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Investigating the Characteristics and Performance of (Organic Material - Metal Oxides) Nanocomposites for Modern Applications

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

((أقْرَأْ باْسمِ رَبِّكَ ٱلَّذِي خَلَقَ ﴿١﴾

خَلَقَ الإِنسَانَ مِنْ عَلَقٍ ﴿٢﴾

أقْراء وَرَبُّكَ الأَكرَمُ ﴿٣﴾ ٱلَّذِي عَلَّمَ بِاْلقَلَمِ ﴿٤﴾

عَلَّمَ الإِنسَانَ مَا لَمْ يَعْلَم" ﴿٥﴾))

صَدَقَ اللهُ العَظِيم

سورة العلق ١– ٥

DEDICATION

To my first and last credit my father and mother

To my esteemed supervisors Dr. Ahmed Hashim

And to everyone who helped me even with a word.

Ola··· ✍

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The first thank to *my God* for helping to complete my study

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Ola... ✍

SUMMARY

The nanocomposites of [Poly (methyl methacrylate)/ Silicon dioxide-Cerium dioxide) were prepared by casting method with different concentrations of SiO_2 and CeO_2 nanoparticles to study the structure, optical and electrical properties of nanocomposites for antibacterial application. The structural properties were studied that include Optical Microscope (OM), Scanning Electron Microscope (SEM), and Fourier Transforms Infra-Red (FT-IR). The optical microscopy images showed that with increasing concentrations of nanoparticles network paths are formed inside the polymeric matrix that act as charge carriers. And SEM measurement results showed a good distribution and homogeneous in surface morphology. The results of FT-IR indicate to a physical interference between the polymer matrix and nanoparticles. While results of optical properties for ($PMMA/SiO_2$-CeO_2) nanocomposite showed that the absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants, as well as optical conductivity increases with increasing in the concentrations of SiO_2 and CeO_2 nanoparticles, while the energy gap and transmittance decrease with increasing concentrations of nanoparticles. It also indicated that the highest absorption of spectrum happened in U.V region. The results of electrical properties of nanocomposites showed that the dielectric constant and dielectric loss increase with increasing concentrations of nanoparticles and decrease with increasing frequency of applied electric field. while the A.C electrical conductivity increases with increasing the frequency and weight concentrations of (SiO_2-CeO_2) nanoparticles . The results of applications of ($PMMA/SiO_2$-CeO_2) nanocomposites against bacteria showed that the inhibition diameter zone increases with increasing concentrations of nanoparticles.

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List of Abbreviations

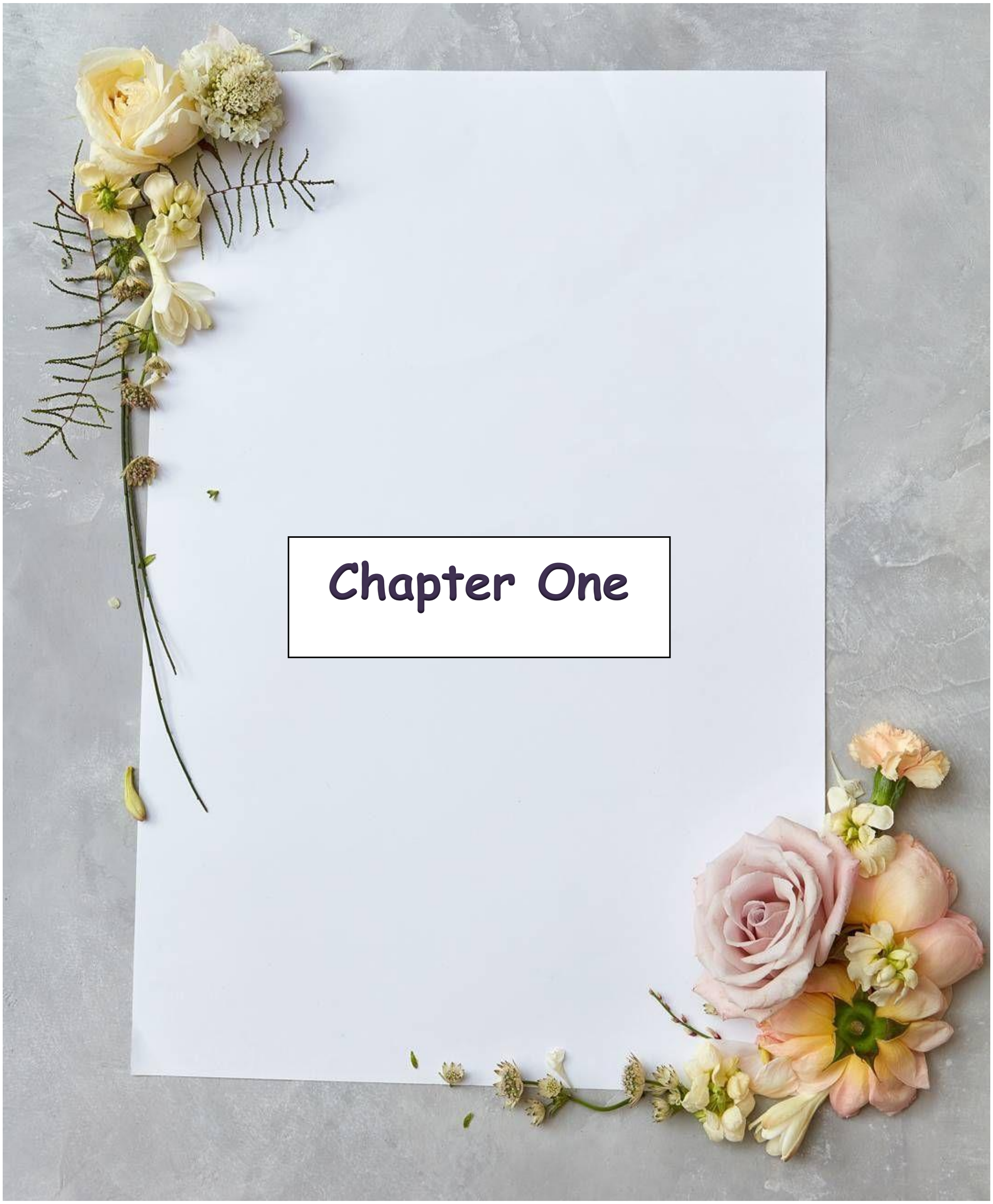
Abbreviation	Physical Meaning
PMMA	**Poly (methyl methacrylate) polymer**
SiO_2	**Silicon dioxide**
CeO_2	**Cerium dioxide**
FTIR	**Fourier Transform Infrared Radiation**
OM	**Optical Microscope**
SEM	**Scanning Electron Microscope**
V.B	**Valance band**
C.B	**Conduction band**
A.C	**Alternative current**

List of Symbols

Symbol	Physical Meaning
A	Absorbance
B_o	Constant depend on type of material
C	Velocity of light
C_o	Capacitance in vacuum
C_p	Capacitance in parallel
D	Dispersion factor
E_g	Energy gap
E_{Phonon}	Energy of phonon
E_{Ph}	Energy of photon
ε'	Dielectric constant
ε''	Dielectric loss
ε_o	Permittivity in vacuum
h	Blank constant
I_A	Intensity of absorbed light

I_O	**intensity of original radiation**
I_T	**Intensity of transmittance ray**
j	**Imaginary number**
k	**Extinction coefficient**
K	**Wave vector**
n	**Refractive index**
R	**Reflection**
r	**Exponential coefficient**
T	**Transmittance**
t	**Thickness of the film**
v	**Velocity of light**
α	**Absorbance coefficient**
ε^*	**Complex permittivity**
ε_1	**Real dielectric constant**
ε_2	**Imaginary dielectric constant**
ε_a	**Real part of complex permittivity**
ε_b	**Imaginary part of complex permittivity**

λ	**Wavelength**
$\sigma_{A.C}$	**Alternating current conductivity**
σ_{op}	**Optical conductivity**
ω	**Angular frequency**
ν	**Frequency**



Chapter One

1.1 Introduction

Polymers are materials consist of many small molecules, these macromolecules may be linear, branched, or highly network[1]. The small molecules used as the building blocks for these larger molecules are known as monomers. Monomers are small molecules can be joined together in a repetitive The process by manner to form more complex molecules called polymers[2]. which monomers are transformed into a polymer is called polymerization[3]. The polymerization process is the process that allows a simple low molecular weight compound to combine and form a high molecular weight complex .The Polymerization process can be classified into two types: condensation polymerization and addition polymerization[4,5]. Polymers can be divided into two categories according to their sources: natural and synthetic, natural polymers include proteins, cellulose, and rubber, while synthetic polymers include nylon, polypropylene, polyester, polycarbonate, and etc.[6]. The nanoparticle includes these particles have different ,particles having size between 1 and 100 nm properties at their atomic level due to their size[7]. Can applied these particles in different fields such as pharmaceutical, nanoelectronics, and cosmetic[8]. The field of nanotechnology is one of the most popular areas of current research and development for basically all technical disciplines, and this obviously includes polymer science and technology[9]. Evan before nanotechnology was recognized as a new scientific field, work on the manufacture and production of nanomaterials and nanostructures began a long time ago[10]. Due to rapid technological advancements, some components currently used in manufacturing have to be replaced with new materials with improved specifications; as a result, studies of electrical and optical properties of polymers have gotten a lot of attention in recent years due to their usage in electronic and optical devices[11,12].

1.2 Polymer Structure

The physical properties of polymer materials depend on the molecular weight and the shape of it as well as on the molecular structure[13]. Polymers are classified according to their chemical composition into three main types (linear ,branched and cross-linking Polymers). Linear polymers these polymers have a linear structure and are generally thermoplastic polymers, the basic of these polymers is a single molecular chain of a certain length connected to each other in a linear form and with the exception of materials with very high molecular weight, they are soluble in solvents. As for the branched polymers, there are branches that arise from the original polymer chain. Branching may result in several physical properties in the polymer such as lower solubility in solvents, higher softening point and also lower properties of thermoplastics and the last type is crosslinked polymers. These polymers have a three-dimensional network structure where chemical bonds are intertwined with each other in a complex manner[14,5].

1.2.1 Classification of polymers according to thermal response

a. Thermoplastic Polymers:

When the temperature increases, these materials becomes elastic and sticky because these molecules in thermoplastic polymers are bound by relatively weak intermolecular forces (Vander - Waals forces), and when lowered they return to their original state. When these molecules heated slide over each other as in polystyrene, polyethylene, polypropylene and polyvinyl alcohol[15]. The polymer chains associate by intermolecular forces, which weaken rapidly with increased temperature yielding a viscous liquid. In this state, thermoplastics may be reshaped[16].

b. Thermosetting Polymers:

Thermosetting polymers (inflexible to heat) are polymers that if exposed to heat experience irreversible reactions, and therefore exposure to heat or pressure does not cause them to soften because heat leads to chemical crosslinking and obtaining thermal hardening, and thus it cannot be returned to its original position. Reversed, whether by heat or cooling[17]. The molecules in this type of polymers are linked by strong covalent bonds, which leads to the formation of polymeric chains with a three-dimensional network structure. Continues of reaction for a longer period of time polymer begins to harden gradually[18].

1.2.2 Classification of polymers according to source

a. Natural polymer: natural polymers refer to polymers they come from nature (plants or animals). It mainly includes carbohydrates and proteins found in plants and animals that primarily provide structural support[19].

b. Synthetic polymer: they are man-made polymers, which can be classified into four main categories: thermoplastics, thermoplastic elastomers, elastomers and synthetic fibers. They are commonly found in a variety of consumer products such as money, glue, etc.[20].

1.2.3 Classification of polymers according to homogeneity

Polymers are classified depending on the homogeneity qof repeating units in to [21,18]:

a. Homo polymers: it is a polymer that consists of the same unit of basic building blocks (monomers), an example of which is polyethylene.

b. Copolymers: when the building blocks of a polymer are more than one type, as in the polymer (styrene – butadiene).

c. Composite polymers: itis the process of adding some material to homogeneous polymers in order to change in some of its characteristics and the entering of new recipes on it[21,18]. Matrix (the base material) and additives are the two basic components of the compound. The additives coat the other ingredients and make them more viscous[22].

1.3 Nanocomposites and their Applications

Nanocomposites are materials in which at least one of the phases has nanoscale dimensions[23]. Their capabilities are so promising that they may be used in a wide range of applications from packaging to biomedicine[24]. Polymer nanocomposites have gotten a lot of attention in academia and industry over the last few decades and they've become a key component in the development of novel advanced materials for a variety of applications including electrical engineering[25]. Nanotechnology is a new science that has developed in which it has been observed that materials exhibit significantly different properties at nanometer sizes compared to properties of the same material at larger particle sizes[26]. Nanotechnology is an emerging multidisciplinary technology that has flourished in many fields during the last decade, including science materials, mechanics, electronics, optics, medicine, plastics, energy and aerospace[27]. Some of the potential applications of nanotechnology are as follows[28]:

1. Nanocomposites and thin film protective coatings for structural and electronic applications.
2. Mini PCs and Non-Volatile Memory.
3. Miniature thin-film photovoltaic solar cells for cost-effective power generation for applications ranging from the laptop to the automobile.
4. Faster, smaller and more efficient semiconductor and microprocessor.

5. Anti-bacterial dressings and coatings

1.4 Nanomedicines Applications

Nanotechnology has opened new horizons in various fields of life, the most important of which is the field of medicine, it is worth noting that nanotechnology depends on physics, chemistry, engineering and biology and pharmacy, so researchers must have a broad base that includes all these disciplines. Nanotechnology has changed the way Looking at the treatment of many diseases and gave great hopes for the cure of many incurable diseases. Nanotechnology promises many medical applications related to accurate diagnosis and high treatment efficiency facing the most deadly diseases human diseases such as cancer will be possible within the next ten years from through nanomedicine[29]. Figure (1.1) shows some nanomaterial commonly used in medicine[30]. Nanomedicine is a rapidly growing area of medical research that is focused on developing nanoparticles (NPs) for prophylactic, diagnostic, and therapeutic applications.1 The unique properties of nanomedicines offer potential solutions for many of the current challenges in treating cancer, cardiovascular, and neuodegenerative diseases, as well as other illnesses.[31,32]. Many nanomedicines and nanodiagnostics are already FDA-approved and on the market, and many more are in clinical trials. Currently, the most active areas of nanomedical research and product development are in cancer treatments, imaging contrast agents, and biomarker detection. Although many nanotherapeutics and nanodiagnostics are already in use, there are many barriers that impede bringing nanomedical products to market[33,34].

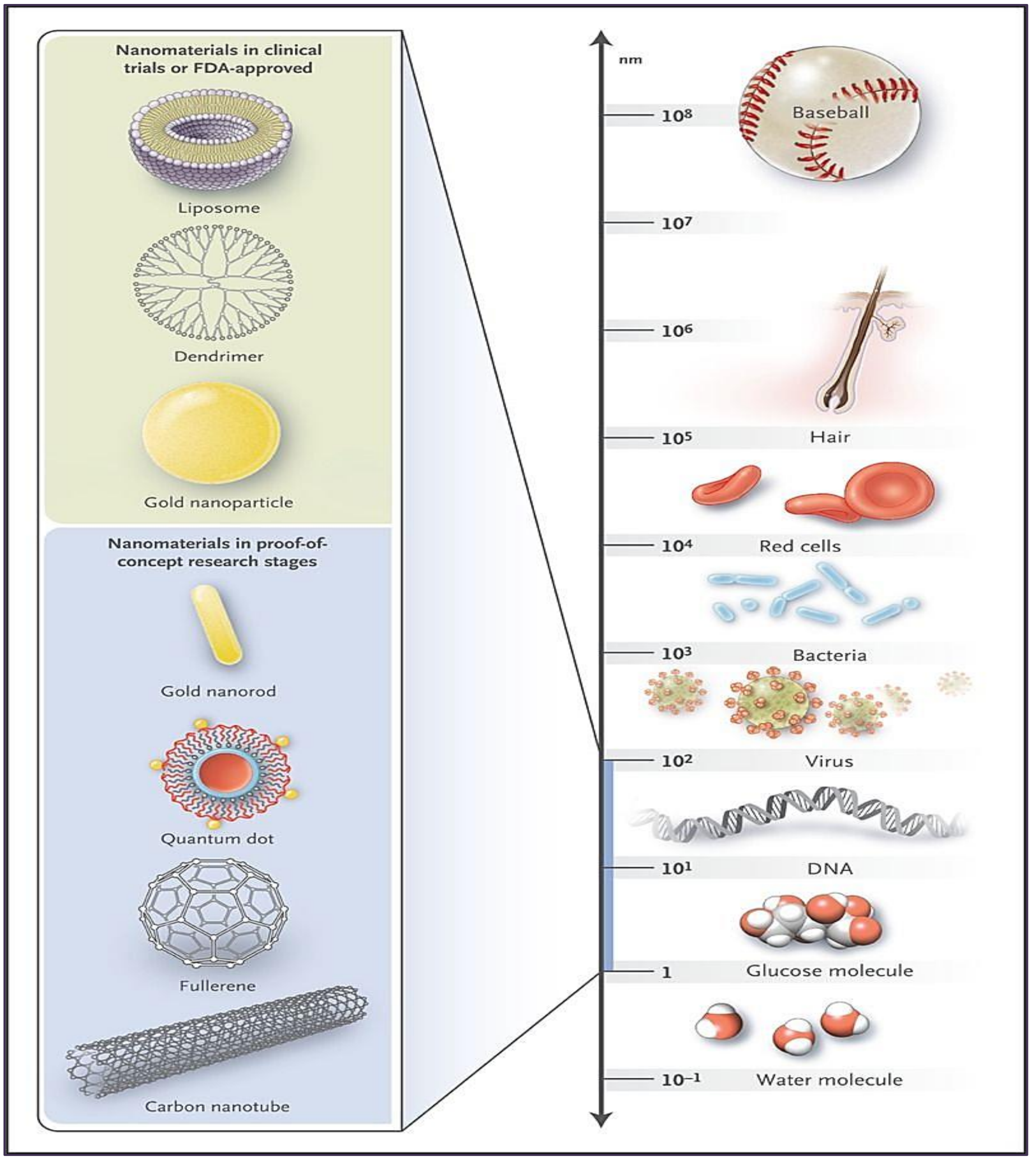


Figure (1.1): Some nanomaterials commonly used in medicine[30]

1.5 Poly methacrylate (PMMA) and its Properties

PMMA is one of the oldest and most popular polymers. This material is one of the toughest polymers, a clear glassy with a glossy finish and good weather resistance[35]. PMMA is an important and interesting polymer due to the attractive physical and optical properties crucial to its wide applications. This is a thermoplastic material with good tensile strength and toughness, transparency, good insulation properties and thermal stability[36]. Figure(1.2) show molecular formula of PMMA[37].

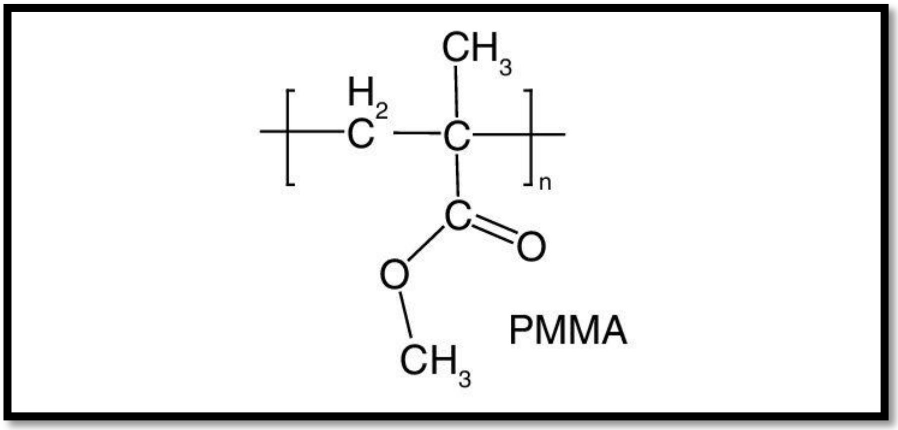


Figure (1.2): Molecular formula of PMMA[37]

Table (1.1): The most important properties of PMMA polymer[38]

Parameters	PMMA
Chemical formula	$CH_2=C(CH_3)COOH_3$
Tg (K)	106 ^{o}c
Refractive index	1.49
Density (g/cm^3)	1.2 g/cm^3
Melting point	213^{o}c

1.6 Silicon Dioxide (SiO_2) Nanoparticles and its Properties

Silicon dioxide or silica is a silicon oxide with the chemical formula SiO_2 and the most common in nature as quartz[39]. It has many forms, but all forms of silica are identical in chemical composition, but with different atomic arrangements. All forms of silica are odorless solids composed of silicon and oxygen atoms. Silica particles become suspended in the air and form non-explosive dust. Table (1.2) show some properties of nanomaterial SiO_2[40].

Table (1.2) : Some properties of SiO_2[40]

Chemical formula	SiO_2
Mole mass	60.8 g/mol
Appearance	Transparent solid (Amorphous) White/whitish Yellow (Powder/Sand)
Density	2.648 (α-quartz), 2.196 (amrophous) $g.cm^{-3}$
Boiling point	2950 °C
Refractive index	1.544

1.7 Cerium Dioxide Nanoparticels (CeO_2)

Cerium oxide is an oxide of a rare earth mineral in the form apale yellow powder with the chemical formula (CeO_2)[41]. Cerium oxide (CeO_2), also known as ceria is used in many technological applications[42]. In the past ten years there has been significant and growing research interest in cerium oxide nanoparticles for its distinctive catalytic properties such as electronic applications and useed it in a wide range of applications in biomedicine, biotechnology, and agriculture[43].

1.8 Literature Review

(M.Abdul-Muhsien *et al.*) in 2010[44], prepared the composite of (PMMA/ TiO_2) with different weight percentages of TiO_2 mamoparticels. The effect of addition of TiO_2 on some optical properties of PMMA has been studied in the wavelengths (from 300 to 850) nm. The extinction coefficient, absorption coefficient, and energy gap of the indirect allowed and forbidden transition have been determined. Results showed that the extinction coefficient and absorption coefficient increase while the energy gap of the indirect allowed and forbidden transition decreases with the wight ratios of TiO_2.

(H. Bahaa) in 2011[45], studied the A.C electrical properties of (PMMA –Al2O3) composites. He found the A.C electrical conductivity of PMMA-Al2O3 composites is increasing with the increasing of the frequency of applied electrical field and Al2O3wt.% content.

(**S. Devikala *et al.***) in 2013 [46], investigated the electrical properties of PMMA-ZrO_2 with a frequency ranging from 50 Hz to 1 MHz. The results were showed that the dielectric constant, dielectric loss and electrical conductivity of AC increased with the increasing of ZrO_2 nanoparticles.

(R. G. Kadhim) in 2015 [47], has studied the effect of TiO_2 nanoparticles on the electrical properties of PMMA polymer. Samples were prepared by using casting method with weight percentages of TiO_2 were (0, 3, 5, 7) wt.%. The results showed that the dielectric constant, dielectric loss, and alternating currwent electrical conductivity of the nanocomposite (PMMA-TiO_2) increase with increasing concentrations of nanoparticles (TiO_2).

(G. Soni *et al.*) in 2018 [48], have fabricated thin films composed of PMMA polymer doped with SiO_2 ,with a thickness of 60 microns using the solution casting method, then they tested the effect of adding nanoparticles on the electrical and structural properties of the thin films. The optical bandgap it was observed that it decreased with increasing concentration of SiO_2 nanoparticles.

(D. Nayak and R. B. Choudhary) in 2019 [49], have studied the optical and electrical properties of PMMA-ZnS nanocomposite. The morphological structure indicated that the nanocomposite was well mixed. For the optical properties obsorved that the energy gap got to a low value (~3.30) with increasing concentractions of ZnS. The dielectric properties of PMMA-ZnS showed a high dielectric constant and high electrical conductivity with increasing the frequencey. The high value of the singlet constant and the decrease in the optical bandgap with increasing conductivity confirmed that it could be used of PMMA-ZnS nanocomposite as an emissive layer in OLED devices.

(S. S. Chiad *et al.*) in 2019 [50], have prepared PMMA films by casting method with various different concentrations of InCl3 (2,4%). It was found that the optical bandgap that determined by using U.V visible spectrophotometer decreased from 3.849 eV of pure PMMA films to 3.230 eV of PMMA at percentage wieght 4 wt.% from $InCl_3$.

(T. S. Soliman and S. A. Vshivkov) in 2019 [51], have Prepared Polyvinyl alcohol (PVA) nanocomposites films and doped with iron (Fe) nanoparticles via solution casting technique. The effect of iron nanoparticles on the optical properties of PVA by using UV-visible spectroscopy. It was found that the refractive index and extinction index of nanocomposites are increased compared to those made of pure PVA. Also, it is observed that the photoconductivity increases with increasing concentration of nanoparticles.

(M. Bafna *et al.*) in 2019 [52] , have studied the variation in optical parameters that occurs when added K_2CrO_4 nanoparticels to polymer PMMA, they added potassium chromate at different weight ratios to the PMMA polymer by solution casting method. The data obtained for films in the wavelength range (300-1100) nm. The optical results showed the absorption coefficient, extinction index, refractive index and real and imaginary of the dielectric constant improvement when potassium chromate was added.

(G. Soni *et al.*) in 2020 [53] , have studied the effect of a mixture of ZnO and SiO_2 nanoparticles on the optical properties of the composite thin film PMMA/ZnO/SiO_2, with a thickness of 50 μm by solution casting method and they observed that the optical bandgap of the composite thin films decreases with increasing concentration of zinc oxide and silica.

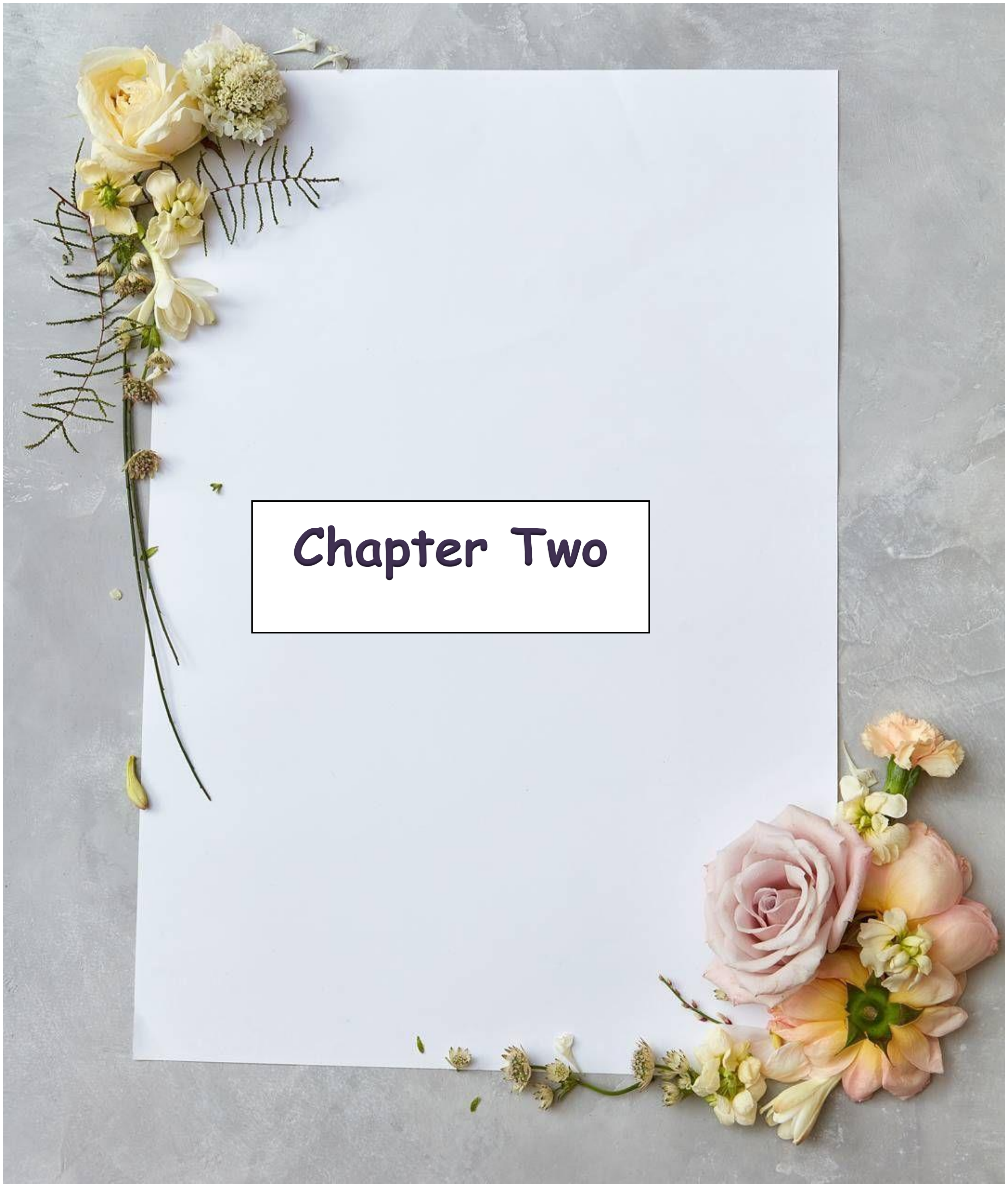
(A. Hazim *et al.*) in 2021 [54], have studied the optical properties of (PMMA–ZrO_2–Au) and (PMMA–Al_2O_3–Au). The results showed value of the energy gap decreased with doping of the ZrO_2-Au and Al_2O_3 – Au.

(M. I. Mohamme *et al.*) in 2022[55], have tested optical properties of the films of PMMA / ZnO nanocomposites and found that the dielectric constant has greater values with increasing in the concentration of (ZnO) nanoparticles that due to the increase of polarization in the polymer matrix, also they found that the conductivity of the alternating current increases with the increase in frequency.

1.9 The Aims of Study

1. Preparation of (PMMA/SiO_2-CeO_2) nanocomposites to use in various photonics, electronics, and medical fields.

2. The bio-medical applications (PMMA/SiO_2-CeO_2) nanocomposites will be tested.



Chapter Two

2.1 Introduction

This chapter includes a general description of a theoretical part of the study's, as well as physical concepts, scientific clarifications, relationships, and rules utilized to understand the findings.

2.2 The Optical Properties

Optical properties can be defined as the interaction between electromagnetic radiation or light with matter that includes absorption, reflection in addition to polarization, etc.[56]. The study of the optical properties of films is of great importance in finding the optical constants through which it is possible Identifying the value of the optical energy gap, as well as we can know the other constants of absorption and transmittance and their coefficients, as well as the damping coefficient and the real and imaginary dielectric coefficients[57].

2.2.1 Absorbance (A) and Transmittance (T) and Reflection

a. Absorbance(A): the absorbance defines as the ratio between the intensity of the absorbed radiation by the membrane (I_A) to the original intensity of the radiation incident on it (I_o) and the absorbance is a unit-free quantity. It is given by the following relationship[58]:

$$A = I_A / I_o \tag{2.1}$$

b. Transmittance(T): it is defined as the ratio between the intensity of the radiation passing through the membrane (I_T) and the original intensity of the radiation incident on it (I_o) , which is also a quantity devoid of units, and is given by the following relationship[59]:

$$T = I_T / I_o \tag{2.2}$$

c. Reflection (R): the reflectivity (R) is defined as the ratio between the intensity of the radiation reflected from the membrane in a particular direction to the original intensity of the radiation incident on it, and it is given in the following equation[60]:

$$R = I_R / I_o \tag{2.3}$$

Also, the value of the reflectivity can be found from the knowledge of the spectral absorption and permeability by adopting the law of energy conservation, In the following relationship[61]:

$$A + R + T = 1 \tag{2.4}$$

2.2.2 The electronic transitions

Electronic transmission are divided into two types[57,58]:

1. Direct Transition

This transition occurs in semiconductors when the bottom of the conduction band (C.B.) is exactly over the top of the valence band (V.B.), that meaning they have the same wave vector value ($\Delta k = 0$). The conservation of energy and momentum was needed for this transition form. There are two types forms of direct transitions[57,58]:

a. Direct Allowed Transition

As shown in Figure (2.1,a), this transition occurs between the top points in the (V.B.) and the bottom points in the (C.B.).

b. Direct Forbidden Transition

This transition happens between near top points of (V.B.) and near points in the bottom of (C.B.), as shown in figure (2.1, b).

2. Indirect Transition

In these transition types the bottom of conductivity band is not over the top of valence band. The electron transits from (V.B.) to (C.B.) not perpendicularly, they in different regions of **(K)** space ($\Delta \mathbf{K} \neq \mathbf{0}$). This type of transition occurs with the help of a particle known as a "Phonon". there are two types of indirect transitions[57,58]:

a. Allowed Indirect Transition

As shown from figure (2.1) these transitions happen between the top of (V.B.) and the bottom of (C.B.) in a different region of (**K-space**).

b. Forbidden Indirect Transition

As shown from figure (2.1) in (d), these transitions occurred between near points in the top of (V.B.) and near points in the bottom of (C.B.). The (Taos's equation) is used to calculate the optical energy gap value of the allowed and forbidden indirect transition[57,58].

$$\alpha h\boldsymbol{\upsilon} = B_o\,(h\boldsymbol{\upsilon} - E_g \pm E_{Phonon})^{r} \qquad (2.5)$$

Where E_{Phonon} means the energy of phonon, (-) when phonon absorption and (+) means when phonon emission, E_g means energy gap, h means blank constant, r means the exponential constant; its value depends on the type of transition, r=2 for the allowed indirect transition, meanwhile r=3 for the forbidden indirect transition.

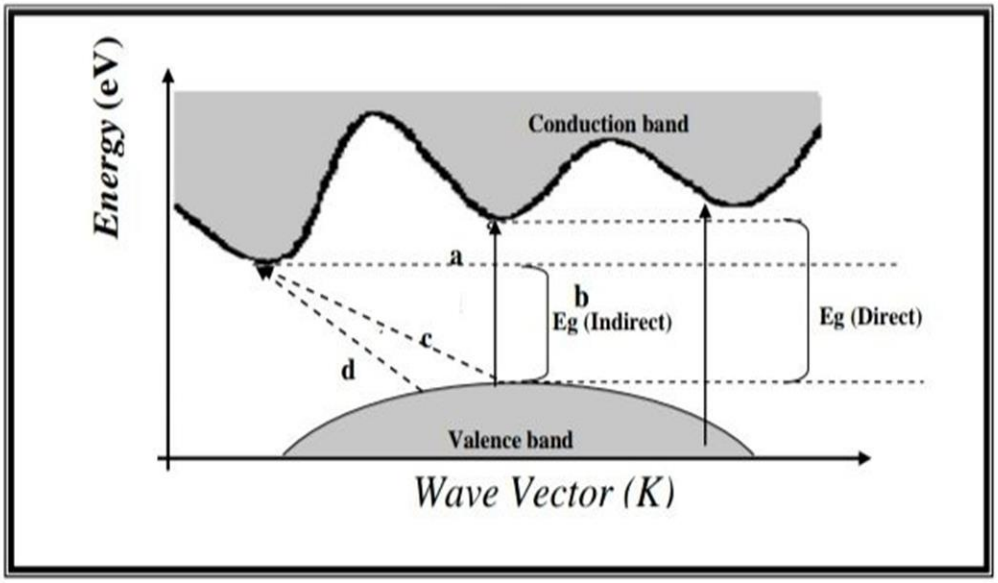


Figure (2.1): Types of electronic transfers [57,58]

(a) Allowed direct transition **(b) Forbidden direct transfers**

(c) Allowed indirect transition **(d) Forbidden indirect transfers**

2.2.3 Optical Constants

1. Optical absorption coefficient (α)

It is the decrease in the radiation energy incident on the material and it depends on the energy of the incident rays and the nature of material that falls on it; and it is measured in cm^{-1} unit. If the energy of the photons (hυ) is equal to the energy gap (E_g), then the photons are absorbed to generate a pair (electron-gap) as shown in (a) from figure (2.2). But if the energy of the photons (hυ) is greater than the energy gap (E_g), then it can be a transition process occurs in the semiconductor and produces an excitation of the electron from the valence band to the conduction band. While the extra energy is dissipated to be in the form of heat, as shown in (b) from figure (2.2). Both (a) and (b) are referred to as self-transition, or packet to packet transition, But if the energy of the photons (hυ) is less than the energy gap (E_g), the absorption will only take place in the presence of localized energy levels in the blocked gap that are caused by chemical impurities and physical defects, as shown in (c) from figure (2.2). This process is called non self-transfer[59,60].

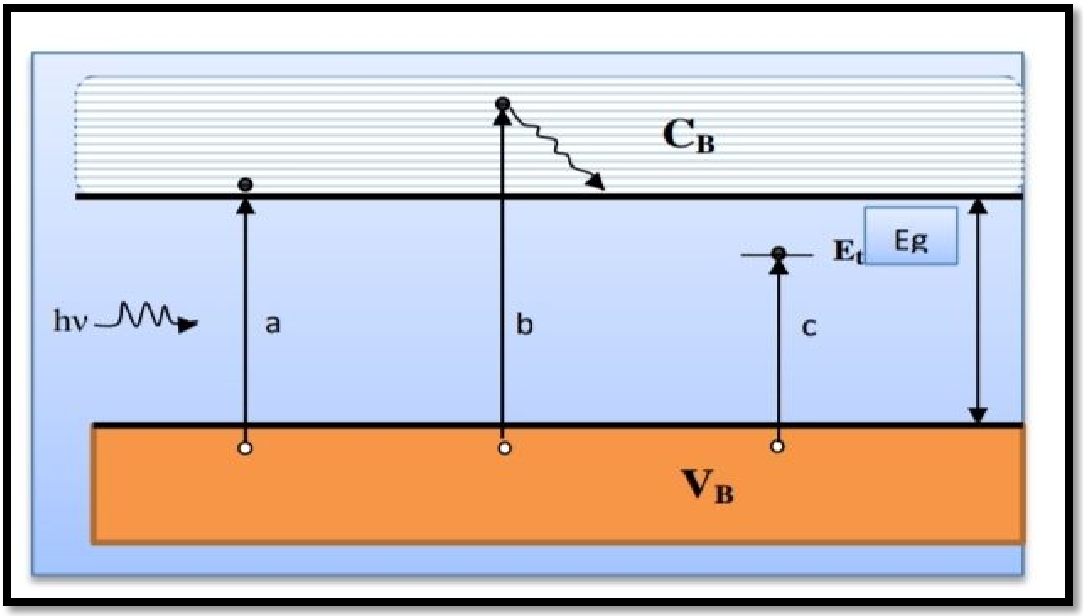


Figure (2.2): Self and non-self-transitions of semiconductors[59,60]

The absorption coefficient can calculate of the relationship called (Per-Lamberts relationship)[66]:

$$I = I_o e^{-\alpha t} \tag{2.6}$$

Where (I_o) and (I) are the intensity incident ray before and after it passes through the material; respectively, (α) is a absorption coefficient, and (t) thickness of film. After reworking the equation (2.6) above we get[66]:

$$\alpha = 2.303\ A/t \tag{2.7}$$

2. Extinction coefficient (k)

It is defined as the amount of attenuation in the intensity of electromagnetic radiation as a result of the interaction of electromagnetic rays and particles of the thin film material, the damping coefficient can be calculated through the following equation, which is related with the absorption coefficient[59]:

$$k = \alpha\lambda / 4\pi \qquad (2.8)$$

Where λ (cm) is the wavelength of the incident radiation and α (cm^{-1}) absorption coefficient.

3. Refractive index (n)

The index of refraction of a material is the ratio of the velocity of the light in vacuum to that of the specimen:

$$n = c / v \qquad (2.9)$$

where (n) refractive index, (c) the velocity of light in a vacuum, and (v) the velocity of light in any material medium[67].Refractive index can be expressed by the following equation[68]:

$$n = [4R/(R-1)^2 - k^2]^{1/2} + (R+1)/(R-1) \qquad (2.10)$$

Where (n) the refractive index, (R) the reflection, and (k) extinction coefficient.

4. Dielectric constant ($\mathcal{E}$)

Represents the ability of a substance to be polarized, when the interaction between light and the charges of the medium occurs the resulting polarization of the charges of this medium is described by the nodal dielectric constant (ε) that defined by the following equation[59]:

$$\mathcal{E} = \mathcal{E}_1 - i\mathcal{E}_2 \qquad (2.11)$$

Where $\mathcal{E}$: complex dielectric constant, $\mathcal{E}_1$:the real part of the dielectric constant, and $\mathcal{E}_2$: the imaginary part of the dielectric determined constant. The real and imaginary part of dielectric constant can be by using equations[69]:

$$\mathcal{E}_1 = n^2 - k^2 \qquad (2.12)$$

$$\mathcal{E}_2 = 2nk \qquad (2.13)$$

2.2.4 Optical conductivity

Is the phenomenon of an increase in the number of charge carriers (electrons or holes) as a result of a light beam incident on a semiconductor. The optical conductivity can be calculated from the equation[70]:

$$\sigma_{op} = \alpha \frac{nc}{4\pi} \qquad (2.14)$$

Where (σ_{op}) the optical conductivity, (α) is the absorption coefficient, (n) the refractive index, (c) the velocity of light.

2.3 Electrical Properties

Polymers are generally insulators, but they are also not completely free of conduction mechanisms. Conduction often occurs due to impurities that include concentrations of charge carriers[71]. Insulators can be used to store electrical energy in the form of charge separation when the electron distributions around the constituent atoms or molecules are polarized by an external electric field[72].

2.3.1 The A.C electrical conductivity

The electric field frequency in the A.C conductivity would be variable during[15]. Dielectric materials can be used to store electrical energy by separating the charge by applying an external electric field. So, when applied a low-frequency electric field on the insulator the permanent or induced dipoles keep pace with the direction of the applied electric field, that is, the material becomes polarized[14]. The complex permittivity of a material (ε^*) can be written as[72]:

$$\mathcal{E}^* = \mathcal{E}_a - j\,\mathcal{E}_b \qquad (2.15)$$

where $\mathcal{E}_a$ and $\mathcal{E}_b$ are value real and the imaginary parts of complex permittivity and Permittivity and j imaginary number equal $\sqrt{-1}$. The real part is determined by[72]:

$$\mathcal{E}_a = \mathcal{E}_o\ \mathcal{E}' \qquad (2.16)$$

The magnitudes of $\mathcal{E}_a$ and $\mathcal{E}_b$ depend on the angular frequency (ω) of applied the electric field. Magnitude of $\mathcal{E}_a$ (or the dielectric constant $\mathcal{E}'$) indicates the ability of material to store energy from applied electric field[72]. The equation can be used to measure the capacitance of a capacitor made up of two parallel plates[73]:

$$C = \mathcal{E}'\,\mathcal{E}_o\ A/t \qquad (\ 2.17)$$

Where $\mathcal{E}'$ is the constant of dielectric, t is the sample thickness and $\mathcal{E}_o$ is Permittivity in vacuum. Dielectric constant is given by the relation[74] :

$$\mathcal{E}' = C_P / C_o \qquad (2.18)$$

Where: C_P is capacitance in parallel and C_o this is vacuum capacitor[74]. The dielectric of loss ($\mathcal{E}''$) is given by[75] :

$$\mathcal{E}'' = \mathcal{E}'\,D \qquad (2.19)$$

Where D is dispersion factor, and this measures the lost electrical energy in the sample from the applied field which is transformed to thermal energy in the sample. The dissipated power in the insulator is represented by the existence of alternating potential as a function of the alternating conductivity is given by [76]:

$$\sigma_{A.C} = \omega\, \mathcal{E}_o\, \mathcal{E}'' \tag{2.20}$$

where ω is an angular frequency ($\omega = 2\pi f$).

2.4 Anti-bacterial Application

Antibiotics have been the preferred treatment method for bacterial infections due to their cost-effectiveness and robust results. In reality, antibiotic overuse has recently resulted in the development of superbugs that are resistant to practically all antibiotics[77]. Because of the emergence and spread of drug resistance in bacterial pathogens, antibiotics often lose their effectiveness over time. The so-called "antibiotic resistance crisis" by drug-resistant bacteria result in additional medical costs of up to billions of dollars annually [78,79]. Faced with this increasingly severe situation, discovering new antibacterial agents and therapeutic strategies is urgently necessary. Nanoparticles provide a universal platform for therapeutic applications based on their own unique physical and chemical properties and provide treatment for drug-resistant bacteria[79]. Antibacterial activity exhibited by nanomaterials such as silver, gold, copper, titanium, zinc oxide, and magnesium oxide is expected to become a substitute for antibacterial agents[80]. The unique properties of gold nanomaterials, such as their adjustable size, shape, surface properties, optical properties, biocompatibility, low cytotoxicity, high stability, and multi-functional potential, make them appealing in many fields of medicine[81]. Figure (2.3) show mechanisms for antibacterial activity of nanoparticles[82].

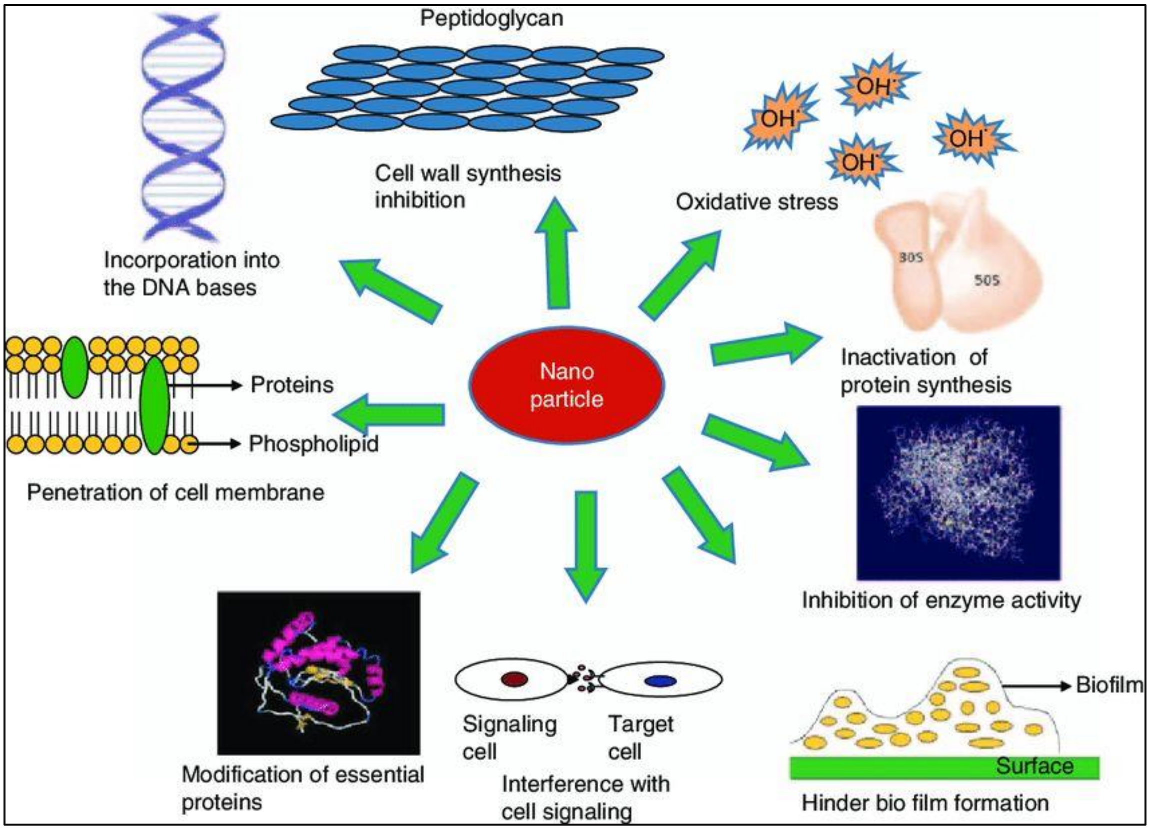
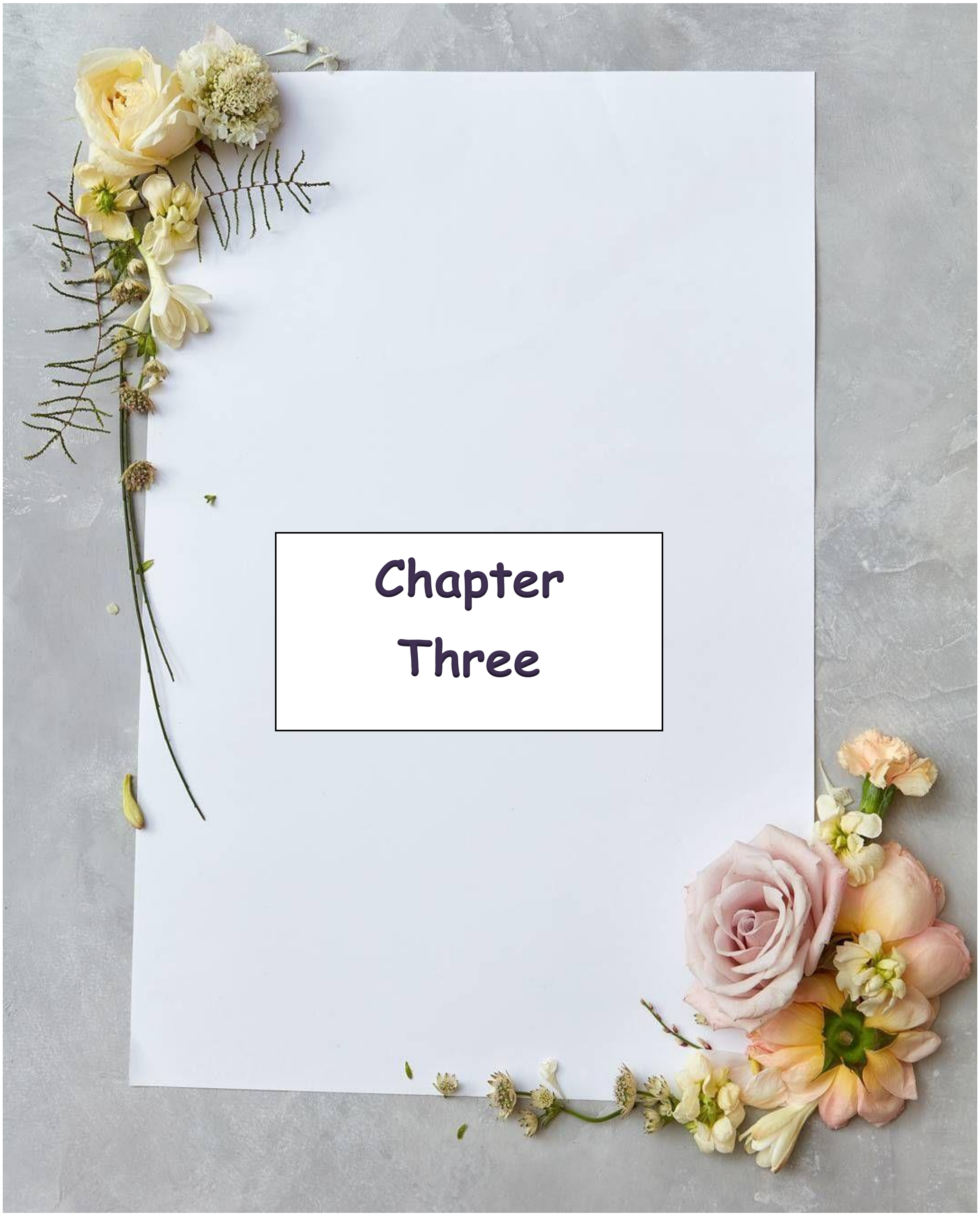


Figure (2.3) Mechanisms for antibacterial activity of nanoparticles[82]



Chapter Three

3.1 Introduction

This chapter includes the steps of sample preparation and processing, as well as a description of equipment and methods used in the preparation nanocomposites and measurement process for structural, optical, electrical properties for anti-bacterial applications.

3.2 The Materials Used in this Work

The materials that used in this study are:

3.2.1 Matrix materials

In this work, as polymer matrix the Poly (methyl methacrylate) (PMMA) was used. It is a kind of thermoplastic polymer. In normal state it is brittle, transparent, and lightweight. It is also called acrylic glass that due to high trans- parent as shown in figure (3.1).

Figure (3.1): poly (methyl methacrylate) Polymer

3.2.2 Additive materials

1. Silicon dioxide (SiO_2)

Silicon dioxide $SiO_{2,}$ also known as nano-silica or silica nanoparticles are the basis for a great deal of biomedical research due to their low toxicity, stability and ability to be functionalized with a range of molecules and polymers. The silicon dioxide nanopowder ($SiO_{2,}$ 98 + %, 60 – 70 nm, amorphous) was obtained from US Research Nanomaterials, lnc. It appear in the form of white powder, as shown in figure (3.2):

Figure (3.2): Silica dioxide nanoparticles

2. Cerium dioxide (CeO_2)

The chemical compound has the formula CeO_2, and it is in the form of white to pale yellow crystals. It is one of the oxides of the rare earth element cerium. It is mostly used in the fabrication of cells, sensors, anti-parasitic, and drug delivery careers. The cerium dioxide nanopowder (CeO2, 99.97, 50 nm) was obtained from US Research Nanomaterials, lnc. As shown in figure (3.3):

Figure (3.3): Cerium dioxide nanoparticles

3.3 Preparation of (PMMA/SiO_2-CeO_2) Nanocomposites

Films of poly (methyl methacrylate) – silicon oxide – cerium oxide nanostructures were synthesized by casting technique. The polymer solution (PMMA) fabricated with dissolve of 1.5 gm in chloroform (30 ml) at room temperature. The SiO_2-CeO_2 nanoparticles added to PMMA solution with contents (1.4, 2.8, 4.2, and 5.6) wt.%..

3.4 Measurements of Optical Properties for Nanocomposites

The absorption, transmittance and reflection spectrum of the nanocomposites (PMMA/SiO_2-CeO_2) films in the wavelength range (220-820)nm were recorded using a dual-beam spectrophotometer (SHIMADZO MODEL UV-1800 UVSPECTROPHOTOMETER) located at the University of Babylon / College of Education for Pure Sciences/Department of Physics. These measurements happened at room temperature.

3.5 Measurements of A.C Electrical Conductivity Properties for Nanocomposites

The A.C electrical conductivity was measured by wavelength ranged (100Hz - 5 MHz) LCR meter (HIOKI 3532-50 LCR Hi TESTER (Japan)) located in the University of Babylon/College of Education for Pure Sciences/Department of Physics. Capacitance (C_P) and dispersion factor (D) were recorded for all samples. The dielectric constant, dielectric losses, and conductivity were measured at room temperature.

3.6 Measurements of Structural Properties for Nanocomposites

3.6.1 Optical Microscope (OM)

Samples of nanocomposites (PMMA) were examined by using the optical microscope named Olympus (top view) type (Nikon 73346) under magnification (10x). This measurement was made at University of Babylon/College of Education for Pure Sciences.

3.6.2 FTIR spectrometer

The Fourier Transform Infrared Spectrometer (FTIR) is a powerful tool for determining the types of chemical bonds. When infrared radiation is shined on a molecule, the molecule can absorb some of these waves and as a result gain energy and vibrate its atoms, resulting in an increase in the length of the bond (bond expands) i.e. a change occurred in the places of the atoms. The FTIR spectra of the (PMMA/SiO_2-CeO_2)nanocomposites were recorded by FTIR(Bruker Corporation, German origin, type vertex-70) in the wavenumber range (1000-4000 cm^{-1}) at University of Babylon / College of Education for Pure Sciences / Department of Physics.

3.6.3 Scanning Electron Microscope (SEM)

The surface morphology of (PMMA/SiO_2-CeO_2) nanocomposites was tested for all samples by using scanning electron microscope. It is characterized by magnifying the image with a high accuracy of about 100,000 times, as a beam of electrons is directed to the surface and gives black and white images of the sample surface because it does not depend on light waves but on electronic emission. Figure (3.4) shows a schematic drawing of (a) the typical Scanning Electron Microscope (SEM) column and (b) sample-beam interactions within a SEM.

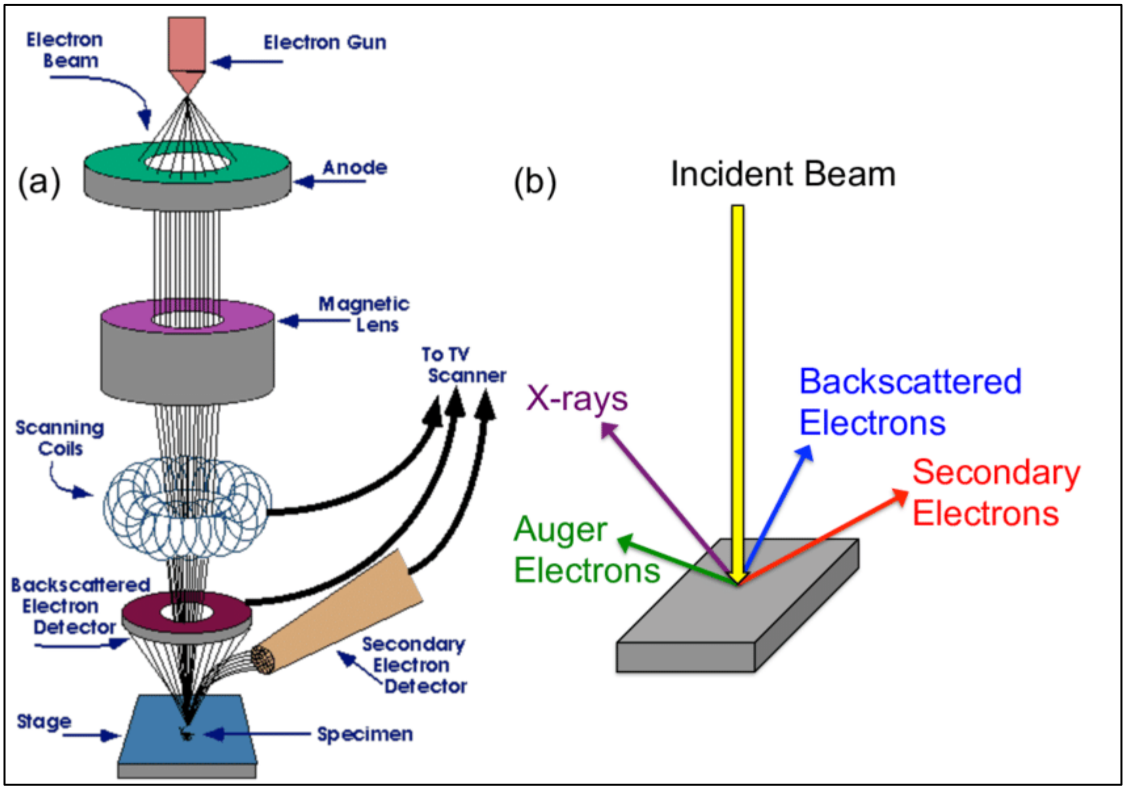


Figure (3.4): Schematic drawing of (a) the typical Scanning Electron Microscope (SEM) column and (b) sample-beam interactions within a SEM.

3.7 Measurements of Anti-bacterial Activity for Nanocomposites

The ($PMMA/SiO_2$-CeO_2) nanocomposites films were tested against two types of clinical bacterial (Staphylococcus aureus) and (Proteus vulgaris) by using agar diffusion method. Bacteria (Staphylococcus aureus and Proteus mirabilis) were cultured in Muller-Hinton Medium. The disks of the ($PMMA/SiO_2$-CeO_2) nanocomposites were placed over the media and incubated for 24 hours. Figure (3.5) shows SEM of (a) staphylococcus colonies (b) Proteus vulgaris.

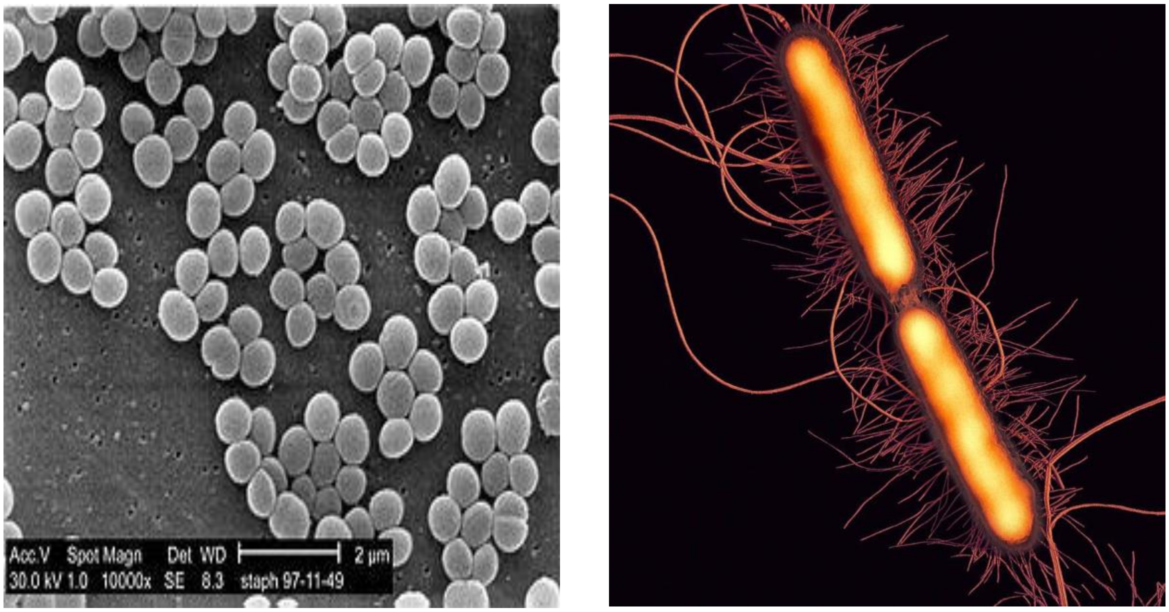
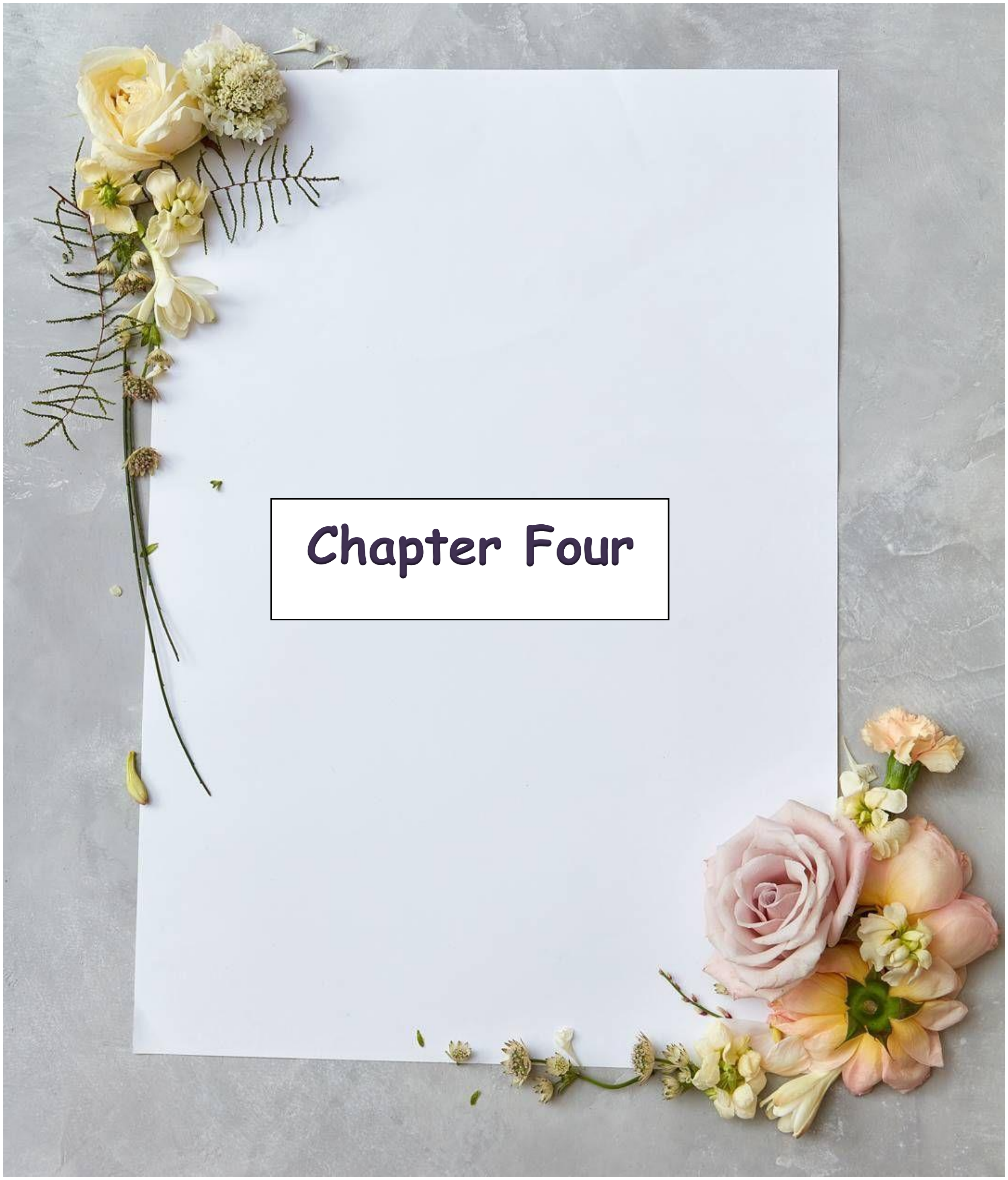


Figure (3.5): Scanning electron microscope images of (a) staphylococcus colonies (b) Proteus vulgaris



Chapter Four

4.1 Introduction

This chapter includes the results and discussion of structural , optical and A.C electrical measurements for (PMMA/SiO_2-CeO_2) nanocomposites. This chapter also studies the application of antibacterial drugs to nanocomposites and their inhibition quantification.

4.2 The Results of Structural Properties

4.2.1 Optical Microscope (OM) and Scanning Electronic Microscope (SEM) of (PMMA/SiO_2-CeO_2)

Figure (4.1) shows the arrangements of SiO_2 and CeO_2 nanoparticles in (PMMA/SiO_2-CeO_2) nanocomposites at magnification power (×10) for all samples. The figure shows that the nanoparticles is aggregated as a clusters at a lower concentrations. when increasing concentrations of SiO_2 and CeO_2 nanoparticles formation a network pathways inside the nanocomposites act as charge carriers into the polymeric structure, causing change in properties of material. This behavior consistent with the results of researchers[83,84]. SEM technology was used to study morphology and arrangement of nanocomposites. Figure (4.2) shows the SEM images for (PMMA/SiO_2-CeO_2) nanocomposites for all samples in various concentrations with the scale (1 µm). Figure (4.2, a) shows a SEM image of the pure polymer, the image shows that the substance is composed of spherical particles randomly distributed in polymeric surface this is maybe come back to the natural of the polymeric structure. With increasing a concentrations of SiO_2 and CeO_2 nanoparticles observed a good distribution and homogenous in surface morphology and the material becomes more softer. Nanoparticles distribution in spherical form as like grain randomly distributed on the surface and close to the rough texture. The SEM images show a network pathways formed of nanoparticles inside a polymer matrix. This behavior consistent with the results of researchers[85,86].

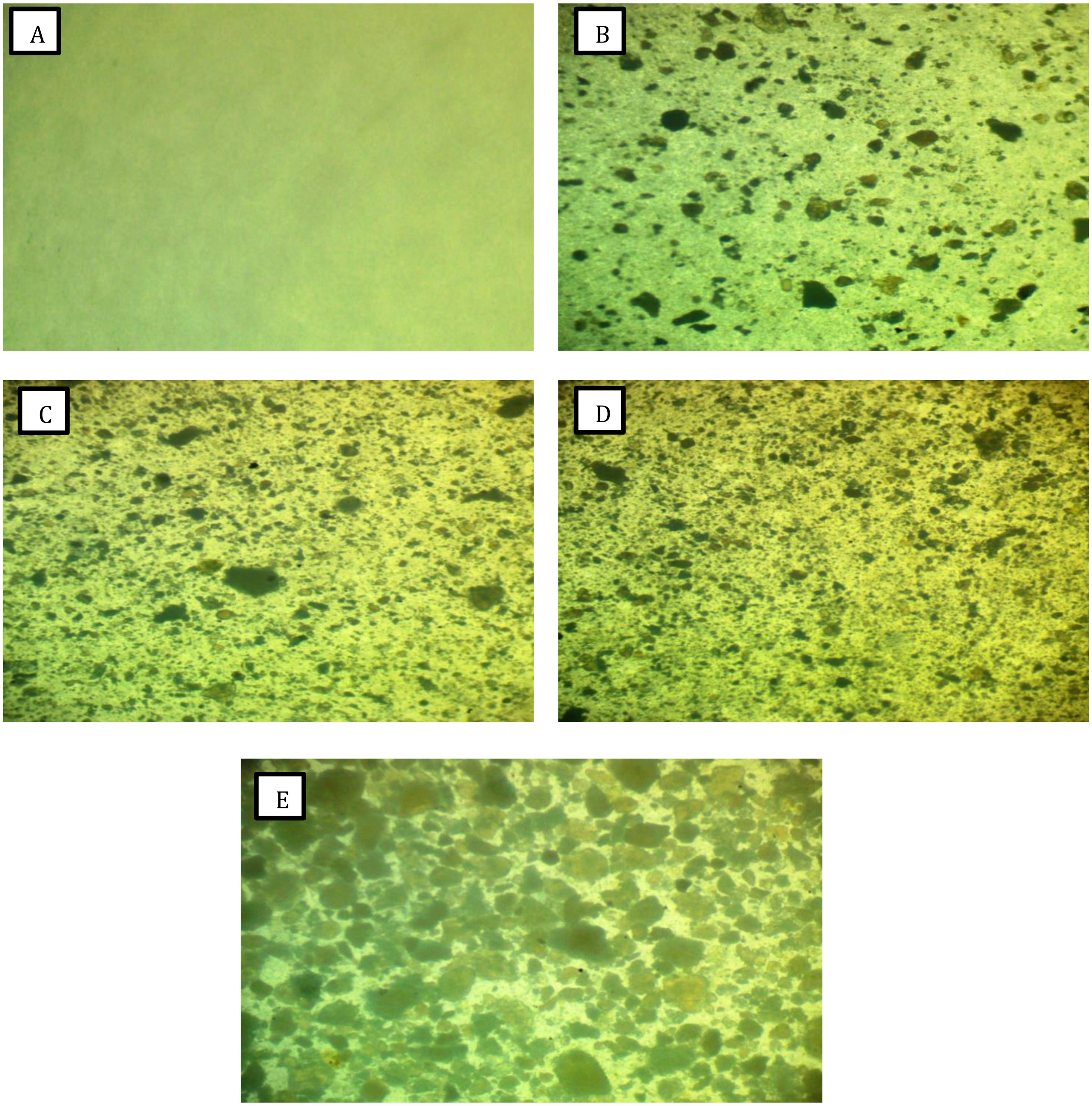


Figure. (4.1): Optical microscope images (×10) for (PMMA/SiO_2-CeO_2) nanocomposites

A. pure polymer, B. 1.4 Wt.%, C. 2.8 Wt.%, D. 4.2 Wt.%, E. 5.6 Wt.%

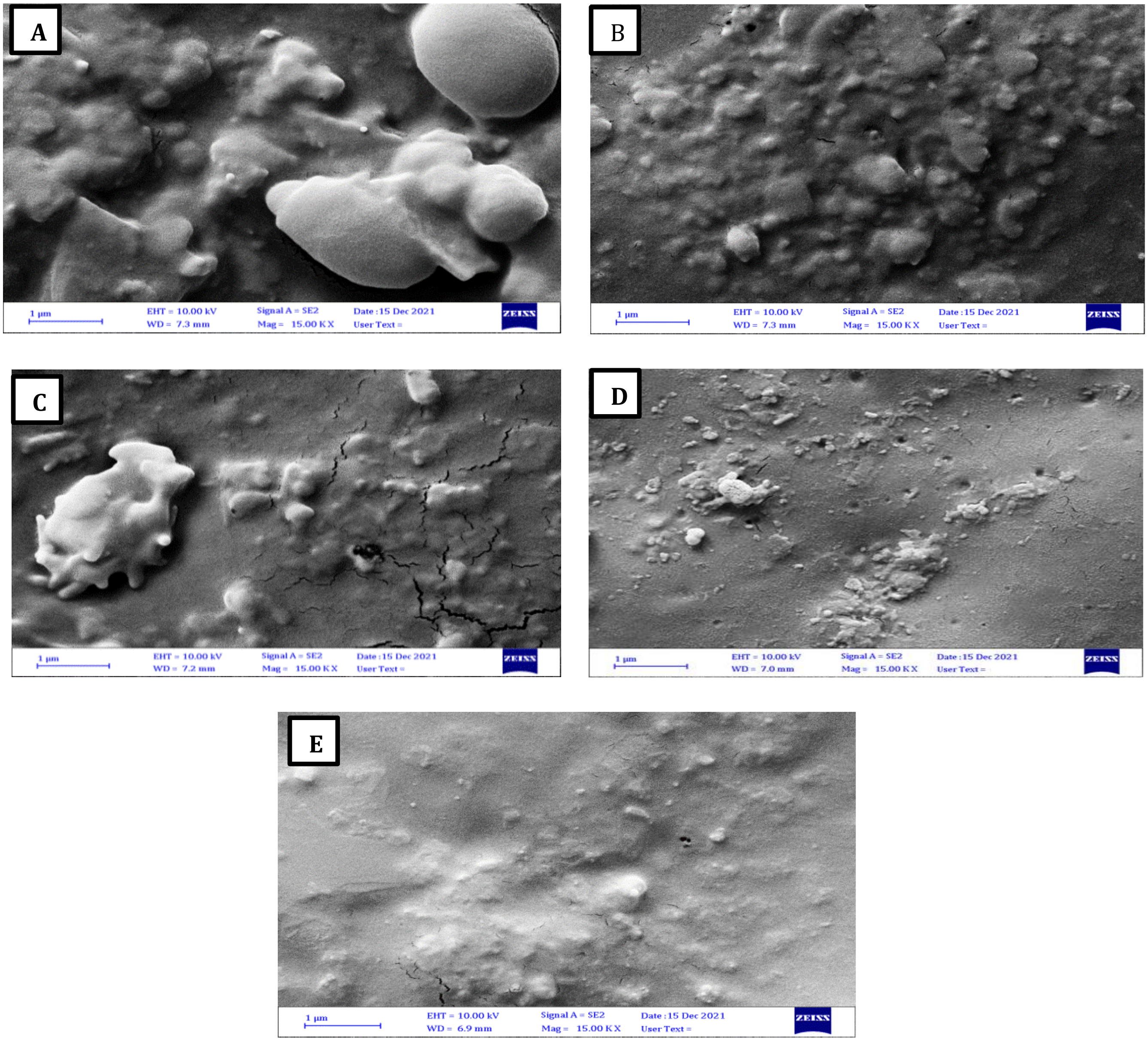
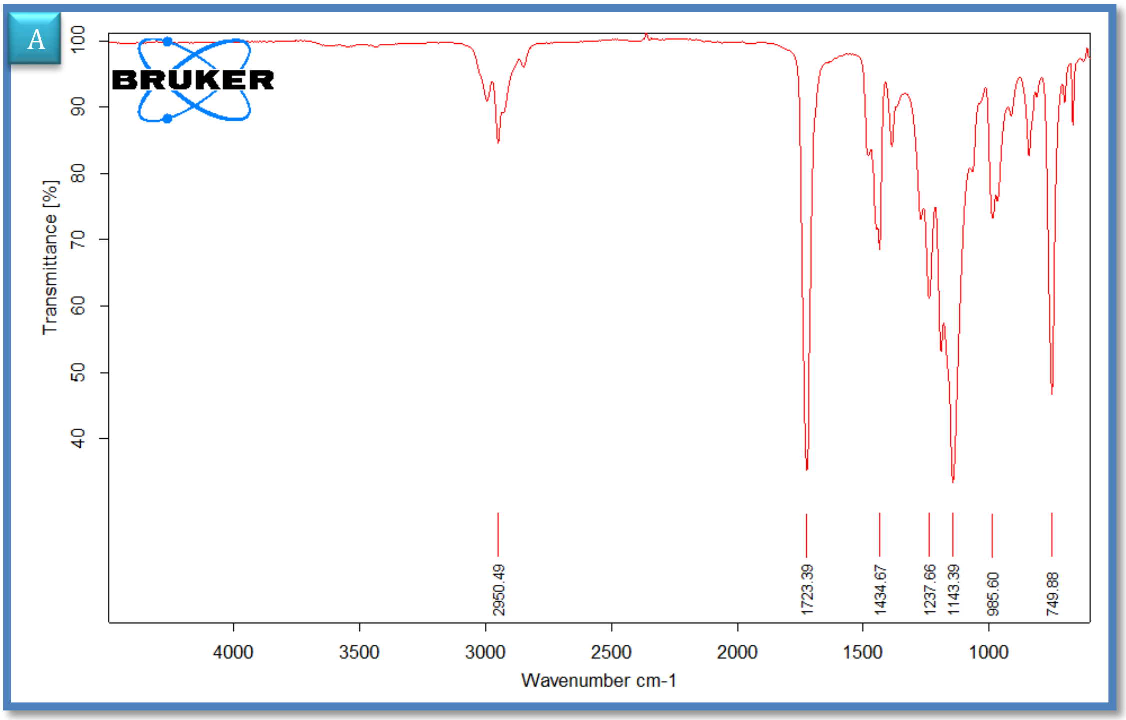


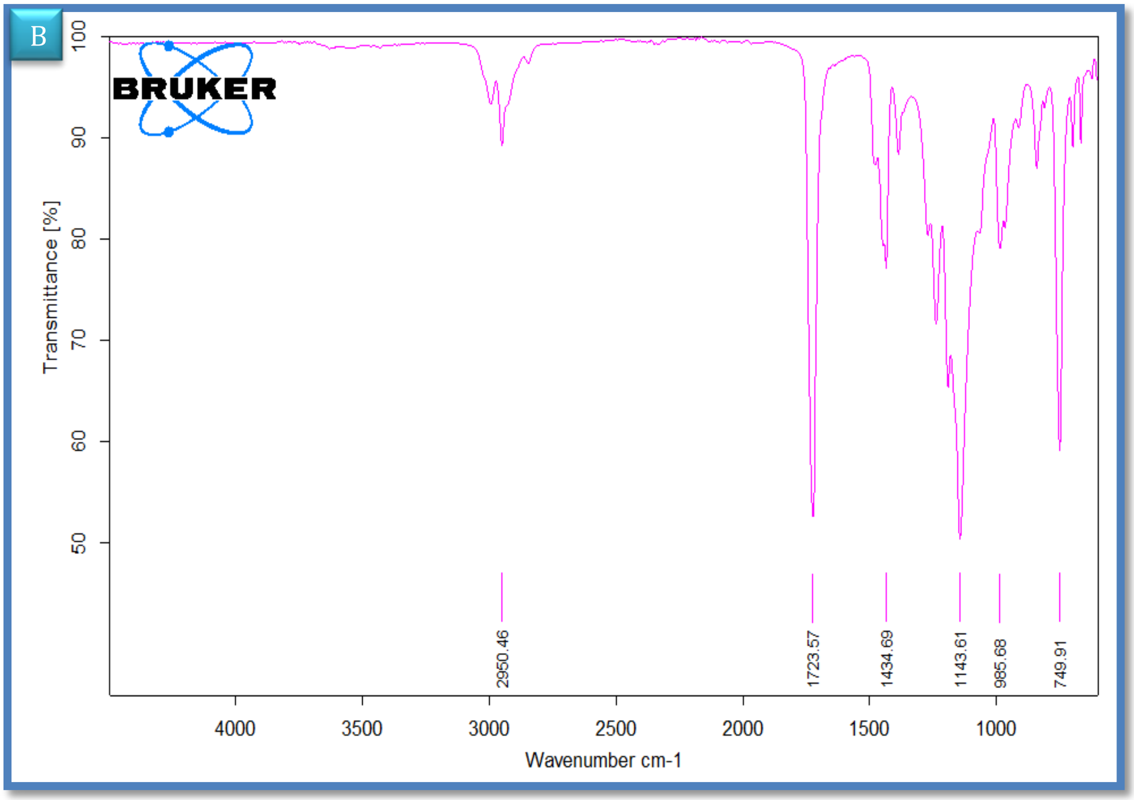
Figure. (4.2): SEM images for (PMMA/SiO_2-CeO_2) nanocomposites

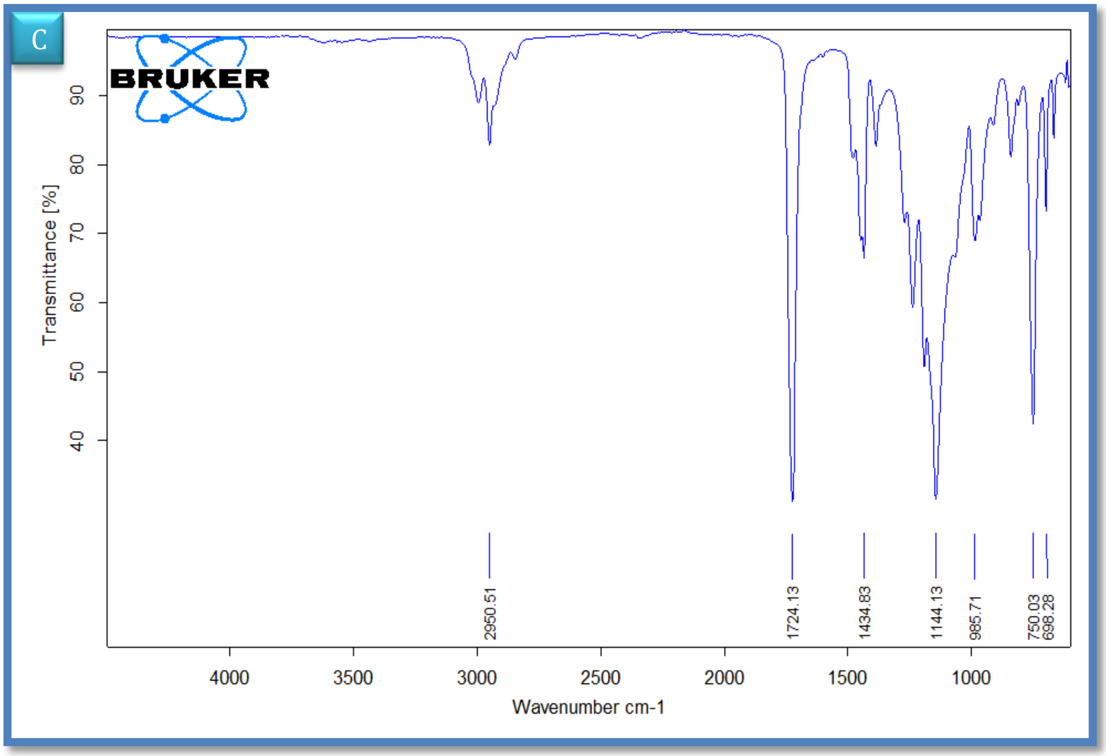
A. pure polymer, B. 1.4 Wt.%, C. 2.8 Wt.%, D. 4.2 Wt.%, E. 5.6 Wt.%

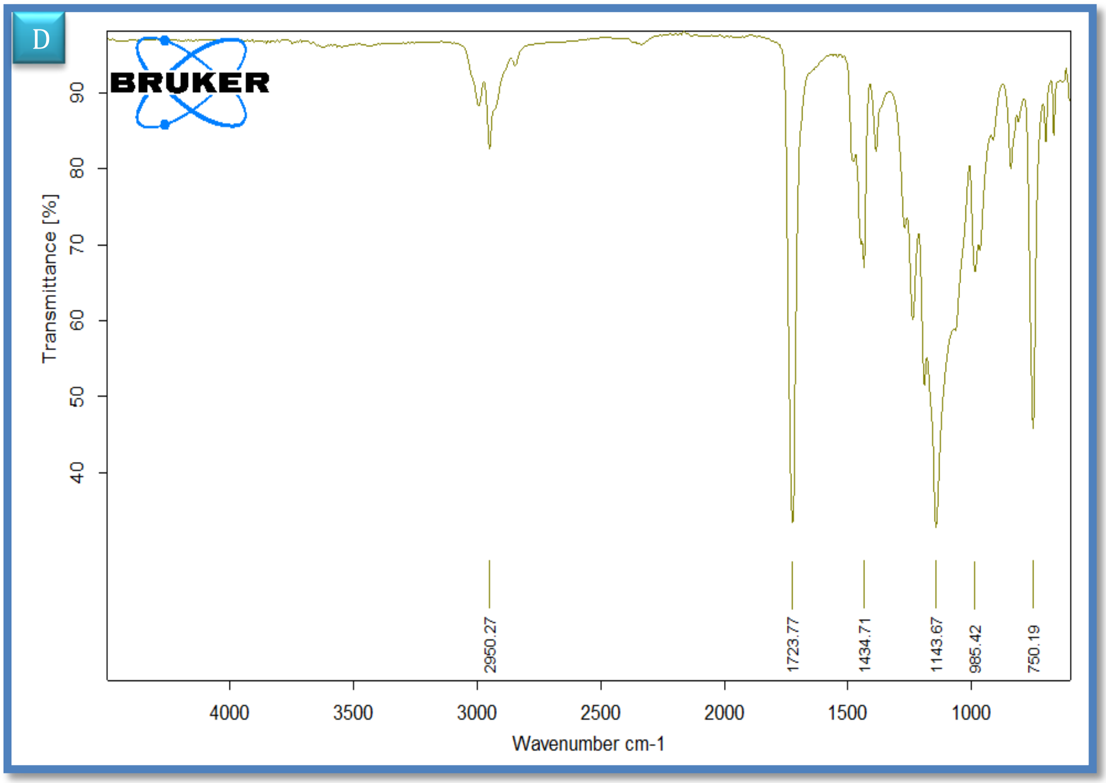
4.2.2 Fourier Transform Infra-Red of (PMMA/SiO_2-CeO_2)

FT-IR spectra of (PMMA/SiO_2-CeO_2) nanocomposites are shown in figures (4.3) at wavenumber range (1000-4000) cm^{-1}. FTIR studies of nanocomposites show the interactions in nanocomposites. FTIR spectra of a polymer (PMMA) are shown in image (A) from figure (4.3). Absorption bands characteristic of pure polymer (PMMA) appear at **(2950.49, 1723.39 cm^{-1})** and bands in the range from **749.88** to **1434.67 cm^{-1}** (fingerprint region). The appearance of the sharp band at 2950.49 cm^{-1} means absorption occurred at this bond and the medium-strength functional group (– C – H) from the Alkane group represents the type of hybridization of the bond (Sp^3), meaning that the bonds are single, and the appearance of the package **1723.39 cm^{-1}** assigned for the stretching bond that (C=H) (Carbonyl) return to the ester group in the polymer. while the last group called the footprint region **(749.88 - 1434.67 cm^{-1})** a range of absorption regions appeared. The appearance of the package **(1434.67 cm^{-1})** at the absorption sites dating back to the stretching bond that (C – O – C) Ether existing within the group in the polymer Austrian. After adding nanoparticles (SiO_2-CeO_2) as shown in image (from B to E) from figure (4.3) observed a slight change in the beam positions was observed because the addition of nanoparticles causes a slight stretching or restriction of the vibrational motion of the polymeric material molecules, but the locations of the peaks did not change. That no new bonds were formed, these results agree with the researchers[87,88].


A
BRUKER
Transmittance [%]
100
90
80
70
60
50
40
2950.49
1723.39
1434.67
1237.66
1143.39
985.60
749.88
4000
3500
3000
2500
2000
1500
1000
Wavenumber cm-1


B
BRUKER
Transmittance [%]
100
90
80
70
60
50
2950.46
1723.57
1434.69
1143.61
985.68
749.91
4000
3500
3000
2500
2000
1500
1000
Wavenumber cm-1


C
BRUKER
Transmittance [%]
90
80
70
60
50
40
2950.51
1724.13
1434.83
1144.13
985.71
750.03
698.28
4000
3500
3000
2500
2000
1500
1000
Wavenumber cm-1


D
BRUKER
Transmittance [%]
90
80
70
60
50
40
2950.27
1723.77
1434.71
1143.67
985.42
750.19
4000
3500
3000
2500
2000
1500
1000
Wavenumber cm-1

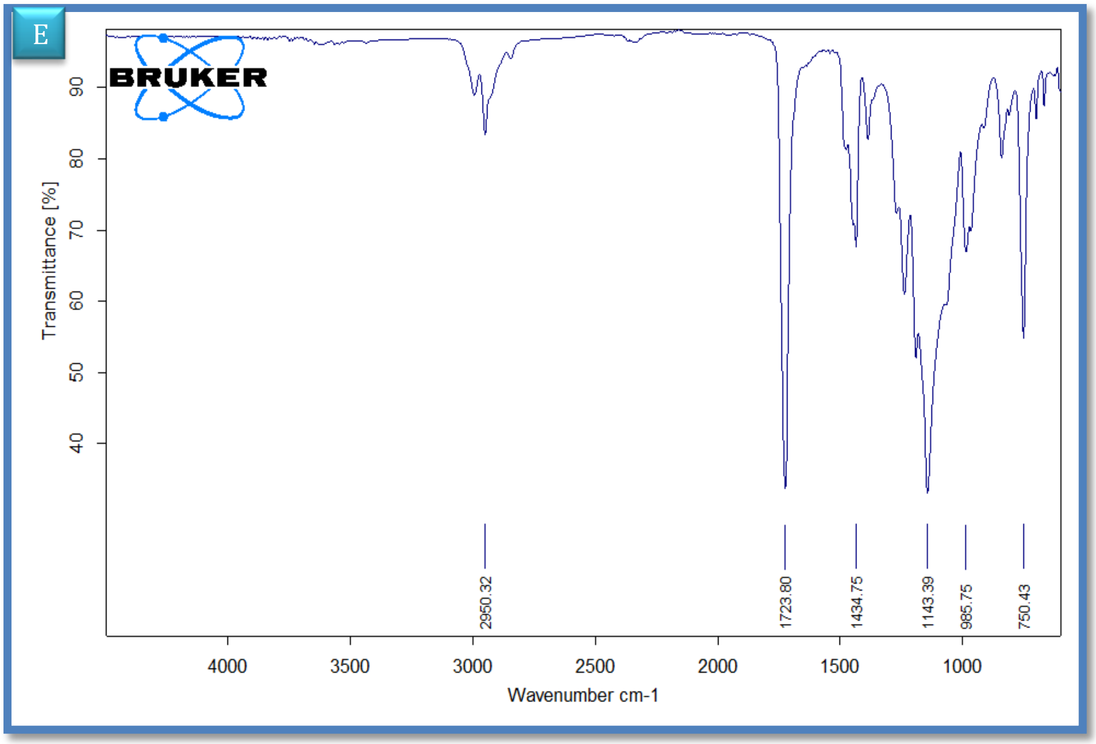


Figure (4.3): FT-IR sprctra of (PMMA/SiO_2-CeO_2) nanocomposites

A. pure polymer, B. 1.4 Wt.%, C. 2.8 Wt.%, D. 4.2 Wt.%, E. 5.6 Wt.%

4.3 The Results of Optical Properties

4.3.1 Absorbance and transmittance of (PMMA/SiO_2-CeO_2) nanocomposites

Figures (4.4) and (4.5) show the absorption and transmittance spectrum for (PMMA/SiO_2-CeO_2) nanocomposites as a function of wavelength of the incident light respectively. Figure (4.4) shows there high absorption for all samples of nanocomposites at U.V. region is due to the energy of photon enough to interact with the atoms as the electron is excited from a lower energy level to a higher one. In the near-infrared and visible regions, the absorption of nanocomposite samples is low, due to the low energy of the incident photons as there is not enough energy to interact with the atoms. The absorption of films is greater at short wavelengths and then decreases with increasing wavelength. Absorption increases with increasing concentrations of SiO_2 and CeO_2 nanoparticles and the charge carries increasing, this is due to the density of the positional levels formed by the impurity atoms between the conduction and valence band. As these levels act as auxiliary levels for the transfer of electrons that absorb photons with an energy less than the value of the optical energy gap of the incident photons, then absorption occurs. This behavior consistent with the results of researchers[89,90].

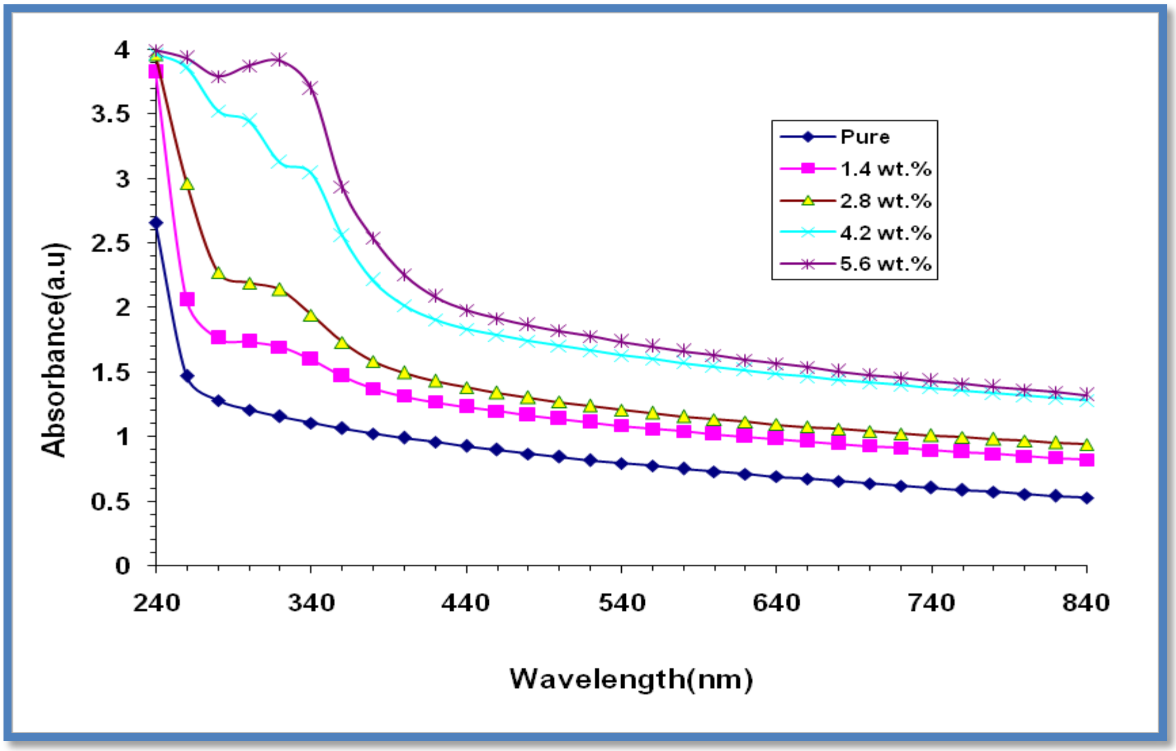


Figure (4.4): Variation of absorbance for (PMMA/CeO_2-SiO_2) nanocomposites with wavelength

Figure (4.5) shows transmittance spectrum for (PMMA/SiO_2-CeO_2) nanocomposites against wavelength. The figure shows the transmittance for all sample nanocomposites is as low as possible at the short wavelengths and increases with increasing wavelength. The transmittance spectrum decreases with the increase in the percentage of doping due to the impurity atoms and the accompanying formation of positional levels within the energy gap between the valence and conduction bands. Thus positional levels make absorbance increasing and decreasing in transmittance. These results have the same behavior that obtained[91][51]. The properties of the prepared film within the indicated wavelength range can be used as a thermally transparent material and as infrared windows.

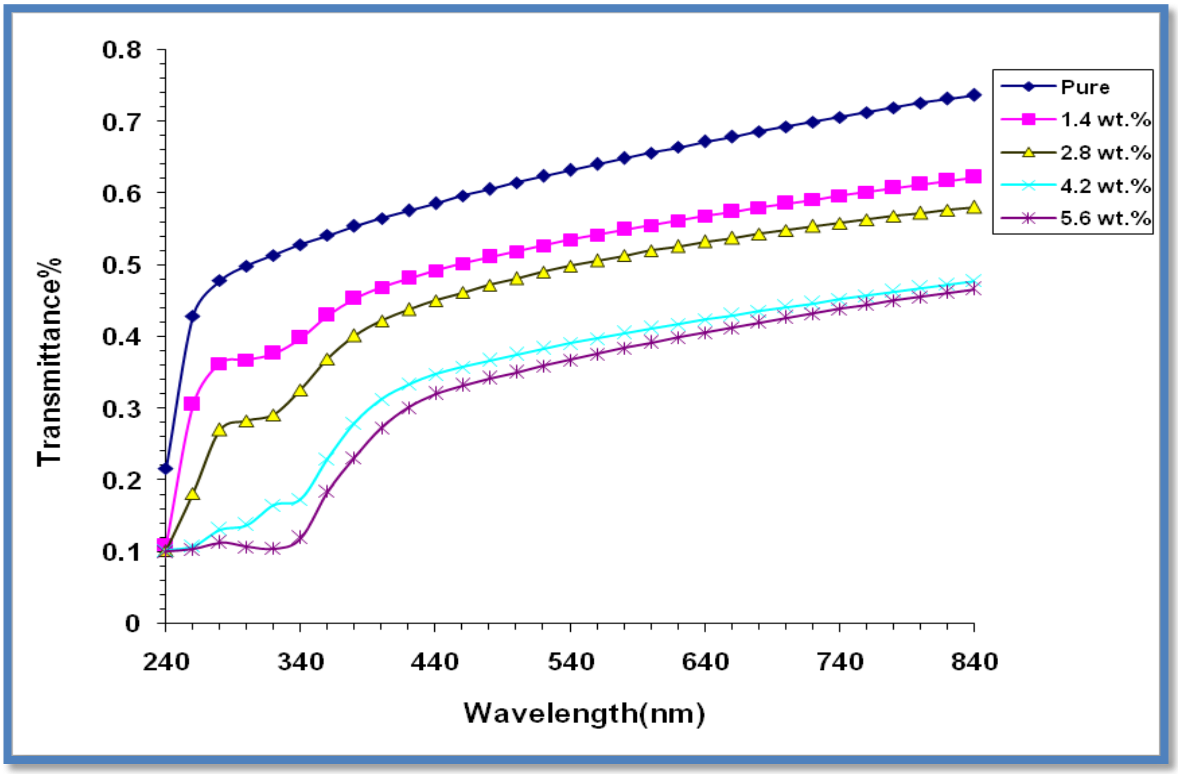


Figure (4.5): Variation of transmittance for (PMMA/SiO_2-CeO_2) nanocomposites with wavelength

4.3.2 Absorption coefficient (α) of (PMMA/SiO_2-CeO_2) nanocomposites

The absorption coefficient of nanocomposites is calculated by using equation (2.7). Figure (4.6) shows the absorption coefficient (α) as a function of the photon energy of the incident light . As shown in the figure the absorbance coefficient of all samples for nanocomposites is lower at low energies. This means that the power is low and insufficient for the electron to move from the valence band to the conduction band, but at higher energies the absorption is high, which indicates a high probability of the electron moving from the valence band to the conduction band. This means that the energy of the incident photon exceeds the forbidden energy gap and therefore conduction occurs. The absorption coefficient helps to know the nature of the electron transfer. When the values of the absorption coefficient of the substance are high (more than 10^4 cm^{-1}), direct electron transfer is expected. Whereas, when the values of the absorption coefficient of the material are low (less than 10^4 cm^{-1}) an indirect electron transfer is expected. The absorption coefficient of nanocomposites increases with the increase in the concentrations of nanoparticles, and this is due to the formation of positional levels within the energy gap near the conduction band which leads to an increase in the absorption from the incident photons, this behavior consistent with the results of researcher[92].

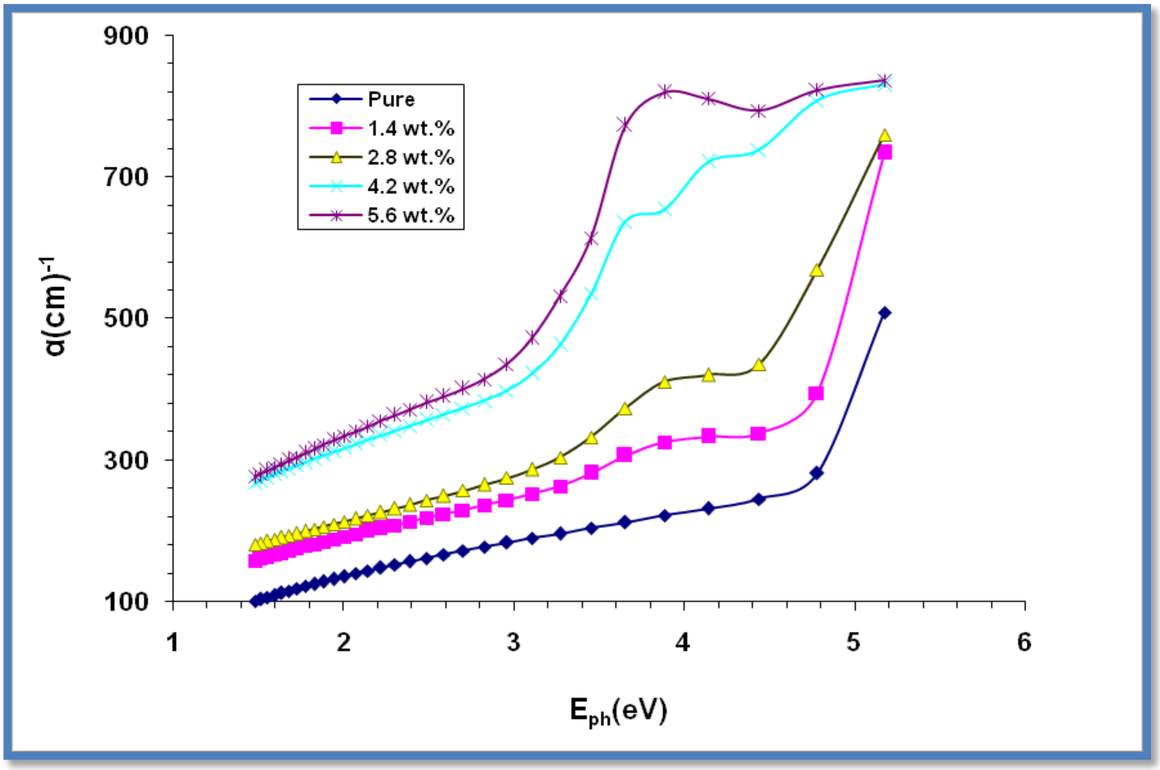


Figure (4.6): Variation of absorbance coefficient (α) for (PMMA/SiO_2-CeO_2) nanocomposites with photon energy

4.3.3 Extinction coefficient (k) of (PMMA/SiO_2-CeO_2)

The extinction coefficient refers to the amount of attenuation obtained by the electromagnetic wave as it passes through a material medium. The natural of the attenuation coefficient curves is almost similar to the behavior of the absorption coefficient curves due to the natural of the relationship between them in the equation (2.8). Figure (4.7) shows behavior the extinction coefficient with wavelength. From the figure was noticed that the values of extinction coefficient increases with the increasing of SiO_2 and CeO_2 nanoparticles concentrations, this is due to the density of levels formed by the impurities inside the energy gap that increase the absorbance of the prepared films. The extinction coefficient of nanocomposites has high values at U.V region this due to high absorbance of all samples of nanocomposites. Also, extinction coefficient of nanocomposites increases with the increasing of the wavelength at visible and near infrared regions which are due to the absorption coefficient of nanocomposites is approximately constant at visible and near infrared region, this behavior consistent with the results of researchers[93,94].

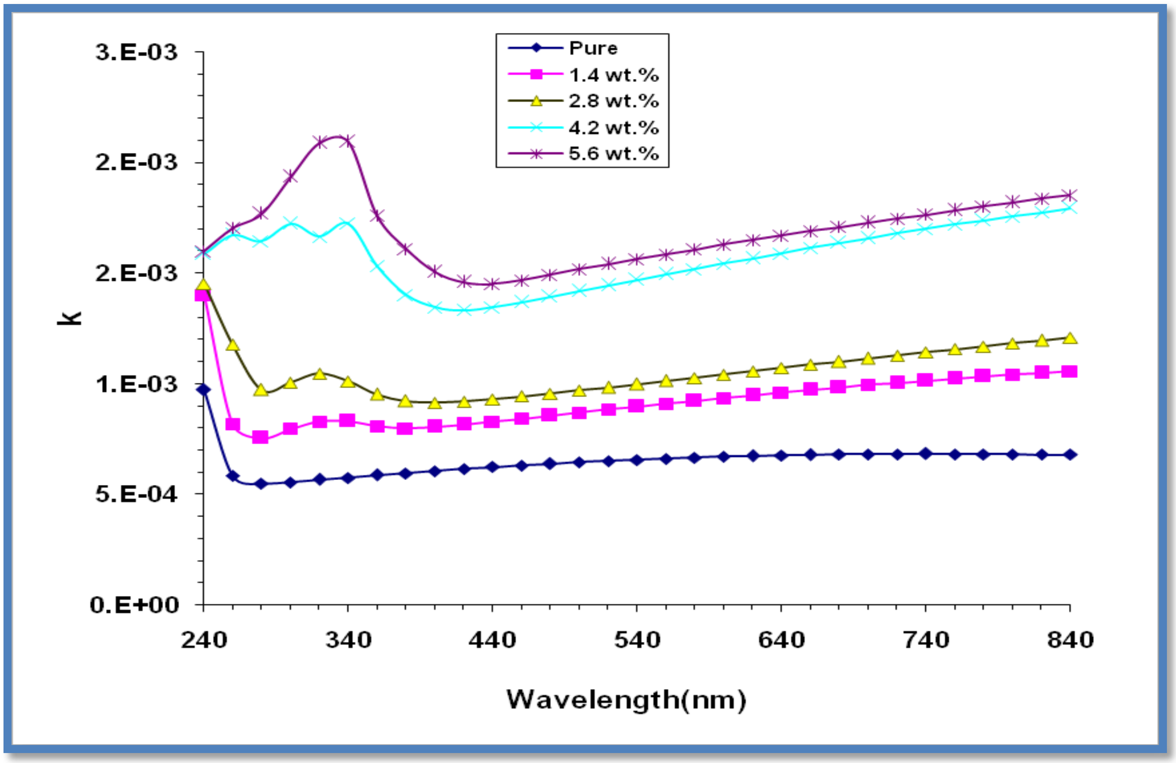


Figure (4.7): Variation of extinction coefficient for (PMMA/CeO$_2$-SiO$_2$) nanocomposites with wavelength

4.3.4 Refractive index (n) of (PMMA/SiO$_2$-CeO$_2$) nanocomposites

Refractive index (n) is calculated by using equation (2.10). The figure (4.8) shows refractive index as a function of the wavelength. From this figure it can be seen that the refractive index increases with the increasing of the SiO$_2$ and CeO$_2$. The reason for this is that the doping process led to the addition of new levels based on reversing the incident rays by more quantity, which increases the intensity of the reflected rays and thus increases the refractive index. In the U.V region observed a high values of the refractive index that due to the little transmittance (T) in this region, but in the visible and near IR regions, due to high transmittance (T) in this field, the values are low. This behavior is consistent with the researchers[95,96].

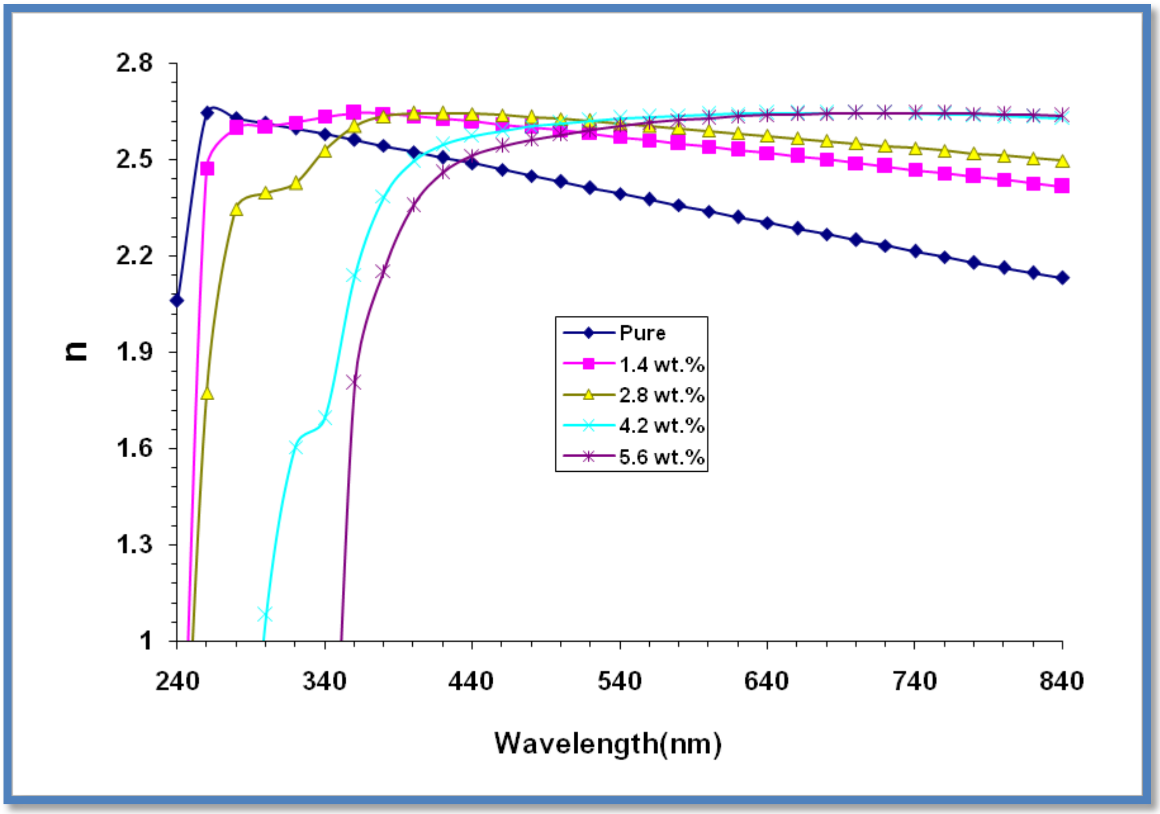


Figure (4.8): Variation of refractive index for (PMMA/SiO_2-CeO_2) nanocomposites with wavelength

4.3.5 Energy gap of (PMMA/SiO_2-CeO_2) nanocomposites

The energy gap of nanocomposites is calculated by using equation (2.5). The energy gap of a pure polymer is always higher than the energy gap of the nanocomposite, i.e. as the doping increases, the energy gap decreases. Figures (4.9) and (4.10) show the energies gap for allowed and forbidden indirect transitions respectively with incident photon energy. Where a straight line is drawn from the top of the curve towards the x-axis at $(\alpha h\nu)^{1/2} = 0$ get allowed energies gap while the value $(\alpha h\nu)^{1/3} = 0$ get the forbidden energy gap. The values for the obtained energy gap are given in table (4.1) . The energy gap values decrease with increasing of the SiO_2 and CeO_2 nanoparticles concentration, this shows us that the doping process led to a decrease in the value of the energy gap, because the doping process this behavior is due to the creation of levels in the energy gap, which leads transition of electron in this case happened in two stages includes transition from valence band (V.B.) to the local levels in energy gap and then to conductivity band (C.B). This behavior consistent with the results of researchers[97,98]

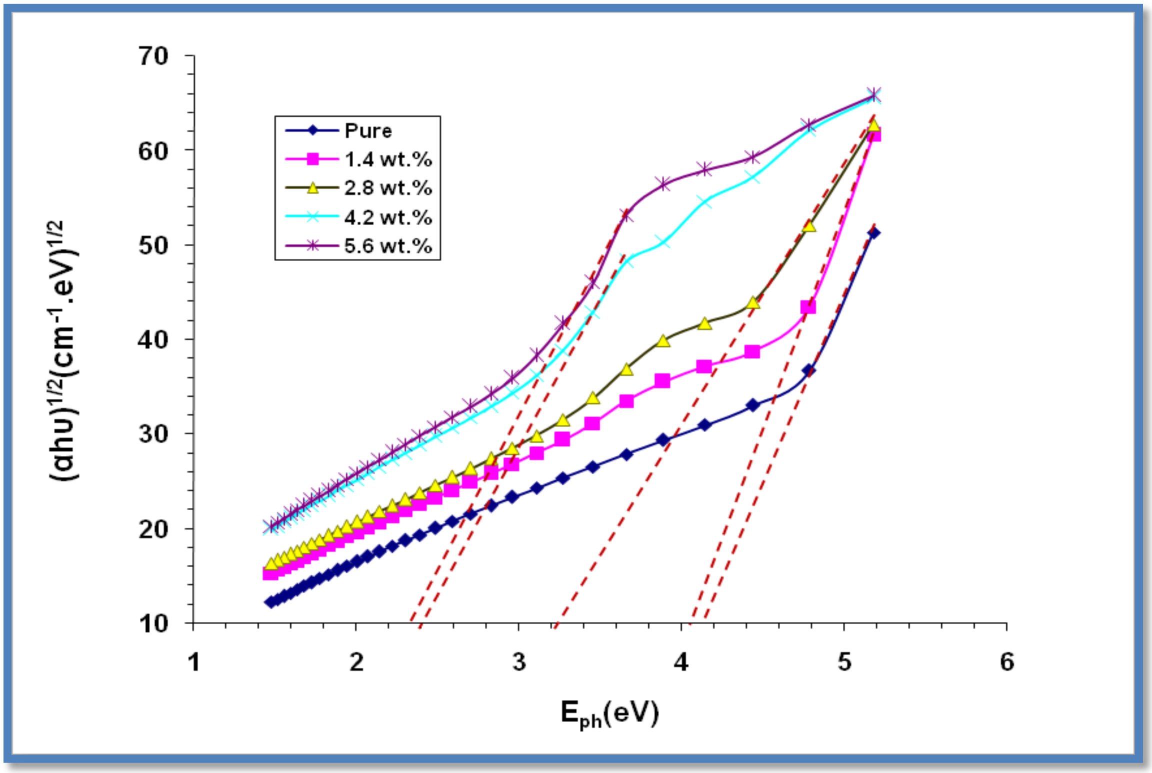


Figure (4.9): Variation of (αhv) $^{1/2}$ for (PMMA/SiO_2-CeO_2) nanocomposites with E_{ph}

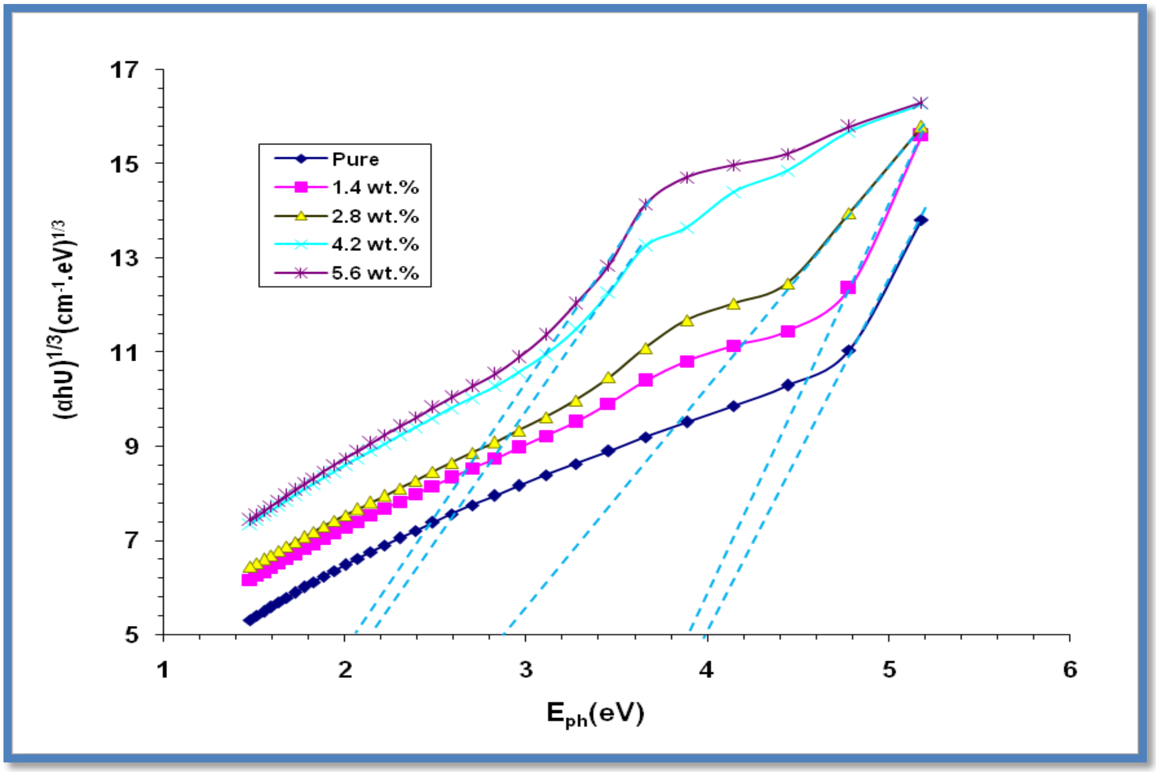


Figure (4.10): Variation of $(\alpha h\nu)^{1/3}$ for ($PMMA/SiO_2$-CeO_2) nanocomposites with E_{ph}

Table (4.1): Values of allowed and forbidden indirect energy gap energy gap.

concentrations of (SiO_2-CeO_2) wt.%	Allowed indirect energy gap (eV)	Forbidden indirect energy gap (eV)
0	4.14	**4**
1.4	4.07	**3.9**
2.8	3.23	**2.9**
4.2	2.4	**2.15**
5.6	2.31	**2.08**

4.3.6 The Real and imaginary parts of dielectric constant (ε_1 and ε_2)

The dielectric constant represents the ability of a material to polarize when electromagnetic radiation is applied to it which divided to two types: the real dielectric constant (ε_1) and the imaginary dielectric constant. These two types were calculated by using equations (2.12) and (2.13) respectively. Figures (4.11) and (4.12) show variation of the real and imaginary dielectric constant with wavelength for (PMMA/SiO_2-CeO_2) nanocomposites. These figures show the real and imaginary dielectric constants increased with increasing of SiO_2 and CeO_2 nanoparticles concentration and this behavior is attributed to the increase in the electric polarization by the nanoparticles, whose increase leads to the generation of high density for the dipoles increasing the dielectric constant. Figure (4.11) shows the similar behavior of the real dielectric constant curves with the refractive index curves due to relationship that connects them according to the equation (2.15) and this similarity is the result of the dependence of the real dielectric constant on the values of n^2 more than the value of k^2 because the values of (k) are very small compare to the value of refractive index especially after squaring. Figure (4.12) shows the change of the imaginary dielectric constant with wavelength, where the imaginary part of the dielectric constant depends on the damping coefficient, especially in the infrared regions near the wavelength and visible radiation, where refractive index (n) is almost constant, while extinction coefficients (k) increases with increasing wavelength. This behavior consistent with the results of researchers[99,100].

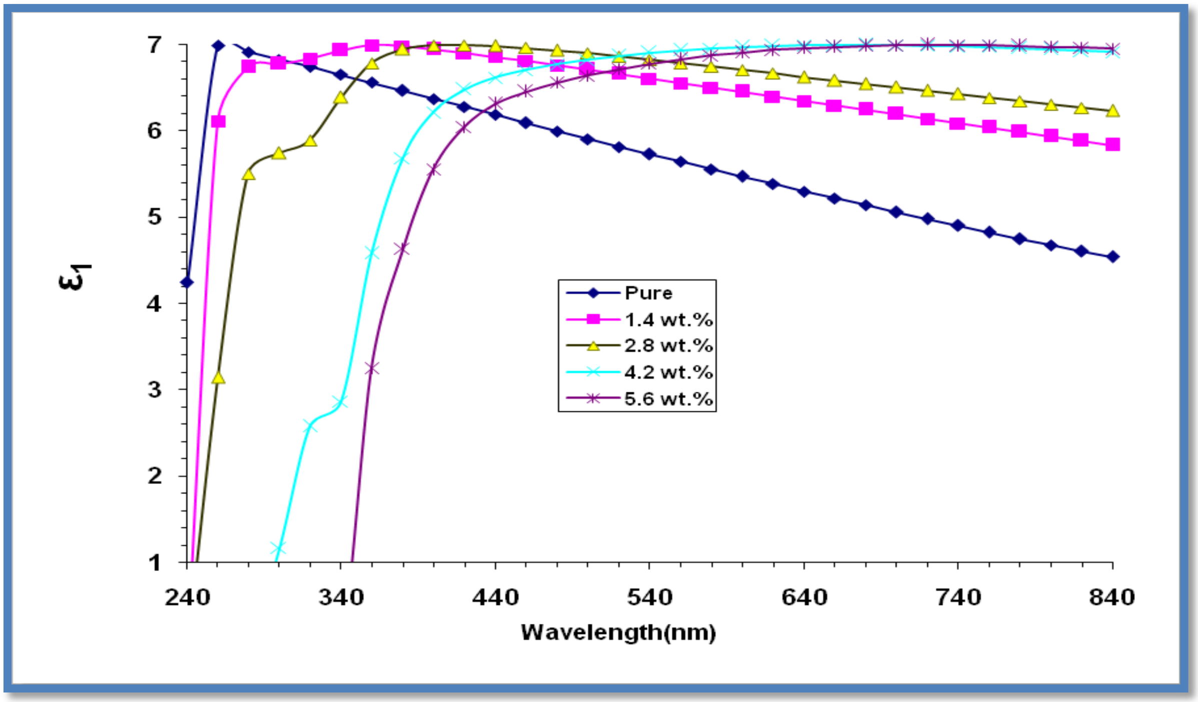


Figure (4.11): Performance of real part of dielectric constant for (PMMA/SiO_2-CeO_2) nanocomposites with wavelength

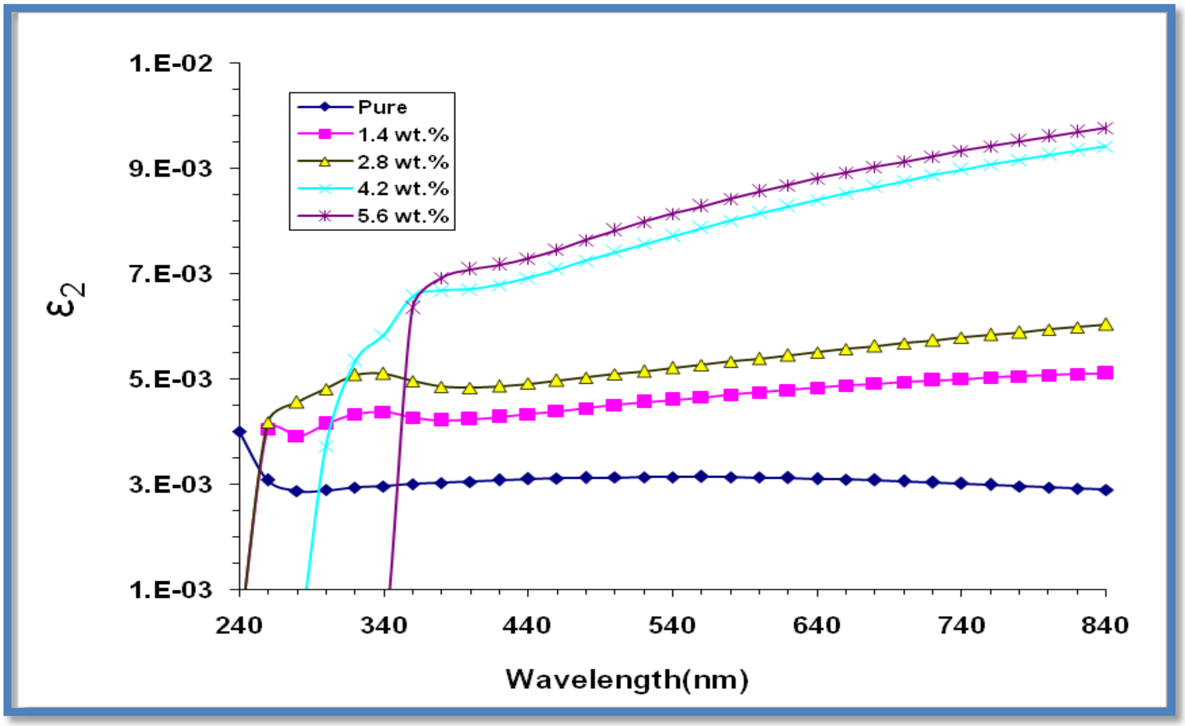


Figure (4.12): Performance of imaginary part of dielectric constant for (PMMA/SiO_2-CeO_2) nanocomposites with wavelength

4.3.7 Optical conductivity (σ) of (PMMA/ SiO_2-CeO_2) nanocomposites

The conductivity was calculated from equation (2.14). Figure (4.13) shows the variation of the optical conductivity as a function of the wavelength of the (PMMA/SiO_2-CeO_2) nanocomposites. The figure shows that the optical conductivity decreased with the increasing of the wavelength for all samples of nanocomposites and increases at low wavelength, The increased optical conductivity at the low wavelength of photon is due to the high absorption of all nanocomposites samples in this region, hence, increase of the charge transfer excitations. Also the spectrums show high transmittance at visible and near IR regions, also the optical conductivity increases with increasing of SiO_2 and CeO_2 nanoparticles concentrations this is due to the creation of localized levels in the energy gap. where the absorption coefficient increasing photoconductivity increases, This behavior consistent with the results of researcher[97].

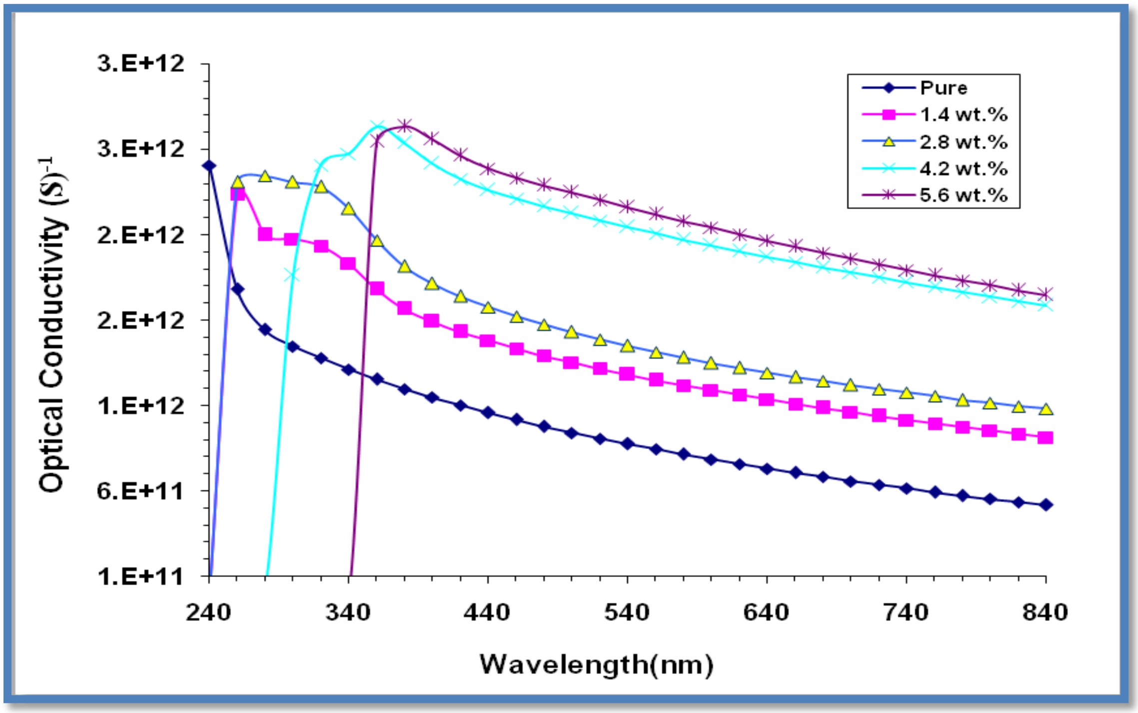


Figure (4.13): Variation of optical conductivity for (PMMA/SiO_2-CeO_2) nanocomposites with wavelength

4.4 The Results of A.C Electrical Properties

4.4.1 Dielectric constant (ε') and dielectric loss (ε'') of (PMMA/SiO_2-CeO_2) nanocomposites

Figures (4.14) and (4.15) show the variation of dielectric constant and dielectric loss of (PMMA/SiO_2-CeO_2) nanocomposites with frequency respectively. The dielectric constant and dielectric loss of nanocomposites was calculated by using equation (2.18) and (2.19) respectively. The results show the dielectric constant and dielectric loss decreases with increasing of the frequency (f) of applied electrical field for all samples. The reason of this at low frequencies the dipoles that resulting from the application of alternating current applied to the insulating material tend to keep up with the direction of the applied electric field, i.e. a charge buildup occurred. Which leads to an increase in polarization and thus an increase in the dielectric constant and dielectric loss. At a high frequencies the dipoles are unable to keep up with the direction of movement of the applied electric field due to the shorter time available for the dipoles to alignment , which leads to a decrease in polarization and thus a decrease in the value of the dielectric constant and dielectric loss. This feature can be used in many applications such as communication antennas and some microwave components. Also, observed from the figures the **(ε')** and (ε'') increases again to the highest value at ($f = 4$)MHz for the nanocomposites, this high value in dielectric constant and dielectrics loss tend to highest absorption was happened. This absorption is caused by a phenomenon called Maxwell-Wagner[101]. This phenomenon produced by alternating current where an externally applied field forces charges to align the field and form large dipoles[102,103].

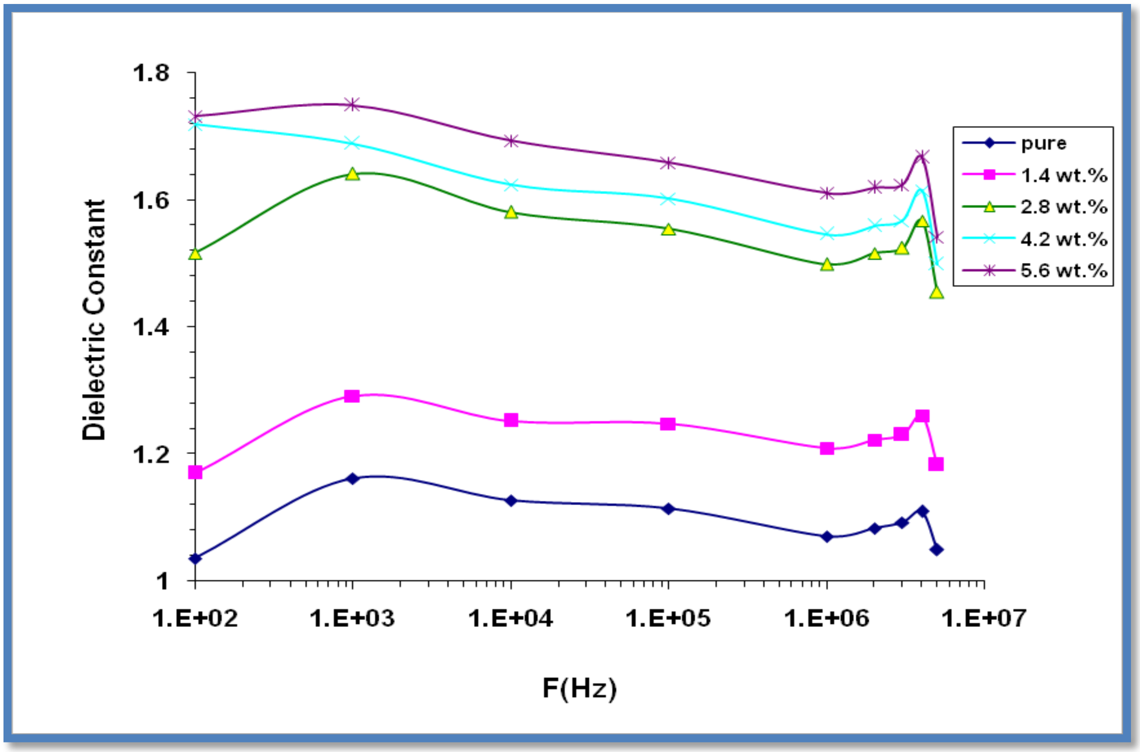


Figure (4.14): Performance of dielectric constant for nanocomposites against frequency

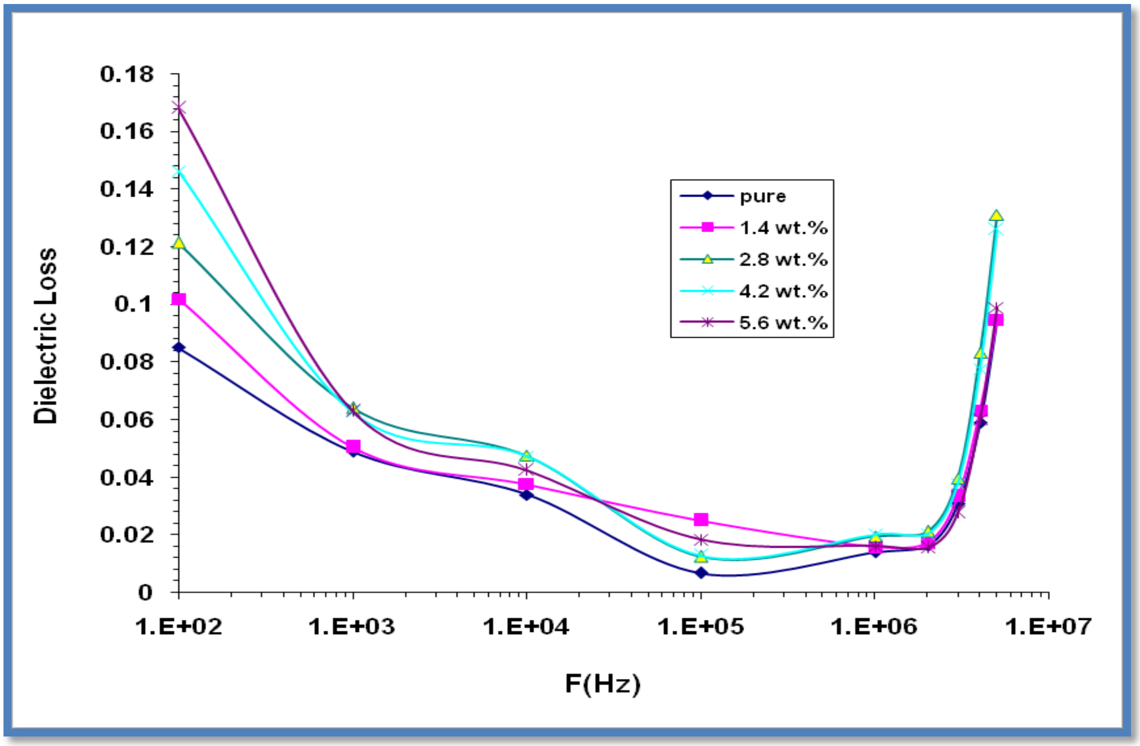


Figure (4.15): Performance of dielectric loss for nanocomposites against frequency

Figures (4.16) and (4.17) show the variation of dielectric constant and dielectric loss with concentrations of nanoparticles for (PMMA/SiO_2-CeO_2) nanocomposites. The figures show how the (ε') and (ε") increases with the increasing of the concentrations of SiO_2 and CeO_2 nanoparticles, this behavior may be return to interfacial polarization inside the nanocomposites in applied electric field and an increase in charge carriers when polarization occurs and thus an increase in the value of the dielectric constant and dielectric loss. This behavior consistent with the results of researchers[104,105].

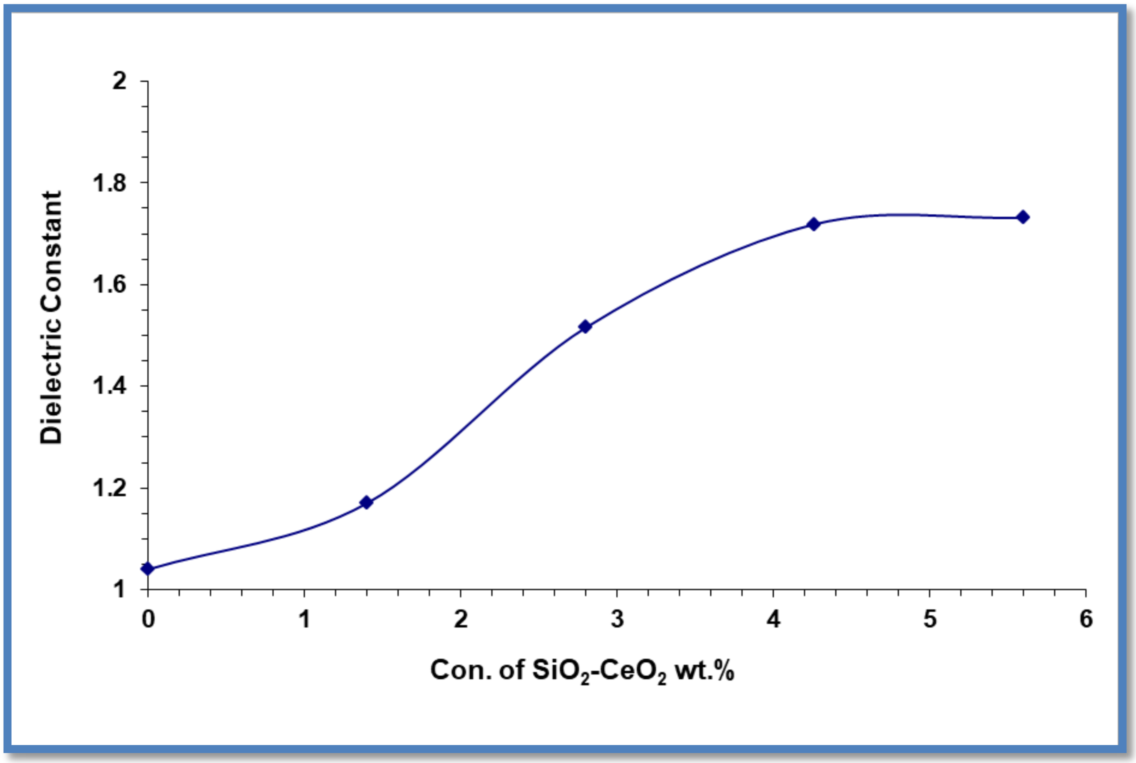


Figure (4.16): Performance of dielectric constant for nanocomposites with concentrations of (SiO_2 & CeO_2) nanoparticles

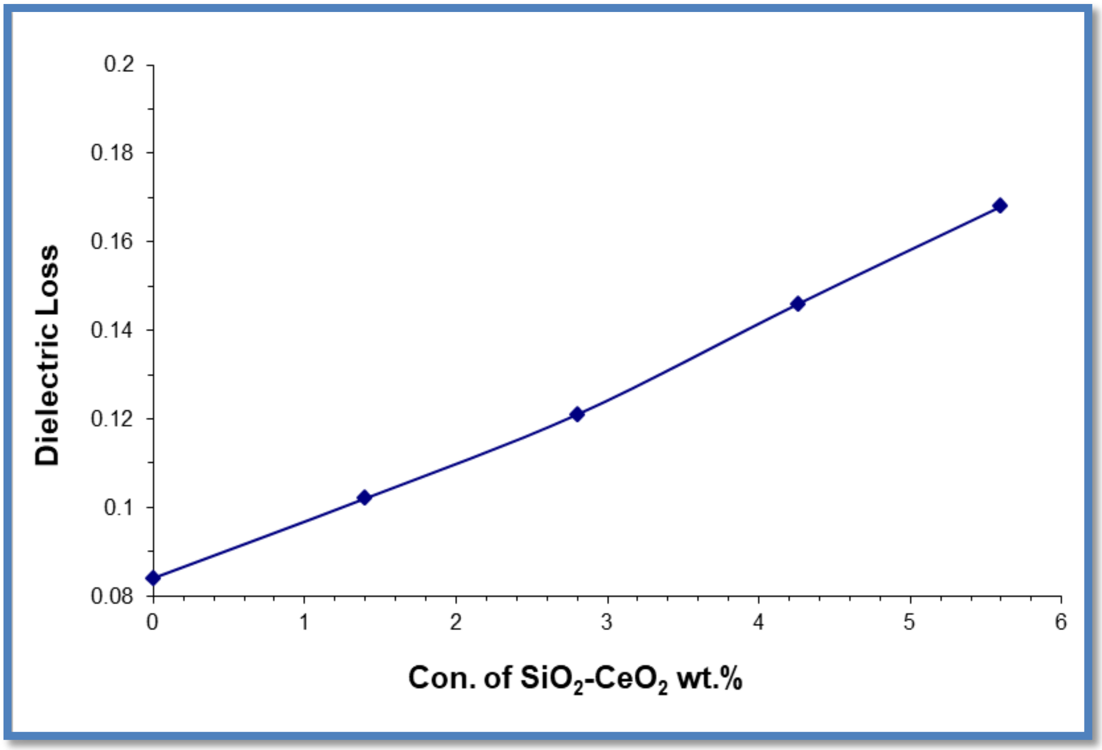


Figure (4.17): Performance of dielectric loss for nanocomposites with concentrations of (SiO_2 & CeO_2) nanocomposites

4.4.2 A.C Electrical conductivity of (PMMA/SiO_2-CeO_2) nanocomposites

A.C conductivity is a measure of the heat generated by rotating dipoles from their positions or the vibration of charges by changing the direction of the alternating field which was calculated by the equation (2.20). Figure (4.18) shows the variation of the A.C electrical conductivity for (PMMA/SiO_2-CeO_2) nanocomposites with frequency of the electric field at room temperature. It was observed that the A.C conductivity increased with increasing of frequency for all samples. In the low frequencies the insulator molecules get polarized which occurred more charge carriers accumulate, leads to a decrease in the number of mobile ions in the conduction band and thus a lead to decrease in A.C electrical conductivity. At high frequency the movement of the charge carriers of the conduction band increases and thus the conductivity value improves. Figure (4.19) shows the variation of A.C conductivity for (PMMA/SiO_2-CeO_2) nanocomposites with concentrations of SiO_2 and CeO_2 nanoparticles. The A.C conductivity increases with the increasing the concentrations of nanoparticles. This is increase caused by the increases in the number of charge carries due to nanoparticles adds a positional levels inside the energy gap and thus increases the conductivity. This behavior consistent with the results of researchers[106,107].

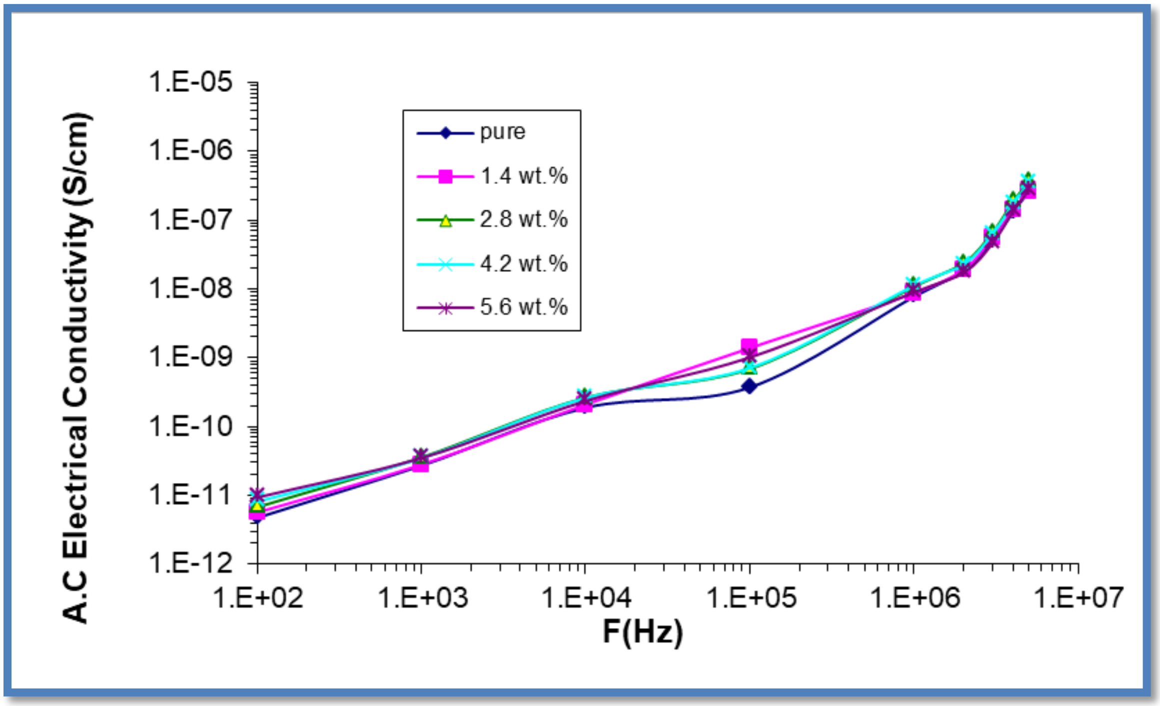


Figure (4.18): Performance of A.C conductivity of of (PMMA/SiO_2-CeO_2) nanocomposites with frequency

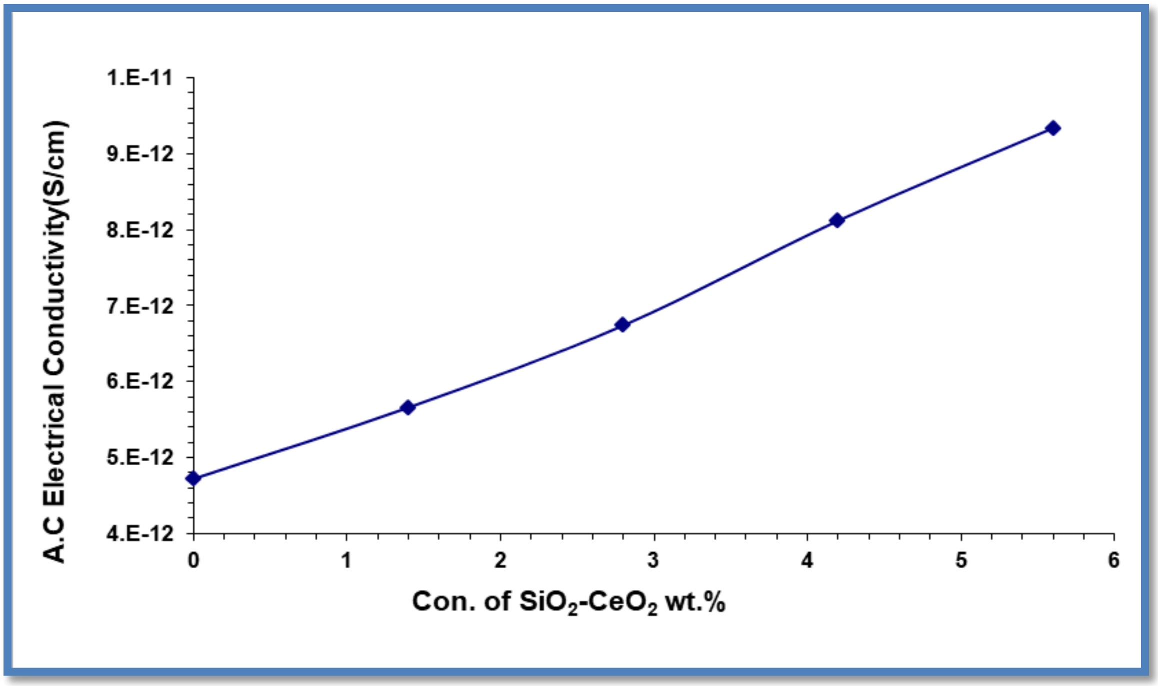


Figure (4.19): Performance of A.C conductivity for (PMMA/SiO_2-CeO_2) nanocomposites with concentrations of (SiO_2 & CeO_2) nanoparticles

4.5 Application of (PMMA/SiO_2-CeO_2) Nanocomposites for Antibacterial Acyivity

In this work, tested inhibition of nanocomposites for antibacterial activity by using the agar diffusion method for two types of bacteria gram-positive (Staphylococcus aureus) and gram-negative (Proteus vulgaris), as shown in figure (4.20) by taking the diameter of the sample equal to (1) cm. Figures (4.21) and (4.22) show inhibition zone diameter of (PMMA/SiO_2-CeO_2) nanocomposites against the concentractions of nanoparticels for all sampels. The inhibition zone increases with increasing the concentrations of SiO_2 and CeO_2 nanoparticles. The antibacterial activity of (PMMA/SiO_2 -CeO_2) may be caused by oxidative stress caused by the reactive Oxygen species (ROS) of SiO_2 and CeO_2 nanoparticles that could damage DNA and proteins in bacteria. The possible mechanism of action is that (PMMA/SiO_2-$CeO_{2)}$ nanocomposites carry positive charges and bacteria have negative charges that create electromagnetic attraction between microbes and nanoparticles of nanocomposites. When the interaction takes place, the microbes oxidize and die instantly. This behavior consistent with the results of researchers [108,109]. Table (4.2) shows the inhibition zone diameter of (PMMA/SiO_2-CeO_2) nanocomposites against Staphylococcus and Proteus bacteria.

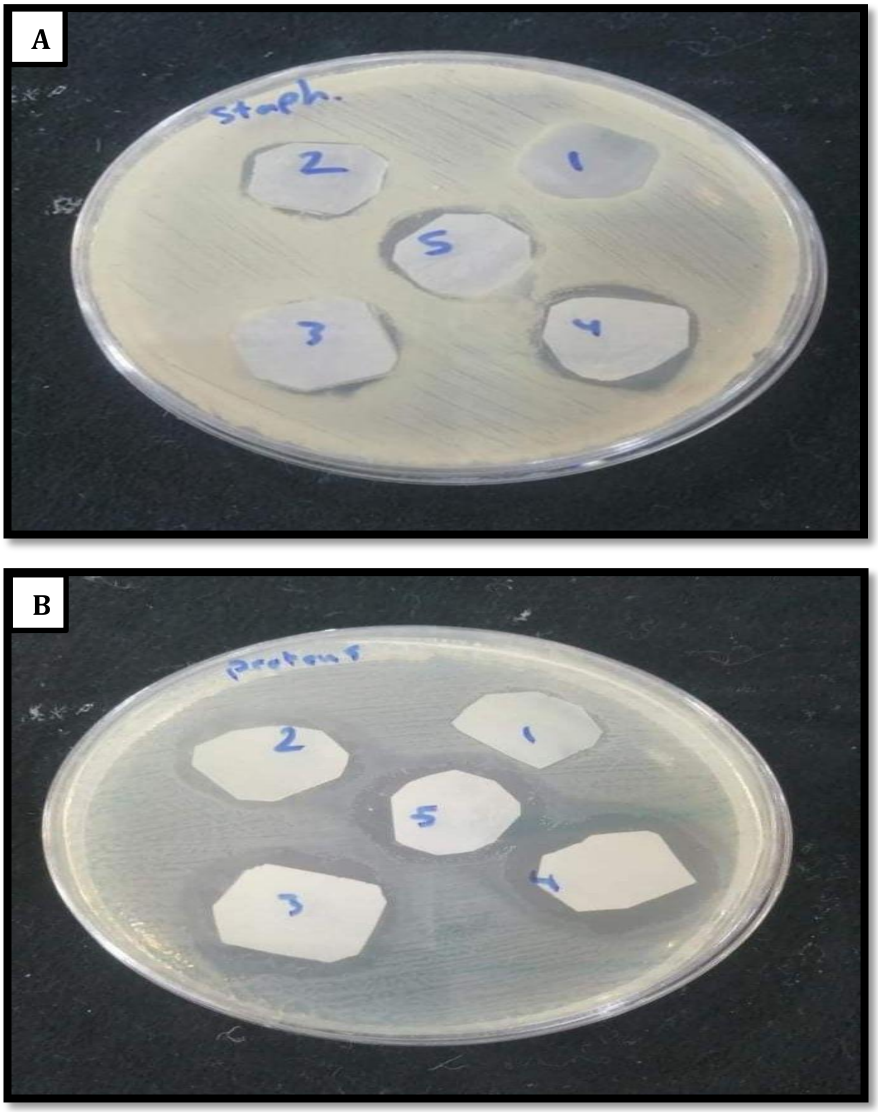


Figure (4.20): Images of inhibition zone for(a) Staph. aureus bacteria

(b) Proteus vulgaris bacteria

Table (4.2): Inhibition zone diameter of (PMMA/SiO_2-CeO_2) nanocomposites against Staphylococcus and Proteus bacteria

concentrations of SiO_2-CeO_2 wt.%	Inhibitions zone diameter(mm) of Staph. aureus	Inhibitions zone diameter (mm) of Proteus vulgaris
0	0	**0**
1.4	18	**24**
2.8	21	**28**
4.2	22	**29**
5.6	23	**30**

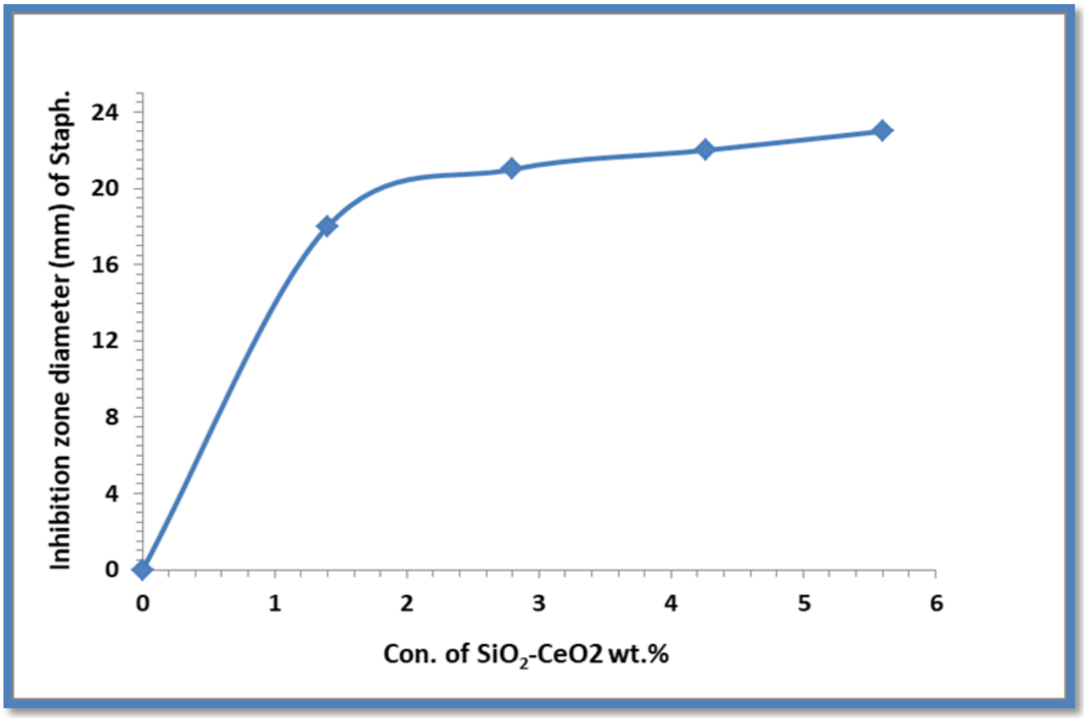


Figure (4.21): Inhibition zone diameter of (PMMA/SiO_2-CeO_2) nanocomposites against Staphylococcus bacterial

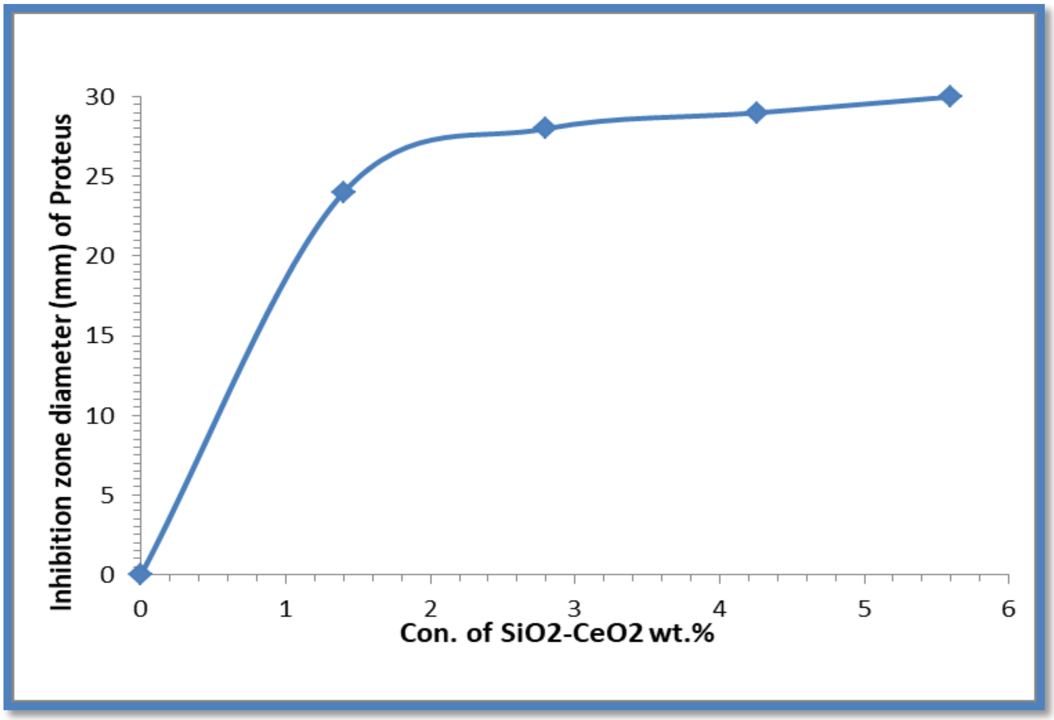


Figure (4.22): Inhibition zone diameter of (PMMA/SiO_2-CeO_2) nanocomposites against Proteus bacterial

4.6 Conclusion

1. The SEM images showed the homogeneous and a good distribution in the surface morphology.
2. The optical microscope images showed the homogeneous distribution of nanoparticles in the polymeric matrix and appearance network paths with increasing the concentrations of the SiO_2 and CeO_2 nanoparticle.
3. The results of the FTIR measurements shown that there is a physical superposition between the polymer and the nanoparticles when mixed it.
4. The absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants of (PMMA/SiO_2-CeO_2) nanocomposite increase with increasing of the SiO_2 and CeO_2 nanoparticles concentrations. The transmittance and energy gap decrease with increasing the SiO_2 and CeO_2 nanoparticles concentrations. The (PMMA/SiO_2-CeO_2)

nanocomposites have high absorbance in the U.V region. These results make the (PMMA/SiO_2-CeO_2) nanocomposites can be used for photonics and electronics applications.

5. The dielectric constant, dielectric loss and A.C electrical conductivity of (PMMA/ SiO_2-CeO_2) nanocomposite increase with increasing the SiO_2 and CeO_2 nanoparticles concentrations. The dielectric constant and dielectric loss of nanocomposites are decreased while the A.C electrical conductivity is increased with increasing the frequency.
6. The inhibition zone for Staph. aureus and Proteus vulgaris increases with increasing the concentrations of SiO_2 and CeO_2 nanoparticles.

4.7 Future Works

1. Studying the D.C electrical properties of (PMMA/SiO_2-CeO_2) nanocomposites.
2. Investigating the mechanical and thermal properties of (PMMA/SiO_2-CeO_2) nanoparticles.

Studying effect of gamma radiation on some physical properties of (PMMA/SiO_2-CeO_2) nanoparticles.

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الخلاصة

تم تحضير المتراكبات النانوية (بوليمر بولي مثيل ميثا كليرات/ أكسيد السليكا/ أكسيد السيريوم) بطريقة الصب لتراكيز مختلفة من الجسيمات أكسيد السليكا وأكسيد السيريوم النانوية لدراسة الخصائص التركيبية و البصرية وكذلك الكهربائية للمتراكبات النانوية لاستخدامه كمضاد للبكتيريا. الخصائص التركيبية التي تشمل المجهر الضوئي (OM), والمجهر الإلكتروني الماسح (SEM), وتحويل فورييه للأشعة تحت الحمراء (FTIR). أظهرت صور المجهري الضوئي أنه مع زيادة تركيزات الجسيمات النانوية تتشكل مسارات شبكية داخل المصفوفة البوليميرية التي تعمل بمثابة ناقلات للشحنة, وأظهرت نتائج قياس SEM التوزيع الجيد والمتجانس للجسيمات النانوية على مورفولوجيا السطح. أما نتائج FTIR فقد أشارت إلى حصول تراكب فيزيائي بين المصفوفة البوليميرية والجسيمات النانوية. أما نتائج الخصائص البصرية للمتراكبات النانوية ($PMMA/SiO_2$-CeO_2) أظهرت أن الامتصاصية والنفاذية ومعامل الامتصاص ومعامل الخمود ومعامل الانكسار وثوابت العزل الحقيقي والخيالي وكذلك الموصلية البصرية تزداد مع زيادة تراكيز الجسيمات النانوية SiO_2 و CeO_2, بينما فجوة الطاقة والنفاذية تقل مع زيادتها. أشارت أيضا أن أعلى امتصاص حدث للطيف في منطقة الأشعة فوق البنفسجية. أظهرت نتائج الخواص الكهربائية للمتراكبات النانوية أن ثابت العزل و فقد العزل الكهربائي تنخفض مع زيادة تردد المجال الكهربائي المسلط وتزداد بزيادة تراكيز الجسيمات النانوية (SiO_2-CeO_2). بينما تزداد التوصيلية الكهربائية المتناوبة مع زيادة التردد ومع زيادة النسب الوزنية لجسيمات SiO_2 و CeO_2 النانوية.أظهرت نتائج تطبيقات المركبات النانوية ($PMMA/SiO_2$-CeO_2) ضد البكتريا أن قطر منطقة التثبيط يزداد مع زيادة تراكيز الجسيمات النانوية.

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قسم الفيزياء

استقصاء خصائص و أداء المتراكبات النانوية (مادة عضوية – أكاسيد المعادن)للتطبيقات الحديثة

رسالة مقدمة الى مجلس كلية التربية للعلوم الصرفة في جامعة بابل

كجزء من متطلبات نيل دراسة الماجستير في التربية / الفيزياء

من قبل

علا باسم فاضل وصيخ

بكالوريوس علوم فيزياء

جامعة بابل (٢٠١٩)

بإشراف

أ. د أحمد هاشم محيسن

أستاذ في جامعة بابل/كلية التربية للعلوم الصرفة/ قسم الفيزياء

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