Electrical and structural properties of isomers aromatic compounds

[1]Mohammed Khalil Ibrahim [2]Assis. prof. Dr. Zeyad Adnan Saleh

Mustansiriyah University, College of Sciences, Department of Physics.

[1]mm 1986320 @ gmail.com [2]zeyad_saleh 1958 @ yahoo.com

Abstract

Electrical and structural properties of the (anthracene and phenanthrene)compounds dissolved in non-polar solvent (cyclohexane)were measured and study in concentration [10^{-2}M].

The study showed of electrical properties of anthracene and phenanthrene that the both compounds are semiconductors and electrical conductivity of phenanthrene is higher than anthracene.

As well as, the study showed structure (anthracene and phenanthrene)thin films were analyzed by (XRD). For anthracene, X-ray diffraction spectrum appears two sharp peaks and three small peaks, while phenanthrene shows X-ray diffraction spectrum appears two sharp peaks and four small peaks . It means that the thin films of (anthracene and phenanthrene) is polycrystalline in nature structure.

الخصائص الكهربائية والتركيبية للمركبات الاروماتية الايزوميرية

محمد خليل ابراهيم أ.م.د .زياد عدنان صالح

الجامعة المستنصرية , كلية العلوم , قسم الفيزياء

الخلاصة

تم قياس ودراسة الخصائص الكهربائية و التركيبية لمركبات (الانثراسين والفينانثرين) المذابة في المذيب الغير قطبي(السايكلوهكسان) وبتركيز [10^{-2} M].

يتبين من خلال دراستنا للخصائص الكهربائية والتوصيلية الكهربائية للانثراسين والفينانثرين ان كلا المركبين اشباه موصلات والتوصيلية الكهربائية للفينانثرين اعلى من الانثراسين.

وكذلك يتبين من خلال دراستنا تركيب الاغشية الرقيقة للانثراسين والفينانثرين والتي حللت

بواسطة جهاز (XRD). بالنسبة للانثراسين يظهر طيف حيود الاشعة السينية قمتين حاده وثلاث قمم صغيرة، بينما الفينانثرين يظهر طيف حيود الاشعة السينية قمتين حاده واربع قمم صغيرة . وهذا يعني لنا ان الاغشية الرقيقة(للانثراسين والفينانثرين) ذات طبيعة تركيبية متعددة التبلور.

1. Introduction

This study concentrate the aromatic molecules , because these molecules important in industry .

The aromatic materials are organic compounds which have rings groups in their structure. The benzene ring is the simplest types of aromatic compounds consisting of six carbon atoms and six hydrogen atoms. In the aromatic series, benzene is recognized as the origin compound . [1]

Isomers are compounds that have the same molecular formula but are structurally different. Therefore, isomers contain the same number of atoms per element, but the atomic order is different. Although there is a molecular formula same, the physical properties of each molecule may vary . Isomerism is the process by which one molecule is converted into another molecule with similar atoms. This may occur automatically or by a reaction may be required to achieve this effect. Example of isomeric aromatic compounds such as (anthracene , phenanthrene). [2]

In previous studies for the (anthracene and phenanthrene) compounds such as in(1963),J.Trotter, study structural properties of phenanthrene. He found phenanthrene structure is multi-crystalline (Polycrystalline)and structure(monoclinic)[3]. In (1964) , S. Matsumoto and T. Tsukada, electrical properties of (anthracene and phenanthrene) were studied. They found that although anthracene is an isomer of phenanthrene, but the electrical properties of the two compounds are different [4]. In(2013) , Hongya wu and Ji zhou ,they were studied

structural properties of anthacene . They found structure was multi-crystalline (Polycrystalline) and structure (monoclinic). [5].

2. Experimental Part:

2.1 Materials

The anthracene (AN) and phenanthrene (PH) compounds dissolved in the solvent (cyclohexane). (AN, PH) prepared with concentration [10^{-2}M] , at room temperature. (AN) purchased from Sigma-Aldrich company and (PH) purchased from british drug houses company in England. These are of the polycyclic aromatic hydrocarbons and also considered an organic semiconductors.

Anthracene **Phenanthrene**

$C_{14}H_{10}$ **$C_{14}H_{10}$**

Figure (1): chemical composition of compounds

2.2 Preparation of solutions:

Solutions were prepared using the following relationship: [6]

$$\mathbf{W} = \frac{[\mathbf{M}]\times\mathbf{V}\times\mathbf{M.W}}{\mathbf{1000}} \quad \text{.....(1)}$$

where:

W: the weight of material in gm.

M.W: molecular weight gm/mol.

[M]: molar concentration (mol/L)

V: the volume of solvent used to dissolve the material in ml.

The prepared solutions were diluted according to the following equation: [6]

$[M]_1V_1 = [M]_2V_2$……………………………………….. (2)

where:

$[M]_1$: primary concentration

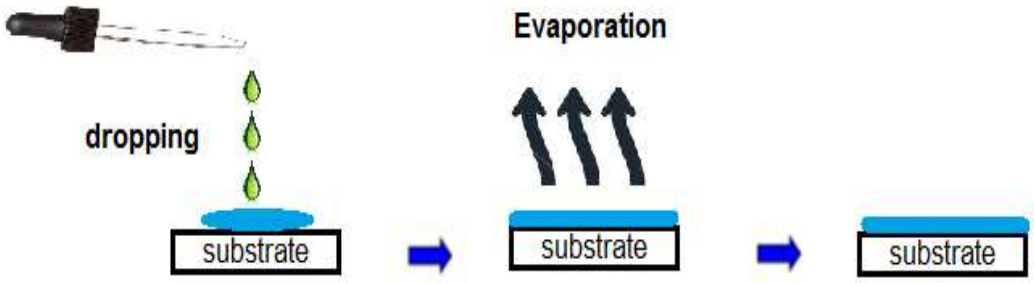
$[M]_2$: new concentration

V_1: the volume before dilution

V_2: the volume after dilution.

2.3 Thin Films Preparation

Anthracene and phenanthrene thin films was deposited on quartz substrates , each of ($2×2.5cm^2$) area, were used as substrates. Thin films of (anthracene and phenanthrene) were prepared using drop-casting method . In this method , a solution with a suitable concentration is prepared by dissolving several milligrams of anthracene and phenanthrene in the cyclohexane solvent. Several drops of it were transported by piptte on a substrate of clean good quartz. It is necessary to place the substrate horizontally to ensure the spread of the thin layer of solution on the entire surface of the substrate and then cover the substrate to reduce the rate of evaporation and to obtain the thickness of thin and crystalline models homogeneous and must avoid any material that can melt in the solvent, because it melts any other substance that affects the purity of the made.



Figure(2): drop-casting method dropping of solution and spontaneous solvent evaporation.

2.4 Thin Films Examination

After the thin films deposition is to choose the best thin films prepared from terms of homogeneity and their surfaces are smooth. They are free of stains and carrots (thin films-free places) and the absence of cracks of the thin films. Is to know the homogeneity of the thin films by optical microscope.

2. 5 The Films Thickness Measurements:

1.The Weight Method:

Thickness is one of the most important thin film parameters since it largely determines the properties of the film .This method is an approximated used to obtain the thickness of the thin films.

The was measured the weight of the quartz substrate before film deposition and after the film deposited over the quartz substrate. The difference(Δm) in weight represented the weight of the film. The thickness can be obtained using the mass law:-

$$t = \frac{\Delta m}{\rho\, d} \quad \text{……..……..(3)}$$

Where ρ is the density of the material used, (d) is the area of substrate for the film.

2.6 D.C Electrical Conductivity Measurements:

It continuous electrical conductivity has measured after the deposition of aluminum poles on the thin films, and then changing of thin film resistance with temperature by using the electrical circuit as shown in figure (3).

The sample was put in an oven heat (GRIFFIN INCUBATOR). After connecting the poles of aluminum deposited on the thin film with wires connect to the ends of device (Keithly 616 Digital Electrometer) to measure changes in resistance thin film with temperature change.

That are measured through wired thermal double , and are recorded resistant thin film for every (10˚) from room temperature (20˚C) to a temperature (120 ˚C).

electrical conductivity (σ_{dc}) is calculated from relation [7]:

$$\sigma_{dc} = 1/\rho_o = L / R_e\ b\ t \quad \text{……..……..……(4)}$$

Where:

ρ_o : Resistivity (Ω.cm).

R_e: Thin film resistance.

b : Width electrode (cm).

L : The distance between the electrodes of aluminum (cm).

t : Thin film thickness (cm)

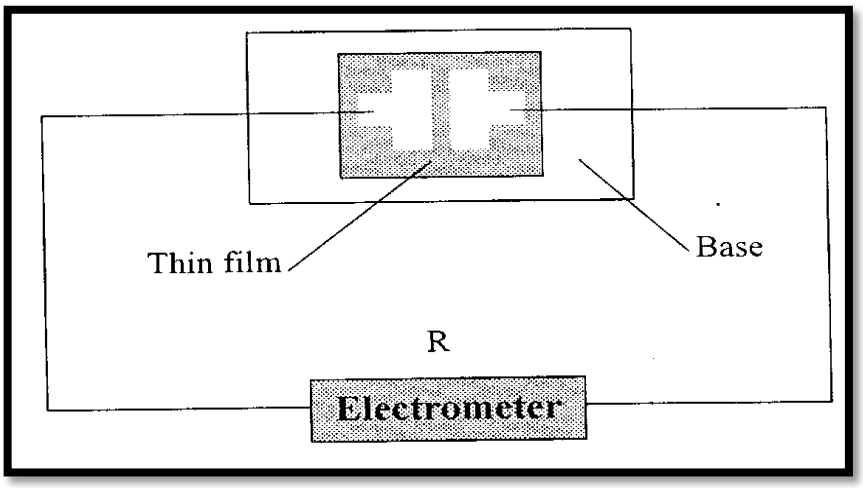


Figure (3) :Electrical circuit used to measure the electrical continuing conductivity [7].

2.7 X-ray Diffraction (XRD) Measurements:

The crystalline structure for any material can be known by studying the phase of (XRD) for that material, when a beam of (XRD) from mono wavelength falling on film surface, will show peaks on limited angels for each material because of reflected of Bragg diffraction on parallel crystalline surface. XRD device is of type (LabX XRD 6000 SHIMADZU XR – Diffractometer) made in Japan .

3. Results and Discussions:

3.1 D.C Electrical Conductivity

The conductivity of the film depends upon several factors such as the preparation technique, the temperature and the measurement conditions. The electrical conductivity $\sigma_{d.c}$ for (anthracene and phenanthrene)films had been measured at a temperature range (20-120 °c) from the reciprocal values of the resistivity (ρ). The resistivity (ρ) was calculated from equation (4). The calculated values of σ_{dc} and the resistivity (ρ) of (anthracene and phenanthrene)films are given in table (1).

Table (1) : Electrical conductivity σ_{dc} and resistivity (ρ) at room temperature .

compound	T °c	R Ω	ρ Ω.cm	σ(Ω.cm) $^{-1}$
Anthracene	50	$8.15*10^{9}$	$20.78*10^{5}$	$0.4*10^{-6}$
	70	$1.98*10^{8}$	$5.04*10^{5}$	$0.1*10^{-5}$
Phenanthrene	50	$7.35*10^{9}$	$27.56*10^{5}$	$0.5*10^{-6}$
	70	$3.84*10^{8}$	$14.4*10^{5}$	$0.6*10^{-5}$

It has been noticed in general in all films from data in table (1) , that the resistivity (ρ) decreases as the temperature degree increases, as well as , can observe that the temperature degree increase will lead reduce resistance. Also ,when the conductivity increases the resistance will reduce and the values of conductivity increases with increasing

temperature . The increasing temperature degree leads to increase the number of pairs electron–hole, i.e the increasing conductivity and this is the general characteristics of semiconductor . This is agreement with[8] . Also ,it is observed the electrical conductivity of phenanthrene is higher than anthracene.

3.2 Structural properties:

The structure of (anthracene and phenanthrene)films were analyzed by a LabX XRD 6000 SHIMADZU XR – Diffractometer with Cu Kα radiation of (voltage 40 kV, current 30 mA, scanning speed = 8°/min), diffraction pattern was obtained with 2θ starting from 10° to 60°.

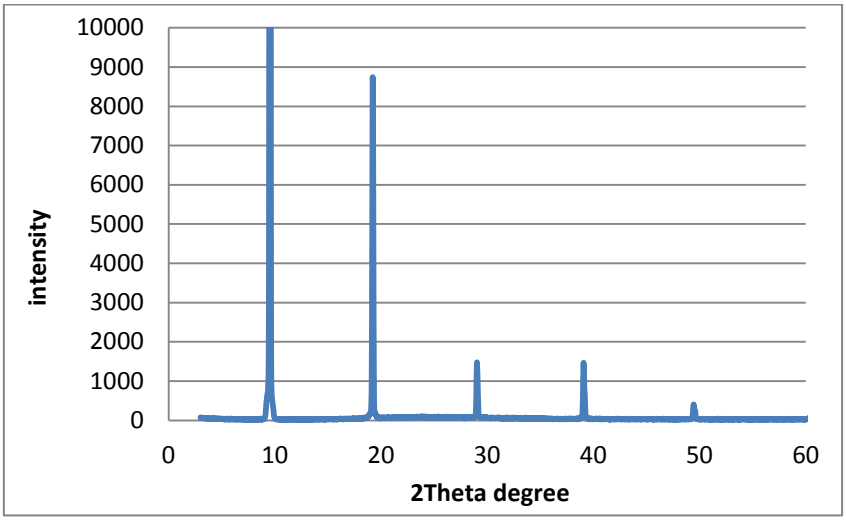


Figure (4) XRD anthracene

In deposited anthracene thin films, figure (4) represented the X–ray diffraction spectrum of anthracene is possess two sharp and three small peaks. It means that the film is polycrystalline in nature structure.

The results shows of examination X-ray (XRD) the nature of the crystal structure of thin films anthracene on the substrate of quartz. They have structure multi-crystalline (Polycrystalline) and structure (monoclinic) . This is agreement with [5].

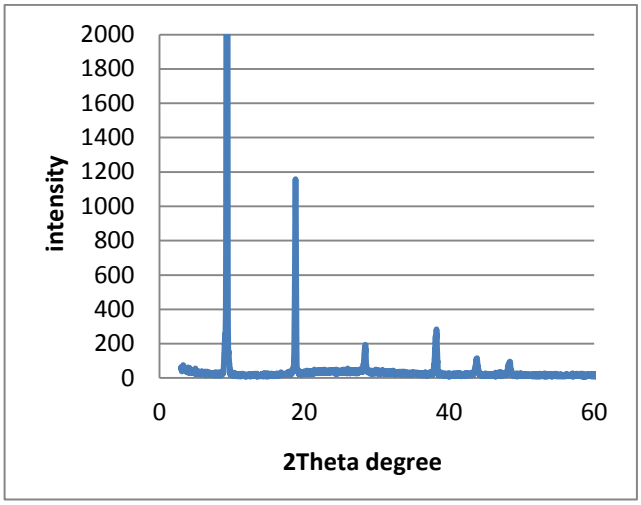


Figure (5) XRD phenanthrene

Also, deposited phenanthrene thin films ,the X–ray diffraction spectrum of phenanthrene was shows in figure(5), possess two sharp and four small peaks. It means that the film is polycrystalline in nature structure.

The results of examination X-ray (XRD) shows the nature of the crystal structure of thin films phenanthrene on the substrate of quartz. They have structure multi-crystalline (Polycrystalline) and structure (monoclinic). This is agreement with [9].

4. Conclusion:

1. A study showed of electrical properties of the two compounds (anthracene and phenethrene) are semiconductors and although anthracene is an isomer of phenanthrene, but the electrical properties of the two compounds are different.

2. The crystal structure of thin films (anthracene and phenanthrene) on the substrate of quartz. They have structure multi- crystalline (Polycrystalline) and structure (monoclinic) and anthracene have two sharp peaks and three small peaks, while phenanthrene have two sharp and four small peaks.

5. References:

1- Carey, F. A., "Organic Chemistry" 4th ed., McGraw-Hill, New York, (2000).

2- Bruice P. Y., " organic chemistry " 4th Edition, pearsons prentice Hall,(2004).

3- J.Trotter " The crystal and molecular stracture of phenanthrene " Acta cryst ,(1963).16.605 .

4- S. Matsumoto and T. Tsukada " Semiconductivity of Phenanthrene Single Crystals " Received June 6, (1964).

5- Hongya wu and Ji zhou " Optical properties of anthracene single crystales Grown by A simple solution technique" Journal of modern Physics B Vol. 27, No. 8 (2013).

6- S. M. sundaram, S. Parthiban, U. R. Pisipaty, G. Madhurambal and S. C. Mojumdar, "Effect of anthracene doping on potassium hydrogen phthalate crystals" Journal of Thermal Analysis and Calorimetry , vol. 100, No. 3, p.p. (821-826(6)), (2010).

7- K. L. Chopra, "Thin Films phenomena", Mc Graw-Hill, New York, (1969).

8- R. Schroeder, "characterization of organic and inorganic optoelectronic semiconductor devices using advanced spectroscopic methods", the Virginia Polytechnic Institute and State University , USA, (2001).

9- S. Ding, Q.Yin, W. Du, X. Sun, G.Li, Y. Mao and H. Hao," Ternary phase diagram of phenanthrene and carbazole in different solvents and its application in the separation of them " , J. Chem. Thermodynamics (2018).