - G_{(0)}$$

$$\dots\dots\dots (17)v_{0 \rightarrow v} = \omega_e U - \omega_e x_e U(U + 1)$$

Substituting the value of v into equation 1,2,3, the main frequency and the main difference can be obtained. Thus, additional vibrational transitions such as 0 → 2 and 0 → 3 can be observed at high and low wavelengths. The beam frequencies above the basic are multiples of the basic beam frequencies. The dissociation energy (D_e) is approximately given by the following relationship.

$$\dots\dots\dots (18)D_e = \frac{\omega_e^2}{4\omega_e x_e}$$

after neglecting all the incompatible constants except ω_ex_e. Thus, we find that:

$$\dots\dots\dots (19)D_0 = D_e - \frac{E_0}{hc}$$

Since D₀ represents the chemical dissociation energy of the bond.

As for the selection rules for non-harmonic vibrational transitions: (Δv= ±1, ±2,±3,...) are very weak and are called over-tone bands and their frequencies are approximately equal to the frequency of the fundamental, band[23-26-27-28].

One of the important characteristics that have been studied in this research are the thermal properties that determine the most important conditions on the basis of an experiment The interactions between the molecules, as the formation temperature of the thermal, enthalpy and entropy capacity of the molecule, as well as the calculations of the free Gibbs energy were calculated when setting the equilibrium using the WinMopac program after obtaining the final molecular matrix and the elementary matrix from the Hyper Chem8.0 software.

A. Heat of formation

The standard formation temperature (ΔH[°]f) of the material is required when forming one mole of the substance from its basic elements under standard conditions at constant temperature [29-30]. The formation temperature is usually

measured in units (J / mol) or (Cal / mol). The formation temperature is an important and distinctive feature of the compound and it is related to its stability. Since a compound whose heat formation is large and positive is unstable, then the reaction absorbs heat and the compound that has a negative heat formation is stable, so the reaction is exothermic [29].

B. Entropy (S°)

Entropy (S) is a measure of the extent of disorder in a system or the probability of a particular combination of parts of the system [31]. It is a thermodynamic quantity of a comprehensive character, which was discovered by the scientist Classius in 1854. The holistic characteristic is the characteristic that depends on the quantity of material in the system [32].

Entropy is the case function of the system and is represented by the following relationship:

$$\dots\dots\dots (20) ds^\circ = \frac{dQ}{T}$$

Where T is the ambient temperature and dQ is the amount of heat or liberated.

C. Heat capacity

Heat capacity is defined for any system as the amount of heat required to raise the system temperature by one temperature [33-34].

If the amount of heat entering the system is ΔQ and the amount of rise in its temperature is ΔT, then the heat capacity is defined by the relationship

$$\dots\dots\dots (21) C = \lim_{\Delta T \rightarrow 0} \frac{\Delta Q}{\Delta T} = \frac{dQ}{dT}$$

He followed a pressure or volume fixation process when performing an operation on the material and so on There are two types of heat capacity. (Cv) for constant volume and heat capacity (Cp) under constant pressure, in the case of gases

In general, the more complex the molecule, the greater its molar heat capacity. and be the effect of temperature is great. As for solids, the heat capacity approaches zero when the temperature drops towards absolute zero [34].

D. Enthalpy

Enthalpy (H) is the sum of the internal energy (U) and the product of pressure and volume (PV) given by the equation: H=U+PV. When a process occurs at constant pressure, the heat evolved (either released or absorbed) is equal to the change in enthalpy OR If a system absorb heat at constant t and p then the heat absorbed equal to the ΔH of system for exothermic process the ΔH is negative sign [35].

In addition to the internal energy and heat capacity, there are a number of thermodynamic functions commonly used due to their practical importance, and among these functions are Enthalpy (and can be defined mathematically [36]

$$H = U + PV \dots\dots\dots (22)$$

Where enthalpy is (H), internal energy (U), pressure (P), volume (V).

It should also be noted that the units of this equation must be in harmony with each other as the product of PV has it Power units, as well as (U). Therefore, (H) power units as well. Equation [22] can be written differently as follows:

$$dH = dU + d(PV) \dots\dots\dots (23)$$

And since H, U, P, and V are state functions, the integral of equation[22] can be found directly as follows:

$$\dots\dots\dots (24) \Delta H = \Delta U + \Delta(PV)$$

This equation is used whenever there is a significant change in the system. Enthalpy is a function of temperature, pressure, and internal energy for all substances except for gases that behave either ideally or close to ideal behavior[38] .

E. Gibbs free energy

For reversible change, occurring at constant p and T the ΔG of a system is equal to the work dose on it. But if a system considered under constant P and T and W is caused by ΔV, the system in equilibrium and G of minus sign or free

enthalpy and it is a quantity used to measure the maximum amount of work done in a thermodynamic system when temperature and pressure are constant. Oh, the indicator that indicates, whether the process occurs automatically, remains in equilibrium, or proceeds automatically in the opposite direction. It is inversely proportional to the temperature with constant pressure [37]. It is denoted by the symbol (G) and a change in it is symbolized by the symbol (ΔG) and from the value (ΔG), the direction of the chemical reaction can be indicated. If (ΔG) is negative this means that the reaction is heading towards the formation of produce, In the case of its positive value, this means that the interaction proceeds in the opposite direction, As the free and enthalpic energy relationship is given by the following relationship [38].

$$G = H - TS \dots\dots\dots(25)$$

Likewise, the changes in the standard free energy can be found from knowing the standard enthalpy values (ΔH°) and standard entropy (ΔS°), at a given temperature, using the following equation [39].

$$\Delta G = \Delta H - T\Delta S \dots\dots\dots (26)$$

III. The employed and software's

Work paper, two basic programs were used to study the thermal properties, first: HyperChem 8.0 program and second WinMopac 7.21. Which depends in their mechanism of work on the principles of quantum mechanics, as the elementary matrix was obtained from the program HyperChem 8.0 using the MNDO-PM3 method after the geometric structure of the molecule was drawn thus, the closest energetically stable form was obtained after several Optimization transformers. The elementary matrix was obtained after obtaining the elementary matrix. It is used in WinMopac 7.21 to obtain the required thermal properties and some other information.

IV. Results and discussion

Some thermal properties related to F4-TCNQ molecule, such as formation heat (H.O.F), heat capacity, entropy, and enthalpy heat were calculated using Win Mopac 7.21 program and by the method of MNDO-PM3, and the final matrix was obtained as shown in Table 1: -

Atom	Distance r(A°)	Opt.	Angle (θ°)	Opt.	Dihedral (φ°)	Opt.	A	B	C	charge
C	0.0000000	0	.000000	0	.000000	0	0	0	0	.0566
C	1.3672643	1	.000000	0	.000000	0	1	0	0	.0569
C	1.4699998	1	121.502020	1	.000000	0	2	1	0	-.0268
C	1.4697913	1	112.741481	1	22.741362	1	3	2	1	.0569
C	1.3672165	1	121.556886	1	-22.697598	1	4	3	2	.0568
C	1.4698435	1	121.594642	1	.165993	1	5	4	3	-.0265
C	1.3590433	1	123.599806	1	-155.457971	1	3	2	1	.2528
C	1.3591289	1	123.638765	1	-156.120025	1	6	5	4	.2528
C	1.4265149	1	123.421249	1	178.464670	1	8	6	5	-.1538
C	1.4264418	1	123.494218	1	-.279566	1	8	6	5	-.1536
C	1.4264905	1	123.404046	1	-.331477	1	7	3	2	-.1537
C	1.4264897	1	123.444860	1	178.376038	1	7	3	2	-.1536
N	1.1595439	1	178.484738	1	165.892022	1	11	7	3	.0384
N	1.1595728	1	178.417599	1	-170.327780	1	12	7	3	.0384
N	1.1595531	1	178.354085	1	174.733564	1	10	8	6	.0384
N	1.1595230	1	178.447438	1	-166.767509	1	9	8	6	.0384
F	1.3364971	1	119.692009	1	179.063798	1	2	1	6	-.0544
F	1.3366548	1	119.590962	1	-179.400796	1	1	2	3	-.0547
F	1.3366427	1	119.650344	1	179.368266	1	5	4	3	-.0547
F	1.3366143	1	118.766843	1	-25.169410	1	4	3	7	-.0545

And from that, the above properties were calculated and thus the graphical relationships between these thermal properties and temperature were drawn, as follows.

A. Heat of Formation (ΔH°_f)

The formation temperature was calculated for variable values of temperature (100-662K) and the standard formation temperature was at a temperature of 298 K was equal to (55.740 Kcal/mol) and as we note that, the formation temperature increases with increasing temperature. the relationship between the formation temperature and temperature was plotted as in Figure (1).

Table (2) shows the relationship between Configuration heat ($\Delta H^{\circ}f$) and temperature

TEMP. (K)	H.O.F. kcal/mol
100	46.539
120	47.167
140	47.872
160	48.652
180	49.503
200	50.420
220	51.400
240	52.437
260	53.528
280	54.669
298	55.740
300	55.857
320	57.090
340	58.364
360	59.677
380	61.027
400	62.413
420	63.832
440	65.284
460	66.767
480	68.278
500	69.818
520	71.385
540	72.978
560	74.596
580	76.237
600	77.902
620	79.588
640	81.295
660	83.023

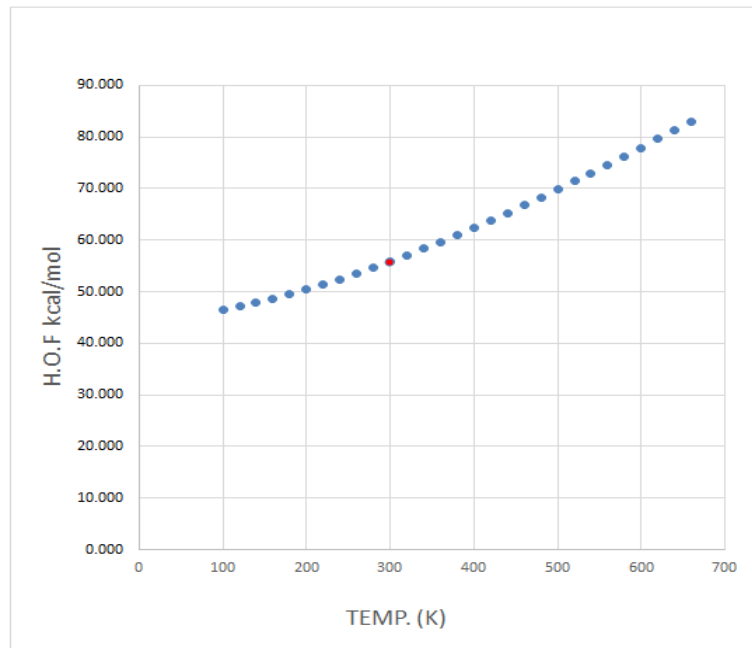


Figure (1) shows the relationship between the heat of formation ($\Delta H^{\circ}f$) and the temperature

B. Enthalpy (H)

It is a result of the sum of the internal energy of the U system with its external energy PV, which is a function of pressure, temperature and internal energy and represents the enthalpy of the system, where the heat content of the temperature was calculated, and the standard formation temperature at a temperature of 298 K was equal to (11045.4722 cal / k / mol) Figure (2) shows that the change enthalpy increases with increasing temperature.

Table (3) shows the relationship between Enthalpy (H), temperature.

TEMP. (K)	ENTHALPY CAL/MOLE
100	1849.9215
120	2477.4940
140	3182.8318
160	3962.8479
180	4813.6675
200	5730.9794
220	6710.3713
240	7747.5747
260	8838.6133
280	9979.8727
298	11045.4722
300	11168.1155
320	12400.4625
340	13032.3646
360	14987.5209
380	16337.9150
400	17723.6977
420	19143.1923
440	19865.0959
460	22077.2743
480	23589.1069
500	25129.1094
520	26696.1038
540	28288.9736
560	29906.6562
580	31548.1386
600	33212.4523
620	34898.6705
640	36605.9055
660	38333.3064

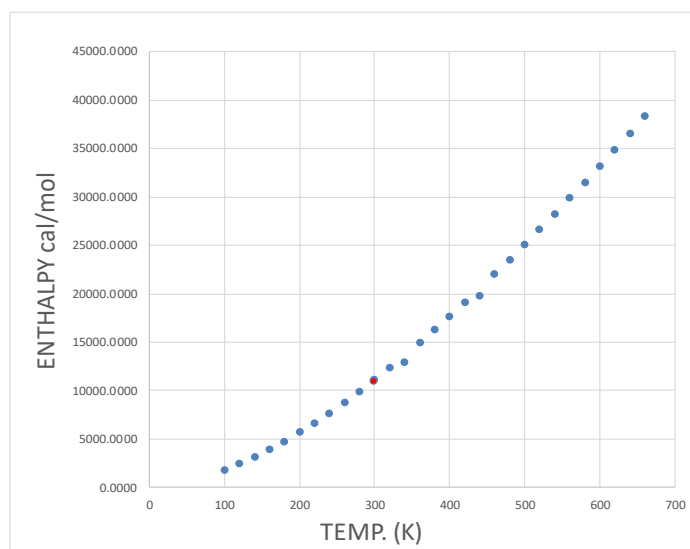


Figure (2) shows the relationship between enthalpy (H) and temperature

C. Heat Capacity (C_p)

It is a function of temperature and directly proportional to it. As the temperature increases, the number of particles in the upper vibration energy level increases and the heat capacity increases for each vibration pattern. The heat capacity was calculated for different values of temperatures 100-662K. The value of the heat capacity was at constant pressure and at a temperature of 298K (60.3194 cal / k / mol), and Figure (3) shows the direct proportion between them.

Table (4) illustrates the relationship between Heat capacity (C_p) and temperature

TEMP. (K)	HEAT CAPACITY CAL/K/MOL
100	29.3949
120	33.3445
140	37.1634
160	40.8056
180	44.2401
200	47.4541
220	50.4494
240	53.2377
260	55.8360
280	58.2630
298	60.3194
300	60.5373
320	62.6761
340	64.6944
360	66.6051
380	68.4190
400	70.1453
420	71.7914
440	73.3635
460	74.8669
480	76.3060
500	77.6845
520	79.0057
540	80.2725
560	81.4874
580	82.6528
600	83.7709
620	84.8436
640	85.8728
660	86.8604

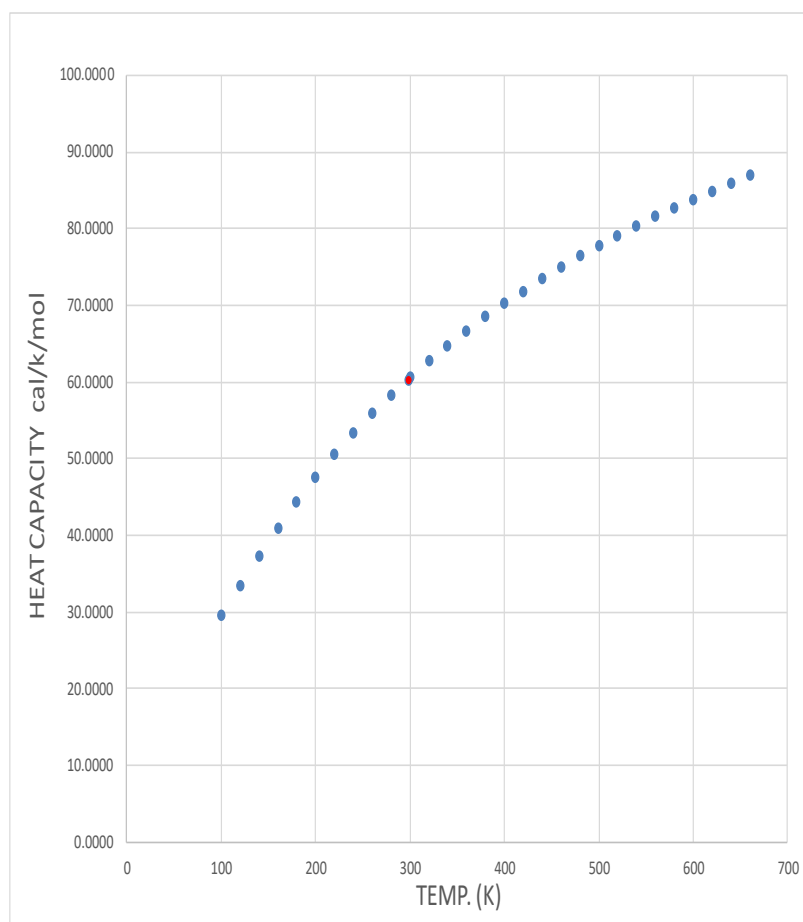


Figure (3) shows the relationship between heat capacity (C_p) and temperature

D. Entropy (S)

Entropy describes the random distribution and the relative regularity of the molecules that make up the system. Entropy was calculated for different values of temperatures 100-662 K. The value of entropy was (138.5499 cal / k / mol) at the standard temperature of 298K and Figure (4) shows the relationship directly between entropy and temperature.

Table (5) illustrates the relationship between Entropy capacitance (S) and temperature.

TEMP. (K)	ENTROPY CAL/K/MOL	ΔS
100	90.9921	-47.5578
120	96.7017	-74.7179
140	102.1302	-36.4197
160	107.3323	-31.2176
180	112.3386	-31.2176
200	117.1678	-21.3821
220	121.8326	-16.7173
240	126.3431	-12.2068
260	130.7080	-7.8419
280	134.9355	-3.6144
298	138.5499	0.0000
300	139.0335	0.4836
320	143.0093	4.4594
340	146.8700	8.3201
360	150.6222	12.0723
380	154.2722	15.7223
400	157.8258	19.2759
420	161.2882	22.7383
440	164.6644	26.1145
460	167.9589	-3.2168
480	171.1757	32.6258
500	174.3187	35.7688
520	177.3914	38.8415
540	180.3969	41.8470
560	183.3382	44.7883
580	186.2181	47.6682
600	189.0391	50.4892
620	191.8034	53.2535
640	194.5134	55.9635
660	197.1710	58.6211

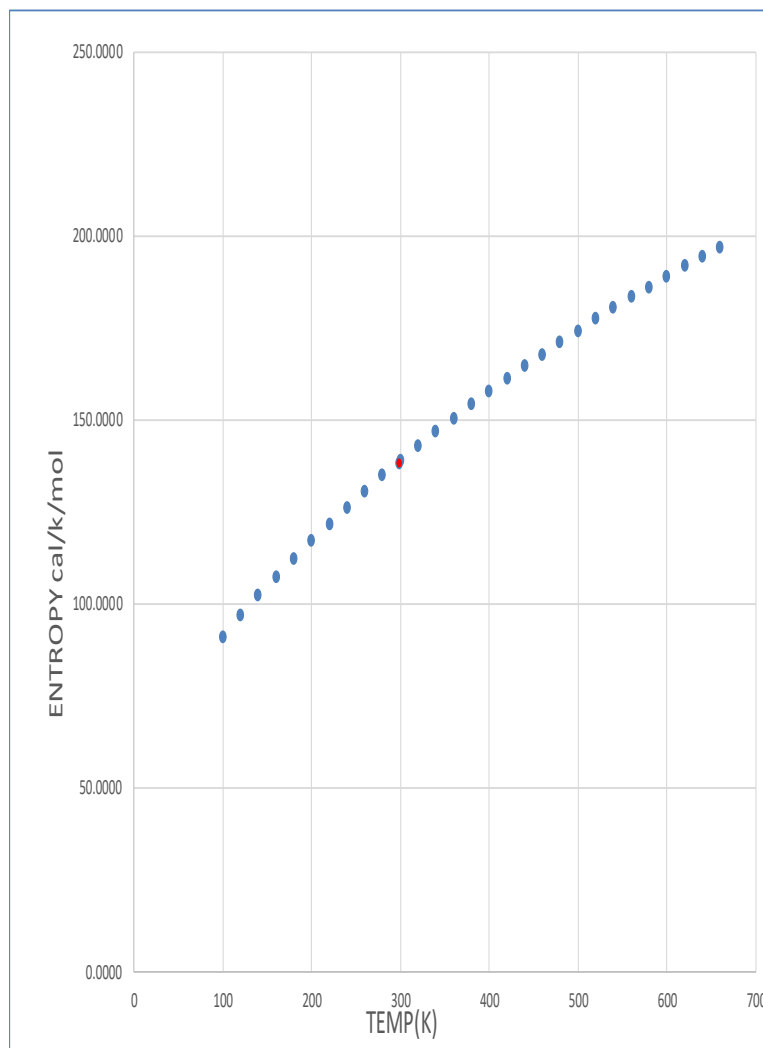


Figure 4 shows the relationship between entropy (S) and temperature

E. Gibbs free energy

After calculating the enthalpy and entropy of the F4-TCNQ molecule, and for different degrees of temperature, it must be known whether the reaction takes place automatically or not. Where the Gibbs energy of the molecule was calculated and for different values of temperature, as well as according to its change. The value of Gibbs energy at the standard temperature was 298K and its was (-30242.3980 cal.mol/k). Figure (5) shows the relationship between Gibbs energy (G) and temperature.

Table (6) illustrates the relationship between Gibbs energy (G) and temperature.

TEMP. (K)	G=H-TS	ΔG
100	-7249.2885	1794.1815
120	-9126.71	16593.9784
140	-11115.3962	25393.026
160	-13210.3201	14760.1785
180	-15407.2805	14060.7723
200	-17702.5806	14978.0842
220	-20092.8007	13026.4971
240	-22574.7693	12673.5901
260	-25145.4667	12420.4997
280	-27802.0673	12261.0189
290	-28881.4059	12066.8234
298	-30242.398	11112.3755
300	-30541.9345	12200.6097
320	-33362.5135	11647.7234
340	-36903.4354	12452.3911
360	-39236.4711	12684.6296
380	-42285.521	12982.7123
400	-45406.6223	13343.2341
420	-48597.8517	13033.3425
440	-52587.2401	14239.4133
460	-55183.8197	24491.9733
480	-58575.2291	15350.881
500	-62030.2406	15981.2614
520	-65547.4242	16658.4666
540	-69125.3524	17380.5102
560	-72762.7358	18145.4852
580	-76458.3594	18951.5887
600	-80211.0077	19797.1489
620	-84019.4375	20680.6225
640	-87882.6705	21600.4434
660	-91799.5536	22569.3963

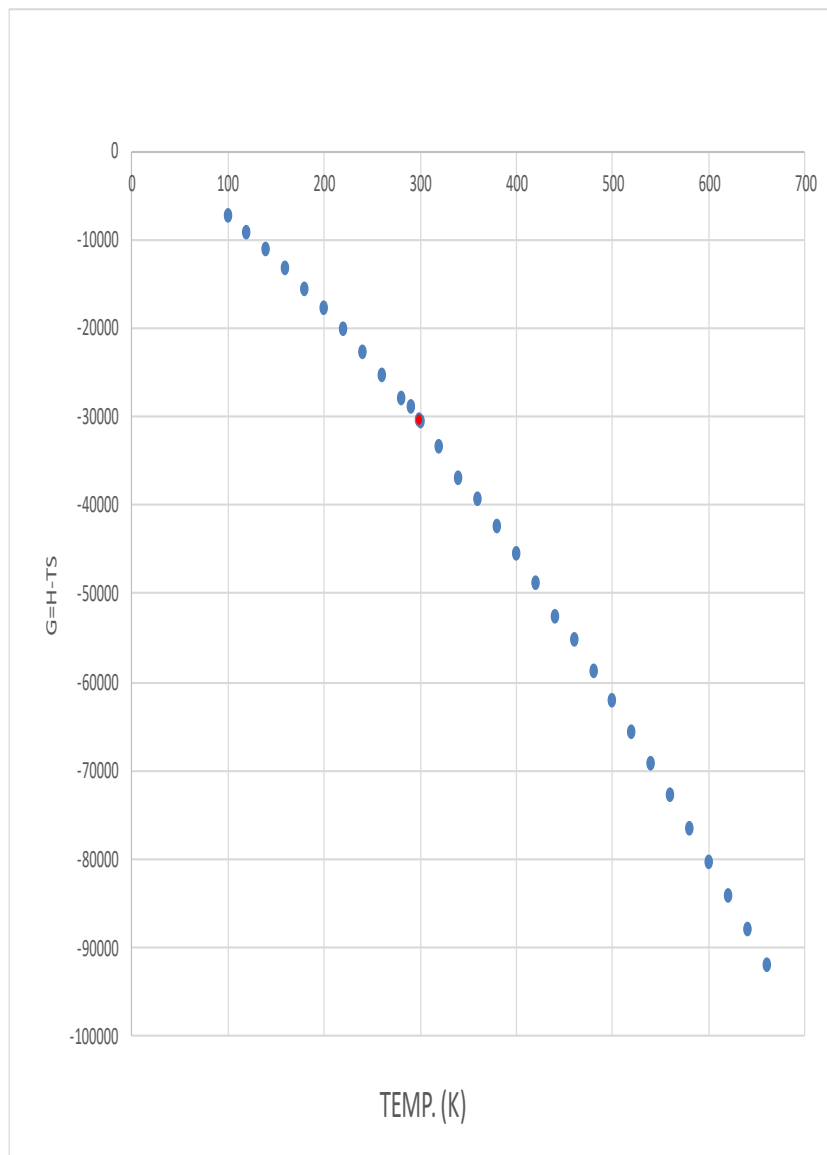


Figure (5) shows the relationship between Gibbs energy (G) and temperature

Table (2) shows the values of each of the thermal properties with the absolute temperature

TEMP. (K)	H.O.F.(HF) KCAL/MOL	ENTHALPY (H) CAL/MOLE	HEAT CAPACITY (CP) CAL/K/MOL	ENTROPY (S) CAL/K/MOL	G=H-TS
100	46.539	1849.9215	29.3949	90.9921	-7249.2885
120	47.167	2477.4940	33.3445	96.7017	-9126.7100
140	47.872	3182.8318	37.1634	102.1302	-11115.3962
160	48.652	3962.8479	40.8056	107.3323	-13210.3201
180	49.503	4813.6675	44.2401	112.3386	-15407.2805
200	50.420	5730.9794	47.4541	117.1678	-17702.5806
220	51.400	6710.3713	50.4494	121.8326	-20092.8007
240	52.437	7747.5747	53.2377	126.3431	-22574.7693
260	53.528	8838.6133	55.8360	130.7080	-25145.4667
280	54.669	9979.8727	58.2630	134.9355	-27802.0673
298	55.740	11045.4722	60.3194	138.5499	-30242.3980
300	55.857	11168.1155	60.5373	139.0335	-30541.9345
320	57.090	12400.4625	62.6761	143.0093	-33362.5135
340	58.364	13032.3646	64.6944	146.8700	-36903.4354
360	59.677	14987.5209	66.6051	150.6222	-39236.4711
380	61.027	16337.9150	68.4190	154.2722	-42285.5210
400	62.413	17723.6977	70.1453	157.8258	-45406.6223
420	63.832	19143.1923	71.7914	161.2882	-48597.8517
440	65.284	19865.0959	73.3635	164.6644	-52587.2401
460	66.767	22077.2743	74.8669	167.9589	-55183.8197
480	68.278	23589.1069	76.3060	171.1757	-58575.2291
500	69.818	25129.1094	77.6845	174.3187	-62030.2406
520	71.385	26696.1038	79.0057	177.3914	-65547.4242
540	72.978	28288.9736	80.2725	180.3969	-69125.3524
560	74.596	29906.6562	81.4874	183.3382	-72762.7358
580	76.237	31548.1386	82.6528	186.2181	-76458.3594
600	77.902	33212.4523	83.7709	189.0391	-80211.0077
620	79.588	34898.6705	84.8436	191.8034	-84019.4375
640	81.295	36605.9055	85.8728	194.5134	-87882.6705
660	83.023	38333.3064	86.8604	197.1710	-91799.5536

V. Conclusions

After studying a molecule in terms of thermal properties, we can conclude the following:

- 1- By noting the value of the formation temperature of the molecule (F_4 -TCNQ) that is under study and in the standard degree of (55.740 kcal/mol), as the formation temperature indicates that the molecule is endothermic. The relationship between the temperature of the formation and the temperature is positive, that is, the temperature of the formation increases with the increase in temperature.
- 2- The more complex the molecule, the greater the value of heat capacity, especially if the temperature effect is greater.
- 3- The entropy of liquids is less than the entropy of gases, as well as the entropy of solids in turn is less than the entropy of liquids. Thus, entropy increases with the increase in the complexity of the chemical composition, and therefore we find that the entropy of the (F_4 -TCNQ) molecule is equal to (138.5499 cal/k/mol).
- 4- Note that the enthalpy of F_4 -TCNQ is equal to (138.5499 Cal.mol) at standard temperature.
- 5- The free Gibbs energy of the molecule was (-30242.3980 cal.mol/k) as the less negative molecules are more stable. The Gibbs energy is inversely proportional to the temperature.

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