

## **Preparation and Study of Electrical Properties and Determined activation energies for Liquid Crystal Materials**

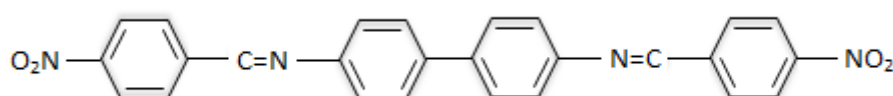
**تحضير ودراسة الخواص الكهربائية وتعيين طاقة التنشيط لمواد بلورية سائلة**

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### **Abstract:**

The electrical properties of compounds (legand and complexes) have been studied, were prepared two complexes of Polymer Schiff's base (legand) with ions Manganese dichloride( $MnCl_2 \cdot 4H_2O$ ) and potassium chloro palatinate ( $K_2PtCl_6$ ) as the following :



( 4,4-dinitrobenzylidene-4,4'-dibenzylidene-1,1'-bi phenyl )

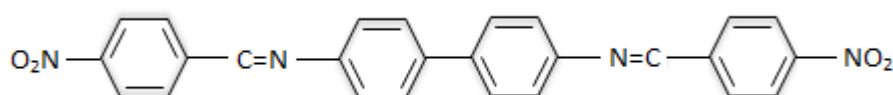
The compounds (legand and complexes) have been characterized by a spectrophotometer Ultra Violet (UV), Infrared (IR). These compounds have been characterized by polarizing microscope equipped with heating stage to study liquid crystalline (LC) behavior, were found that the compounds have (LC) properties with the nematic phase( enantiotropy).

Electrical properties for compounds are include determining of the electric conductivity DC and AC at a temperature ranged from (343 - 463)K, and calculate of the activation energy by using values of the exponential factor.

**Keywords:** Liquid crystals compounds, Electric conductivity, Activation energy.

### **الخلاصة :**

تضمن هذا البحث تحضير ودراسة الخواص الكهربائية لمعقدين لبوليمر قواعد شيف (ليكاند) مع ايونات كلوريد المنغنيز المائي الثنائي التكافؤ وكلوروبلاتينيت البوتاسيوم السداسي التكافؤ ( كما في الصيغة التركيبية التالية:



( 4,4-dinitrobenzylidene-4,4'-dibenzylidene-1,1'-bi phenyl )

تم تشخيص المركبات المحضرة بواسطة مطياف الأشعة تحت الحمراء، مطياف الأشعة فوق البنفسجية . هذه المركبات شخّصت بواسطة المجهر ذي الضوء المستقطب لدراسة الحالة البلورية السائلة. وقد تبين بانها تمتلك الصفة البلورية السائلة ذات الطور النيماتي ثنائي الحالة الوسطية.

الخواص الكهربائية للمركبات تضمنت حساب التوصيلية الكهربائية المستمرة والمتناوبة لمدى درجات حرارة K(343 - 463) وحساب طاقة التنشيط باعتماد قيم العامل الأسّي.

**الكلمات المفتاحية :** مركبات بلورية سائلة، التوصيلية الكهربائية، طاقة التنشيط.

**Introduction:**

liquid crystal polymers is athermoplastic polymers have unparallel structure and sepcial physical properties.It consiste of solid and flexible monomer group that connect one to other. When flow in liquid crystalline status, solid parts of the molecules lined up with each other toward of shear flow , Their orientation and structure continue to exist with orientation formation even when liquid crystal polymer is cooled under the melting temperature. liquid crystal polymer offers mechanical, electrical, chemical, and thermal properties not found in other engineering polymers because of its unique structure [1].

In 1970 the idea of liquid crystalline semiconductors was invented .Detailed studies of electrical conductivity were carried out in smectic, nematic, and cholesteric phases, and it was discovered that ionic conduction happens only in liquid crystalline phase. Several researchers have investigated in the electrical conductivity of the nematic liquid crystals because of increasing use nematic liquid crystals in industrial production of display devices.

The semiconductors have many properties that can be used to achieve high performance devices in various fields, and Many semiconductors are constantly developed, so it studied in this research their electrical properties for the purpose of knowing its electrical conductivity [2].

**Theoretical part:**

The semiconductor at (T=0°C) is the valence band filled with electrons totally and The conduction band is unfilled totally. At the rise of temperatures, electron is excited from the filled band to the unfilled band. Both the electron and the hole contributed to the electric conduction. Partially filling of the conduction band with electrons causes flowing an electric current if the electric field is apply. Therefore, holes in valence band contribute to electrical conductivity ( $\sigma$ ) and the electrons in this band will be able to move to these holes, thus gaining the drift velocity ( $v_d$ ) [3].

$$J_e = - e n v_d \dots\dots\dots (1)$$

Where( e) is the electrical charges ,( n) is density of electrons, ( $J_e$ ) is current density. the solution of the semi-classic equation for the applied electric field (E), giving a drift velocity [4] .

$$v_d = - \mu_e E \dots\dots\dots (2)$$

[  
Were ( $\mu_e$ ) is The proportionality constant which is empirically defined by the equation [5] :

$$\mu_e = v_d / E \dots\dots\dots (3)$$

The drift mobility giving also by the equation ( $J= \sigma E$ ) [4].

$$\sigma = e n \mu_e \dots\dots\dots (4)$$

The activation energy for the thermal activation phenomenon is obtained by fitting data of the dc electrical conductivity ( $\sigma_{dc}$ ) with the Arrhenius relation [6] :

$$\sigma_{dc} = \sigma_0 \exp (- E_\sigma / k_B T) \dots\dots\dots (5)$$

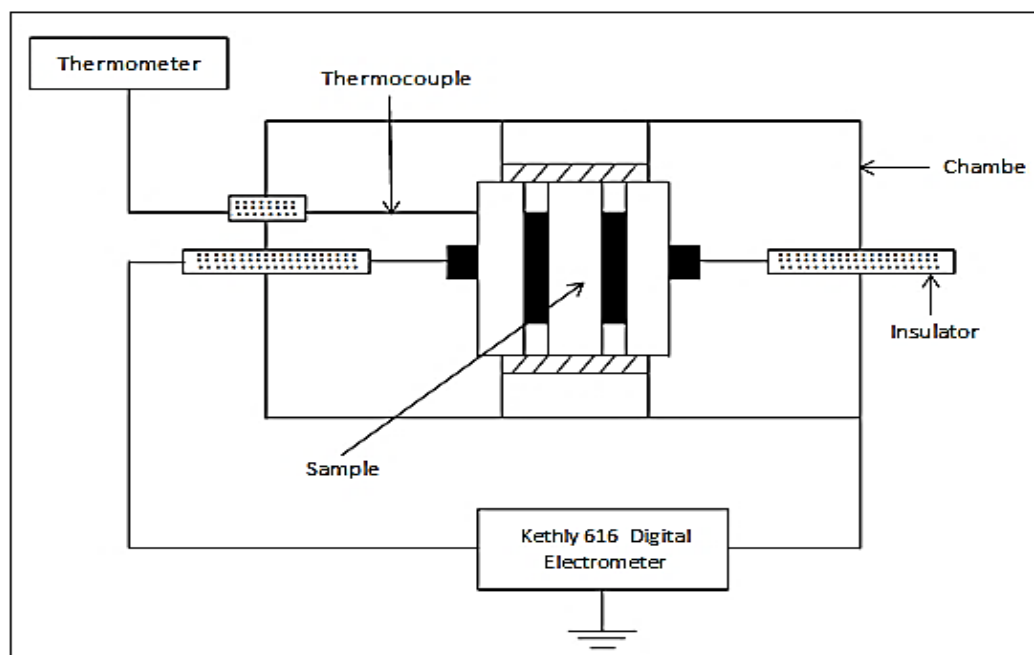
where ( $\sigma_0$ ) is the pre-exponential factor, ( $k_B$ ) is the Boltzmann constant, ( $E_\sigma$ ) is the activation energy, and ( T) is the absolute temperature.

Ac conductivity ( $\sigma_{ac}$ ) is related to the dc conductivity ( $\sigma_{dc}$ ) and total conductivity ( $\sigma_t$ ) by the relation [7] :

$$\sigma_{ac} = \sigma_t - \sigma_{dc} \dots\dots\dots (6)$$

**Expeimmental part :**

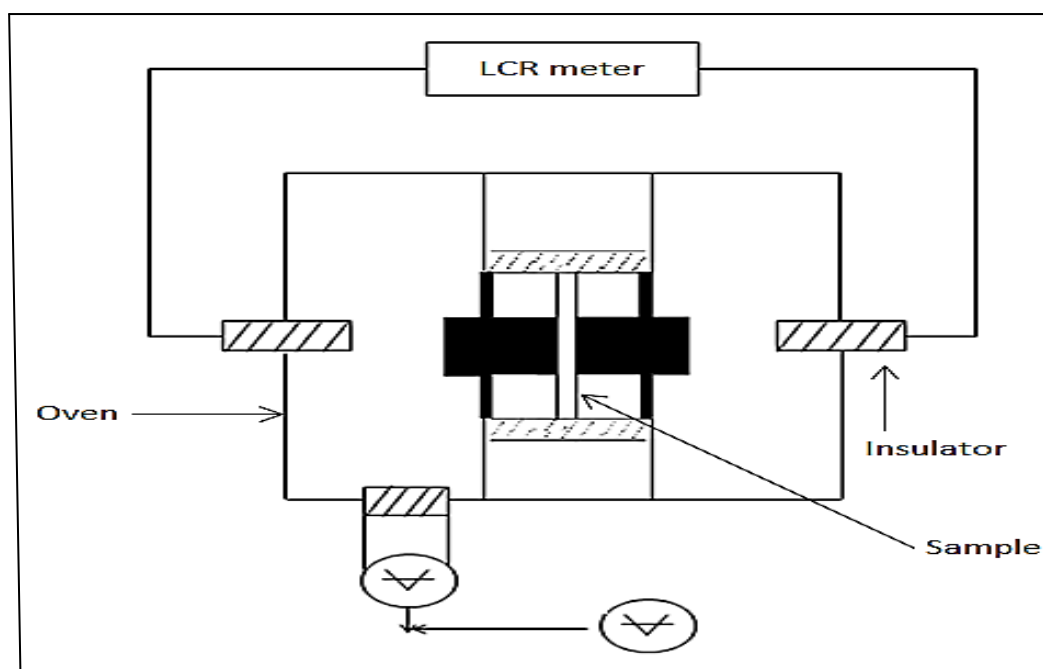
- 1- Preparation of the polymer legan( 4,4-dinitrobenzin-4,4-dibenzylidene-1,1<sup>-</sup>bi phenyl ) by mixing one mole of (4-nitrobenzaldehyde) and two mole of (benzidine) using Ethanol as a solvent during reflux process.
- 2- Preparation of the complexes (1) by mixing the prepared legand and metal ion of Manganese dichloride ( $MnCl_2 \cdot 4H_2O$ ) using molar ratio (1:1) and Ethanol as a solvent during reflux process.
- 3- Preparation of the complexes(2) by mixing the prepared legand and metal ion of potassium chloro palatinate ( $K_2PtCl_6$ ) using molar ratio (1:1) and Ethanol as a solvent during reflux process [8,9].
- 4- Preparation of samples for electrical measurements:  
The electrical measurements of compounds are prepared in their volumetric form and the form of circular disks [10] , The discs were used with diameter (1cm) and thickness ( $0.05 \pm 0.2$ )cm for electrical measurements (AC,DC) ,These samples were prepared using a hydraulic piston type (Specac)with power ( $1-15 \text{ Tn./cm}^2$ ), The material powder after weight by a sensitive balance type (Mettler AE.166) is placed in a special template type (PyeUnicam) In the piston container, the pressure is applied on it until ( $4 \text{ Tn./cm}^2$ ), The following are the steps used in preparation of samples :
  - a- Masks: Aluminum foil was used with thickness ( $2000 \text{ \AA}$  ) to prepare the used masks in the preparation of electrodes that are equal to the area of the circular disk used and its inside the drilling of geometric shapes required for the purpose of electric conduction and both side of each disc
  - b- Thermal evaporation system in vacuum: The evaporation system unit was used type (Edward Speedvac Unit) .In the preparation of electrodes used in the ohm connection, the sample was evaporated under pressure ( $10^{-6} \text{ Toor}$ ) on liquid crystal compounds and their complexes.
  - c- Preparation of electrodes :The electrodes used in the ohm connection were prepared as sandwich by evaporation high-purity aluminum wires(99.99%)and placed inside a wire of tungsten which is shaped as a spiral ,aluminum electrodes have been deposited in this thermal evaporation system, the samples are covered with their own masks and placed in the base of the system(substrate), the deposition of aluminum after reaching the required value of pressure and then the flow of high electricity through the tungsten wire ,after completion of the preparation of the electrodes on one face of the samples, samples are turned again to prepare the electrodes of the other face and in the same way mentioned above.
- 5- DC Conductivity measurement:  
The DC conductivity of the compounds was measured using a device (Kithly 616 Digital Electrometer) where used a measuring cell made from teflon material and two electrodes from the brass material in a circular form, use thermocouple to measure the temperatures which touches sample on side and is connected to a counter on the other, The figure (1) shows the electrical circuit used in DC electrical measurements.



**Figure (1) : Electric circuit used in DC electrical measurements.**

**6- AC Conductivity measurement:**

The AC conductivity of the compounds was measured using a device (HP.LCR)(Multi Frequency LCR Meter 4284 A) where the circuit consists of a compartment or a container with a heat oven connected to power supply to control of the temperature , and measuring container connected to a thermocouple that touches the sample on one side and connects to the other with counter type (Eurothem 1601),the two cell electrodes carrier sample are connected with the two electrodes of the device by conduction wires using a material (Silver best) ,the measuring container is connected to a mechanical emptying device (Rotary), the figure (2) shows the electrical circuit used in AC electrical measurements.



**Figure (2) : Electric circuit used in AC electrical measurements.**

**Results and Discussion:**

The liquid crystalline phase of the compounds prepared using the polarized optical microscope was diagnosed by heating and cooling. All compounds were shown to have a nematic phase (Enantiotropic).

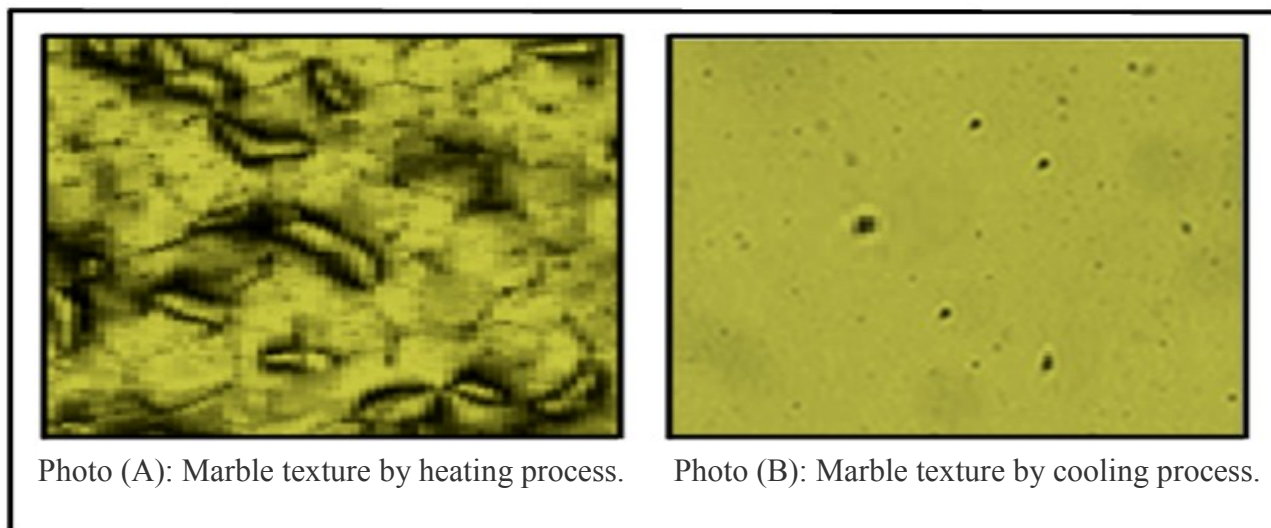


Figure (3): Marble of nematic phase for legand by heating and cooling process.

The electric conductivity DC and AC measurement for the compounds(legand and complexes )at a temperature ranged from (343 - 463)K . the values of the electric conductivity DC and AC shown in Table (1) .

**Table(1): Values of the electric conductivity DC and AC of compounds.**

<b>Compound</b>	<b>The electric conductivity DC (ohm.cm)<sup>-1</sup></b>	<b>The electric conductivity AC (ohm.cm)<sup>-1</sup></b>
Legand	$10^{-12} - 10^{-9}$	$0.71 \times 10^{-8}$
Complex (1)	$10^{-10} - 10^{-6}$	$0.83 \times 10^{-7}$
Complex (2)	$10^{-10} - 10^{-7}$	$0.79 \times 10^{-6}$

It observed from the table (1) that the electric conductivity DC and AC for complexes are increased due to complexity , the effect of complexity was evident in improving its conductivity. The DC electrical conductivity for compounds is increasing with rise of temperatures, increased of temperatures causes increases the number of pairs (electron - hole) formed and then increases its conductivity. the AC electrical conductivity for compounds dependents on frequency and temperature where conductivity increases with increasing frequency and temperature.

Increase electrical conductivity with increasing temperature due to having the temperature coefficient negative of resistance and this is a characteristic of a semiconductor.

The relation between the DC electrical conductivity with temperature for compounds are shown in Figures (4),(5),(6)

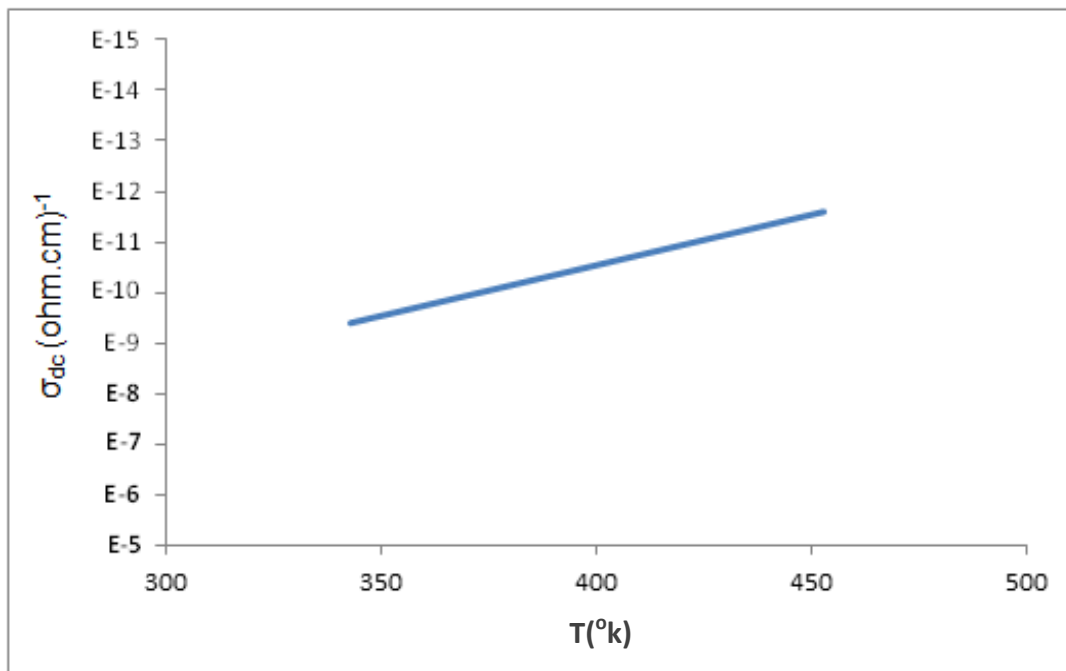


Figure (4) : The DC electrical conductivity as a function of temperature for legend.

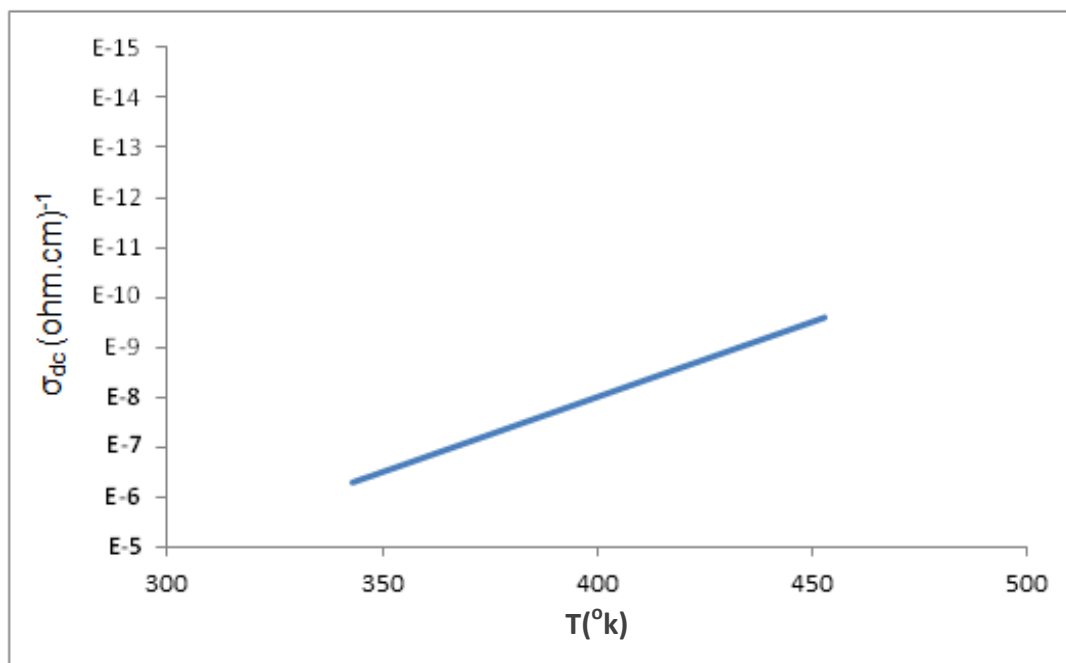


Figure (5) : The DC electrical conductivity as a function of temperature for complex(1).

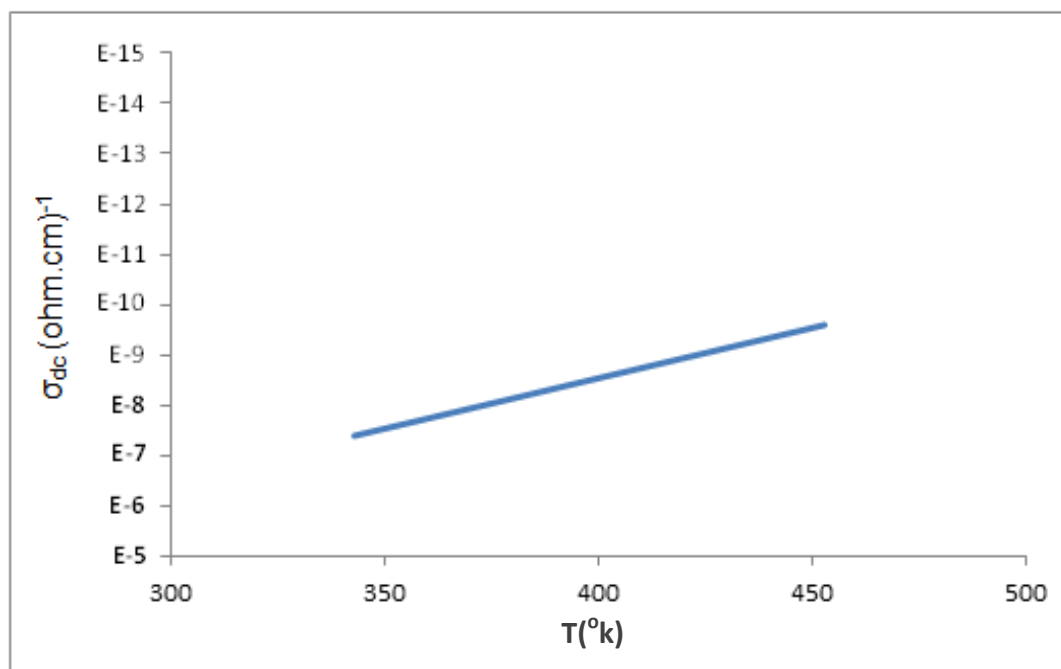


Figure (6) : The DC electrical conductivity as a function of temperature for complex(2).

The relation between ( $\ln\sigma_{dc}$ ) with reciprocal temperature for compounds are shown in figures (7),(8),(9)

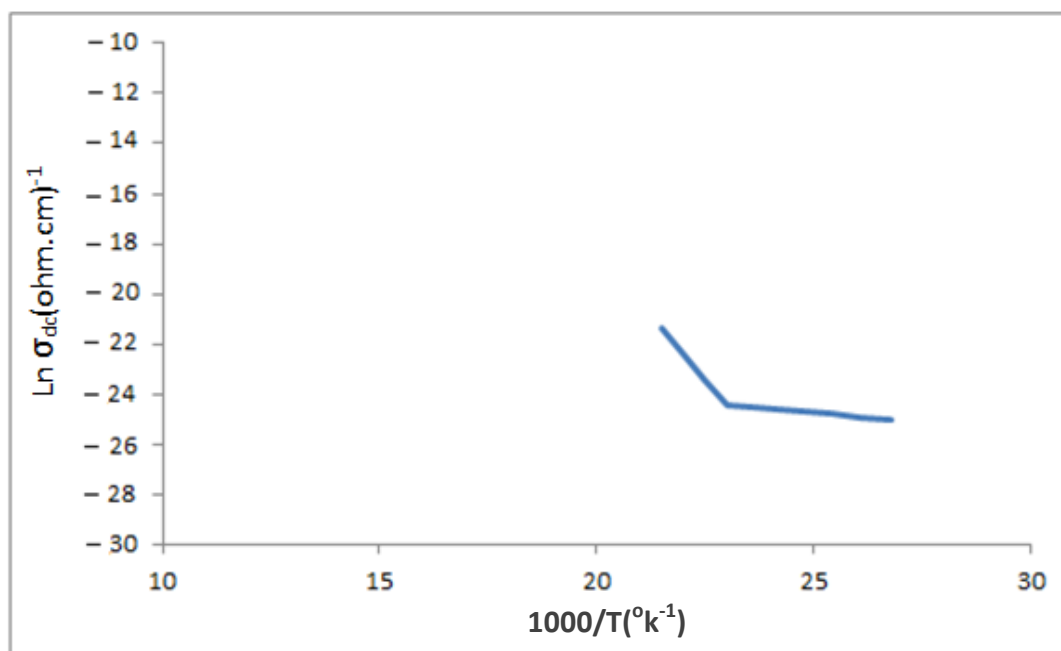
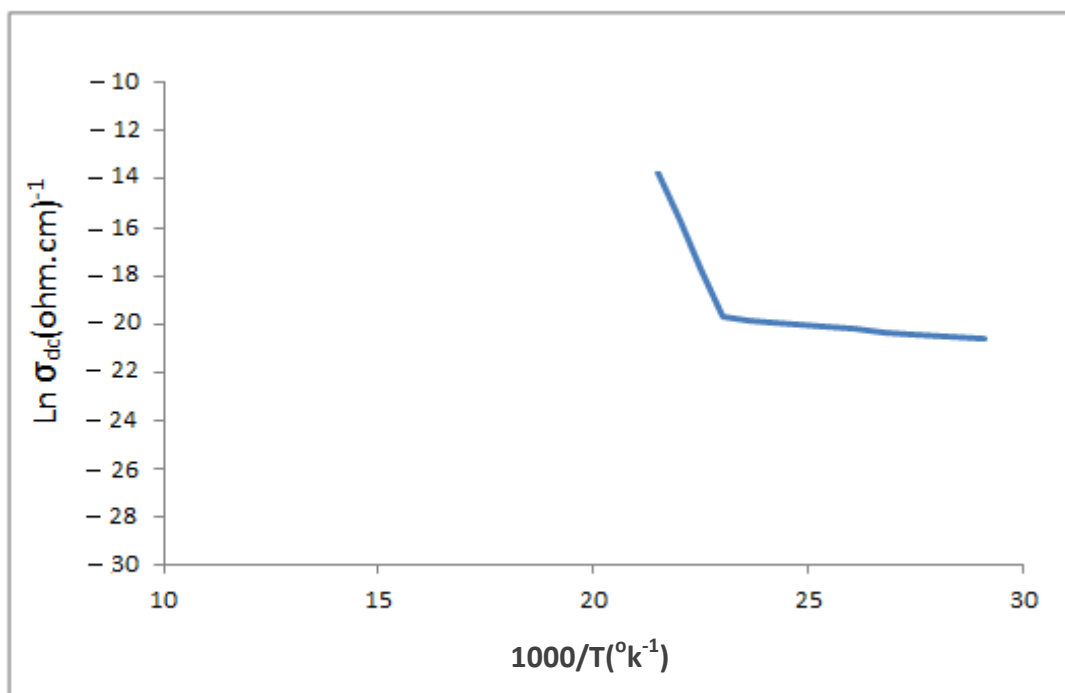
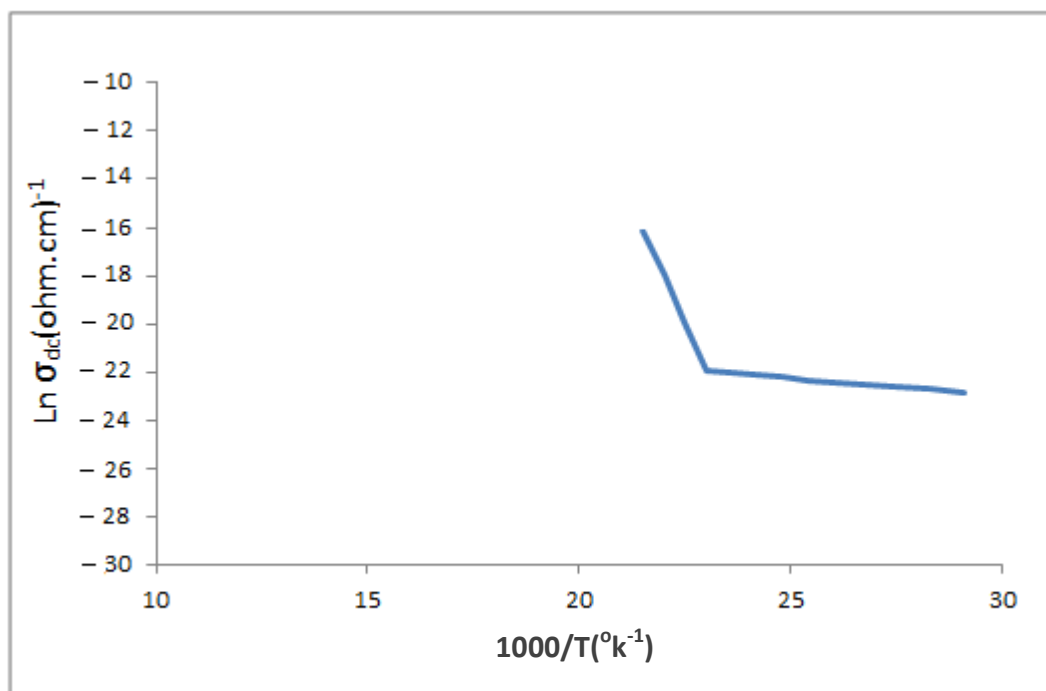


Figure (7): The variation of  $\ln\sigma_{dc}$  with reciprocal temperature for legend.



**Figure (8): The variation of  $\ln\sigma_{dc}$  with reciprocal temperature for complex(1).**



**Figure (9): The variation of  $\ln\sigma_{dc}$  with reciprocal temperature for complex(2).**

The values of ( $E_{act.1}$ ) ( $E_{act.2}$ ) obtained by selecting slope of a better line for these curves and use equation (5) , values of ( $E_{act.1}$ ) ( $E_{act.2}$ ) recorded in table (2).

**Table(2): Values of activation energy of compounds.**

Compound	Activation Energy (eV)	
	( $E_{act.1}$ ) for temp (343-393) <sup>o</sup> K	( $E_{act.2}$ ) for temp (403-463) <sup>o</sup> K
Legand	0.48	2.01
Complex (1)	0.93	4.22
Complex (2)	0.82	3.86

at low temperature occuring the first activation energy (  $E_{act.1}$  ) and its values vary between (0.48-0.93) eV are attributed to the hopping processes , while at high temperature occuring ( $E_{act.2}$ ) by the charge transmit because of the thermal excitation of the carriers at the grain boundaries, and its values ranged from (2.01 - 4.22) eV where reduced with increasing double bond conjugation in compounds prepared. in general the results agree with the source [11].

### **Conclusions:**

- 1- From studying the texture of compounds (legand and complexes) by a polarized optical microscope, it was observed that it exhibited nematic liquid crystal mesophases (enantiotropic)
- 2- From studying the electric conductivity  $A_c$  and  $D_c$  of the prepared compounds, it was found that organic semiconductors and it has low electrical conductivity, while their conductivity was improved by complexity and increased with the rise of temperatures.
- 3- All charge transfer for complex (1) and complex (1) show reduced in values of (  $E_{act.1}$  ) and ( $E_{act.2}$ ) comparing with that of either components.

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