

# Structural, Optical, Dielectric and Ferroelectric Studies of Yttrium Oxide Nanoparticles Synthesised by Hydrothermal Method

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# Abstract

Yttrium Oxide ( $\text{Y}_2\text{O}_3$ ) is a chemically stable rare-earth oxide having unique optoelectronic and dielectric properties.  $\text{Y}_2\text{O}_3$  nanoparticles are of great interest in various fields due to their unique properties and potential applications in advanced technologies. The present study focuses on the synthesis of  $\text{Y}_2\text{O}_3$  nanoparticles by a surfactant-assisted hydrothermal method with a view to incorporating them in polymer matrices for biosensor applications. The synthesized nano materials characterized by XRD for structural analysis, confirming the formation of  $\text{Y}_2\text{O}_3$  with an average crystallite size of 19 nm determined by the Scherrer method and 23 nm from Williamson–Hall analysis. FESEM with energy-dispersive X-ray (EDX) was performed to elucidate the morphology and elemental composition. The FTIR spectroscopy confirms the formation of  $\text{Y}_2\text{O}_3$  from its precursors. Band gap energy and optical constants were evaluated from the UV/VIS/NIR absorption spectrum, which showed a direct band gap of 3.87 eV and a refractive index of 2.14. Photoluminescence measurements exhibited a prominent emission peak at 365 nm, attributed to oxygen-vacancy-related radiative recombination. Dielectric studies revealed frequency-dependent behaviour with an average dielectric constant of 5.68 and low dielectric loss. The obtained results demonstrate that the synthesised  $\text{Y}_2\text{O}_3$  nanoparticles possess favourable optical and dielectric characteristics, making them promising candidates for optoelectronic devices, phosphors, sensors and polymer-based functional composites.

## 1 Introduction

Yttrium oxide ( $\text{Y}_2\text{O}_3$ ) is a significant rare-earth compound and has been studied with great interest in recent years.  $\text{Y}_2\text{O}_3$  is widely used in diverse fields owing to its fascinating optical, electrical and thermal properties [1–7].  $\text{Y}_2\text{O}_3$  exhibits excellent thermodynamic stability, corrosion resistance, high chemical stability and hardness [8–10]. This stable composite material is biocompatible and can be used in biomedical applications [11–13]. The high surface area and stability of  $\text{Y}_2\text{O}_3$  nanoparticles contribute to excellent luminescent properties, which make them remarkable candidates in applications such as phosphors in display technologies and bio labeling in medical diagnostics [12–14].  $\text{Y}_2\text{O}_3$  nanoparticles are explored for their potential use in solid-state lighting and as additives in ceramics to enhance mechanical strength and thermal resistance [12–15]. Their biocompatibility further opens avenues for biomedical applications, including drug delivery and imaging [15,16]. Yttria could be synthesised via several methods, including cathodic electrodeposition, gas-phase condensation, precipitation, sol–gel, pyrolysis, solvothermal and hydrothermal syntheses [17,18]. The hydrothermal method has proven to be effective for the synthesis of nanoparticles due to extensive milling, high phase purity and narrow particle size distribution [19–21]. As reported before, the hydrothermal technique can not only provide a homogeneous nucleation process to control the size and morphology of crystallites but also significantly reduce the aggregation levels [22–24]. Therefore, hydrothermal synthesis was adopted in the present study to obtain highly crystalline  $\text{Y}_2\text{O}_3$  nanoparticles with controlled morphology and desirable optical and dielectric properties while maintaining a simple and cost-effective fabrication process. As research

continues to explore its potential, yttrium oxide nanoparticles play a key role in the development of novel technologies in various fields.

Despite considerable attempts to synthesise  $Y_2O_3$  nanostructures using a variety of techniques, most published investigations focus on structural, morphological, or optical characterisation. There aren't many comprehensive studies that relate the optical, dielectric, and ferroelectric properties of hydrothermally generated  $Y_2O_3$  nanoparticles to their structural features. In particular, it is necessary to comprehend the multifunctional characteristics of  $Y_2O_3$  nanoparticles in order to evaluate their viability in polymer matrices for biosensor applications, optoelectronic devices, dielectric components, and polymer-based functional composites. In order to fully investigate the optical, dielectric, ferroelectric, structural, and morphological features of  $Y_2O_3$  nanoparticles, this work aims to synthesise them through a surfactant-assisted hydrothermal approach. The findings provide additional insight into the structure-property relationship of  $Y_2O_3$  nanoparticles and their potential technological applications.

## 2. Experimental Procedure

Nanoparticles of Yttrium Oxide ( $Y_2O_3$ ) are synthesised by the hydrothermal method. The precursor solution was prepared using 0.1 M aqueous yttrium nitrate ( $Y(NO_3)_3 \cdot 6H_2O$ , purchased from Thermo Fisher Scientific) and sodium hydroxide solutions, while 0.15 mL of polyethylene glycol was added as a surfactant to control particle growth and agglomeration. About 20 mL of  $Y(NO_3)_3 \cdot 6H_2O$  (0.1 M) was taken in a beaker. 20 mL of NaOH was added and stirred vigorously for 30 minutes to make a homogeneous solution. The homogeneous mixture was poured into a Teflon-lined autoclave and heated at a temperature of 180°C for 4 h. The autoclave was allowed to cool. The final solution was washed several times with distilled water and subsequently dried at 200°C for 2 h. X-ray diffraction study and FTIR were performed to evaluate the crystallinity and structure. The morphology and purity of the products were tested by SEM and EDAX. The optical properties were analysed by UV-Visible spectroscopy and photoluminescence studies. The dielectric and ferroelectric properties were also analysed.

## 3 Results and Discussion

### 3.1 Structural characterization

#### 3.1.1 X-ray Diffraction Analysis

The X-ray diffraction (XRD) pattern of the  $Y_2O_3$  nanoparticles is shown in Fig. 1. The analysis was carried out using Cu-K $\alpha$  radiation ( $\lambda = 1.54 \text{ \AA}$ ) from 5° to 90°. The characteristic Bragg diffraction at  $2\theta$  values of approximately 20.42°, 29.10°, 33.77°, 48.50° and 57.45° are indexed to the (211), (222), (400), (440) and (622) planes, respectively, by comparison with JCPDS card No. 41-1105 [24]. The distinct and sharp peaks signify that the synthesised yttrium oxide nanoparticles are highly crystalline and pure. No

impurity peaks are detected, which indicates the formation of pure Y<sub>2</sub>O<sub>3</sub> nanoparticles. The crystalline size of the nanoparticles is calculated using the Scherrer formula [25],

$$d = \frac{0.94 \lambda}{\beta \cos \theta} \quad (1)$$

where d is the diameter of the crystalline particle, λ is the wavelength of the X-ray radiation, θ is the angle of diffraction, and β is the full width at half maximum of the peak (FWHM). The average crystallite size of the nanoparticle is found to be 19 nm. The term βcosθ is plotted with respect to 4sinθ, and the peaks of Y<sub>2</sub>O<sub>3</sub> and the Williamson-Hall (W-H) plot are obtained as in the inset of Fig. 1. From the obtained slope and y- intercept of the fitted line, strain is obtained as 0.01411 and crystallite size is 12 nm, as calculated by the W-H equation, which is given by,

$$\beta_{hkl} = \frac{K\lambda}{D} + 4\epsilon \sin\theta$$

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where ε is the lattice strain. The W-H method assumes a uniform strain distribution throughout the crystallites, whereas the actual strain distribution may vary along different crystallographic directions. The negative slope observed in the present plot suggests a compressive-type apparent lattice strain in the Y<sub>2</sub>O<sub>3</sub> crystallites. Nevertheless, the overall linear trend confirms the coexistence of size-induced and strain-induced broadening in the synthesised Y<sub>2</sub>O<sub>3</sub> nanoparticles. The dislocation density is calculated using the equation,

$$\delta = \frac{1}{D^2}$$

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where D is the crystallite size obtained from the Scherrer equation. The dislocation density is found to be 0.833 × 10<sup>15</sup> m<sup>-2</sup>.

### 3.1.2 SEM and EDX Analysis

The surface features and morphology of the synthesised Y<sub>2</sub>O<sub>3</sub> nanoparticles were examined using a Hitachi SU6600 Variable Pressure Field Emission Scanning Electron Microscope (FESEM). Representative micrographs and the corresponding EDX spectrum are presented in Fig. 2 and Fig. 3. At a magnification of 40,000×, the FESEM image reveals that the particles tend to cluster densely, forming assemblies composed of thin, irregular plates. These plate-like units resemble stacked or partially overlapped sheets, producing a lamellar configuration. The sheets possess uneven textures and appear brittle, with some edges showing fragmentation into sharper, angular pieces. In several regions, the layered structures fold or accumulate into rosette-like aggregates, suggesting a growth process in which

rapid nucleation is followed by expansion along planar directions. The lateral spread of these sheets generally falls within the 100–400 nm range, while their thickness is considerably smaller, consistent with nanoscale lamellae. Overall, the morphology points to densely compacted nanosheets with minimal open porosity.

The EDX analysis confirms the elemental composition of the sample. Only yttrium and oxygen peaks are detected in the spectrum, indicating that the synthesised material corresponds to phase-pure  $Y_2O_3$  without any noticeable elemental contaminants.

### 3.1.3 FTIR

Fourier Transform Infrared spectra of the sample synthesized in the present investigation were recorded using a JASCO (FT/IR 4700LE) spectrometer. Figure 4 shows the FTIR spectrum of  $Y_2O_3$  nanoparticles. The bands at 740 and 856  $cm^{-1}$  are attributed to the absorption of  $CO_3^{2-}$  [26,27]. The broad band at 3500  $cm^{-1}$  is associated with the –OH stretching vibration mode [28]. The bands at 1510  $cm^{-1}$ , 1411  $cm^{-1}$  and 1052  $cm^{-1}$  are assigned to different vibrations of the carboxylate group, which may originate from  $CO_2$  absorption when exposed to air [29–31]. Absorption bands corresponding to the Y-O stretching mode appear at 555  $cm^{-1}$  and 464  $cm^{-1}$ , indicating the formation of  $Y_2O_3$  nanoparticles [31]. In the present work, the thermal treatment at 200°C corresponds to a drying process rather than a high-temperature calcination step. The weak absorption bands associated with the  $CO_3^{2-}$  and -OH groups suggest the presence of residual surface species originating from atmospheric  $CO_2$  adsorption and adsorbed moisture. Similar features have frequently been reported for hydrothermally synthesised rare-earth oxide nanoparticles [32]. Although calcination at higher temperatures can further eliminate these surface hydroxyl and carbonate groups [8, 33], the XRD analysis confirms the formation of crystalline cubic  $Y_2O_3$  without detectable secondary phases. Therefore, the residual carbonate and hydroxyl species can be attributed to surface-adsorbed groups rather than incomplete phase formation.

## 3.2 Optical Characterisation

### 3.2.1 UV-Visible spectroscopic analysis

The optical studies of the synthesised  $Y_2O_3$  nanoparticles were analysed by UV-Visible spectra using a JASCO V570 spectrophotometer. The UV-Visible absorption spectra of the prepared sample of the  $Y_2O_3$  nanoparticles are shown in Fig. 5a. The UV spectra between 200 and 800 nm were analysed. It shows a sharp peak at 289 nm. This indicates good absorbance in the UV region. The energy gap is calculated using the Tauc method. The Tauc relation is,

$$(\alpha h\nu)^n = A(h\nu - E_g) \quad (4)$$

where  $\alpha$  is the absorption coefficient,  $h$  is Planck's constant,  $\nu$  is the frequency,  $A$  is a constant that depends upon the transition probability, and  $E_g$  is the band gap energy.  $n$  is an index that assumes the

values 1/2, 3/2, 2 and 3 depending on the nature of electronic transitions responsible for absorption.  $Y_2O_3$  is widely reported to exhibit a direct band-gap electronic structure. Band-structure calculations and optical studies have shown that the valence band, mainly composed of O 2p states, and the conduction band, predominantly formed by Y 4d states, allow direct optical transitions at the fundamental absorption edge [34]. Therefore, the Tauc relation for direct allowed transitions ( $n = 2$ ) was employed, and a plot of  $(\alpha h\nu)^2$  versus  $h\nu$  was used to estimate the optical band-gap energy. In direct transitions, electrons and holes can recombine directly with a photon, conserving both energy and momentum. A graph of  $(\alpha h\nu)^2$  vs.  $h\nu$  is plotted, and the band gap is obtained by linear fitting. The Tauc plot is obtained as in Fig. 5b. The value of  $E_g$  is obtained as 3.87 eV. The obtained band-gap value is lower than that generally reported for bulk  $Y_2O_3$ , ranging between 5.6 eV and 6 eV [34]. This reduction may be attributed to defect states associated with oxygen vacancies, surface states introduced by the nanoscale dimensions of the particles, and localised energy levels arising from residual hydroxyl and carbonate species identified in the FTIR spectrum. These defect-related states can extend into the forbidden energy region, facilitating lower-energy electronic transitions and resulting in an apparent narrowing of the optical band gap. The refractive index ( $n$ ) of the prepared sample can be determined using the Dimitrov – Sakka formula given by,

$$\frac{n^2 - 1}{n^2 + 2} = 1 - \sqrt{\frac{E_g}{20}}$$

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The value of refractive index is obtained as 2.14 for the synthesized  $Y_2O_3$  nanoparticles. This implies that the material is a high-index optical material, indicating that the nanoparticles are well crystallised and packed, leading to significant light refraction. This is significant in nanocomposites, as adding  $Y_2O_3$  nanoparticles to a polymer matrix, such as polyvinylidene difluoride, increases the overall refractive index of the composite membrane, which is crucial for advanced optical devices and sensors [35–37]. The transmittance spectrum in Fig. 5c reveals that the synthesized nanoparticles are highly non-absorbing in the visible spectrum, which is a desirable feature for host materials in phosphors or laser ceramics. The sharp decline in the transmittance spectrum, which is the absorption edge, is observed in the ultraviolet region between 200 nm and 350 nm. This indicates the onset of fundamental absorption, in which photons have sufficient energy to excite electrons from the valence band to the conduction band. The optical conductivity is a crucial parameter as it provides insights into the electronic structure and dynamics of a material. The variation of optical conductivity against photon energy is illustrated in Fig. 5d. The obtained spectrum indicates that the optical conductivity increases with photon energy up to 4.33 eV, and thereafter it declines. This variation in optical conductivity is similar to the variation in optical density with photon energy, which is depicted in Fig. 5e. Higher optical density implies a higher absorption coefficient. The optical conductivity is proportional to the absorption coefficient and the refractive index ( $n$ ) of the material, expressed by the relation,

$$\sigma_{opt} = \frac{\alpha n c}{4\pi}$$

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where  $c$  is the speed of light. When optical density increases, more photons are absorbed, generating more free charge carriers to participate in conduction. When optical density decreases, the material becomes more transparent, meaning fewer electronic transitions are occurring.

### 3.2.2 Photoluminescence studies

The photoluminescence spectra of  $Y_2O_3$  nanoparticles were recorded using Shimadzu RF-5301PC at the excitation wavelength of 288 nm. This specific value was selected to coincide with the sharp absorption peak observed at 289 nm in the UV absorption spectrum. Excitation under these near-resonant conditions ensures efficient absorption of incident photons, thus maximising the luminescence signal and enabling a reliable correlation between the absorption and emission properties of the material. The Photoluminescence spectrum is presented in Fig. 6. The spectrum shows a broad band in the range of 340–400 nm, in agreement with previous reports [38]. The emission spectrum shows a peak at 365 nm. The luminescence band with a peak at 365 nm might be due to the presence of oxygen vacancies related to radiative recombination of excitons [38]. The electrons get trapped in the intermediate energy levels created by the oxygen vacancies within the band gap. When the electron drops from these vacancy levels back to the valence band, it releases energy in the form of light. Since the synthesized sample emits in the UV-blue range, it could potentially be used in phosphors, sensors or photocatalysis.

### 3.3 Dielectric studies

Frequency-dependent dielectric measurements of the synthesized  $Y_2O_3$  nanoparticles were carried out using Keysight Technologies Impedance Analyser E4990. Figure 7a and Fig. 7b show the variation of dielectric constant and loss factor, respectively, with  $\log F$ . The dielectric constant has frequency dependence. It was observed that the dielectric permittivity measured at lower frequency is greater than that at higher frequency. The average value of the dielectric constant is found to be 5.68. The value changes from 7.3 at a frequency of 100 Hz to 4 at a frequency of 5 MHz. These values are lower than those typically reported for bulk  $Y_2O_3$  ( $\approx 10$ –15). This can be explained by several features common to nanostructured materials. Since the nanostructures have a very high surface area compared to their volume, a large portion of the atoms are located at or near the surface, where the regular atomic arrangement needed for strong dipole alignment is disrupted [39]. The SEM image shows that the synthesised sample consists of irregular, plate-like particles that are tightly clustered together, leaving noticeable voids between them. When this powder is pressed into a pellet for dielectric measurement, these gaps create a porous structure, meaning the pellet is much less dense than a solid bulk ceramic. Since the air filling these pores has a dielectric constant close to unity, the overall measured dielectric constant of the pellet is lower than that of dense bulk  $Y_2O_3$ . In addition, boundaries between particles disrupt the regular crystal structure at these points, which also reduces the material's ability to polarise

compared to the well-ordered interior of the particles. The observed decrease in dielectric constant with increasing frequency is consistent with the Maxwell- Wagner interfacial polarisation. At low frequencies, charge carriers have sufficient time to migrate toward and accumulate at grain boundaries and particle interfaces, enhancing the dielectric constant through space-charge polarisation, whereas at higher frequencies, these charges can no longer follow the rapidly alternating field, causing this contribution to diminish [40]. The decrease in dielectric constant with an increase in frequency may be attributed to the electrical relaxation process [26]. Dielectric loss for  $Y_2O_3$  nanoparticles was observed to decrease with frequency, indicating that energy dissipation is relatively low. The variation of real and imaginary parts of the dielectric modulus is shown in Figs. 7b and 7c, respectively. The frequency dependence of the real part of the dielectric modulus ( $M'$ ) showed a significant increase in the lower frequency region before reaching saturation. This indicates that at high frequencies, the dipole orientation could not follow the rapid field oscillations, leading to a constant modulus value. Concurrently, the imaginary part of the dielectric modulus exhibited a decreasing trend with frequency given in Fig. 7d, which can be attributed to the dominance of the carrier hopping mechanism. Figure 7e shows that the AC conductivity increased with frequency. The conductivity values range from  $1.8 \times 10^{-10}$  at low frequencies upto  $2.47 \times 10^{-7}$  S/cm at higher frequencies. Higher frequencies promote the buildup of charge carriers, leading to an increase in AC conductivity. Figure 7f represents the change in real electrical impedance with growing frequency. The magnitude of  $Z'$  falls with rising frequency upto 10 kHz. The change becomes independent of frequency above 10 kHz. The reason could be the space charge polarisation at the grain and grain-boundary interface. The magnitude of  $Z'$  comes to a steady state, and conductivity increases in the high-frequency region because of the liberation of space charges [41,42].

### 3.4 Ferroelectric studies

The ferroelectric behaviour of the  $Y_2O_3$  nanoparticles was evaluated through Polarization- Electric field (P-E) hysteresis measurements, as shown in Fig. 8. The material exhibits a characteristic leaf-like loop rather than a perfectly saturated loop, indicating a paraelectric nature typical of metal oxide nanostructures. At an applied field of  $\pm 200$  kV/cm, the sample reaches a maximum polarisation ( $P_s$ ) of approximately  $0.0015 \mu C/cm^2$ . The non-zero area enclosed by the loop represents the energy dissipated per unit volume per cycle. This energy dissipation may be attributed to the lag in dipole orientation and the hopping of charge carriers under the oscillating external field [43]. The oxygen vacancies create localised dipoles and provide pathways for leakage current, which contributes to the measured dielectric loss.

## 4 Conclusion

Yttrium oxide nanoparticles have been synthesized by the hydrothermal method. The structural, optical and electrical properties of the synthesized nanoparticles are analysed. The X-ray diffraction studies revealed that the synthesized nanoparticles are highly crystalline and pure. The FESEM image shows densely compacted nano sheets with minimal open porosity. The peaks of the EDAX pattern confirm that

the synthesised nanoparticles are pure. The absorption bands of FTIR spectroscopic analysis indicate the formation of  $Y_2O_3$  nanoparticles. The UV-Visible spectroscopic analysis shows good absorbance in the UV region. The synthesized nanoparticles are highly non-absorbing in the visible spectrum, which is a desirable feature for host materials in phosphors or laser ceramics. The variation in optical conductivity is similar to the variation in optical density with photon energy, and the study implies a higher absorption coefficient. The photoluminescence studies indicate that the synthesized material can potentially be used in phosphors, sensors or photo catalysis. The synthesized  $Y_2O_3$  nanoparticles exhibited good dielectric properties. The P-E hysteresis measurements indicate a Para electric nature typical of metal oxide nanostructures. The study shows that the synthesized  $Y_2O_3$  nanoparticles are suitable for optoelectronic applications.

## **Declarations**

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### **Authors' contributions**

Nimisha Babu Raj: Data curation, Investigation, Writing- Original draft preparation, Software. Arun K. J: Conceptualization, Methodology, Investigation, Supervision, Writing- Original draft preparation, Editing, Reviewing, Software, Validation. Asha. K: Visualization, Software. M.D. Aggarwal: Visualization, Software, Validation. Padmaja Guggilla: Visualization, Software, Validation.

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### **Data Availability**

Data sets generated during the study are available from the corresponding author on reasonable request.

### **Ethics approval and consent to participate**

The authors state that the research involves no human participants and/or animals.

### **Consent for publication**

Not applicable.

### **Competing interests**

The authors declare no competing interests.

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## Figures

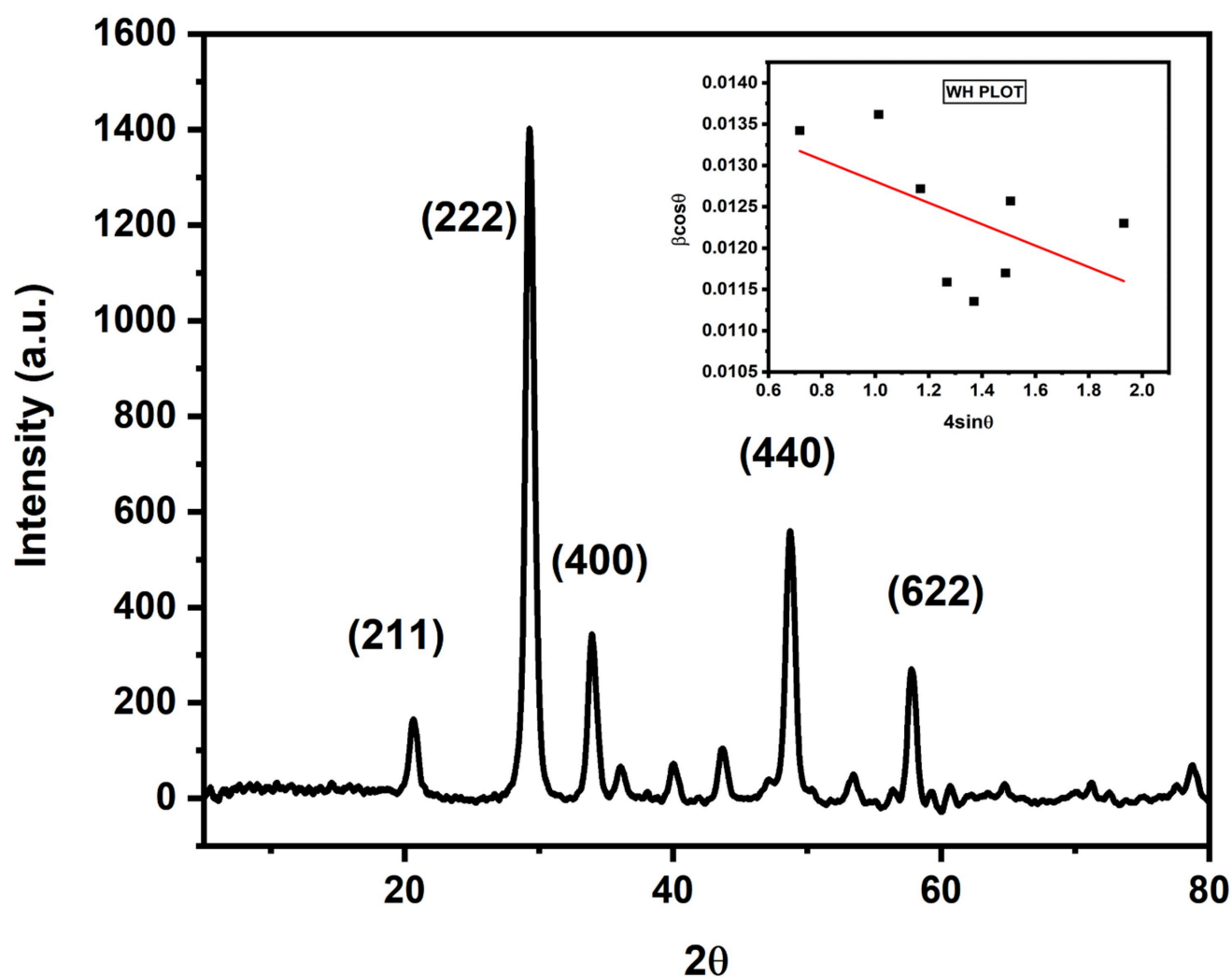


Figure 1

a) XRD image b) W-H plot of prepared  $\text{Y}_2\text{O}_3$  nanoparticles

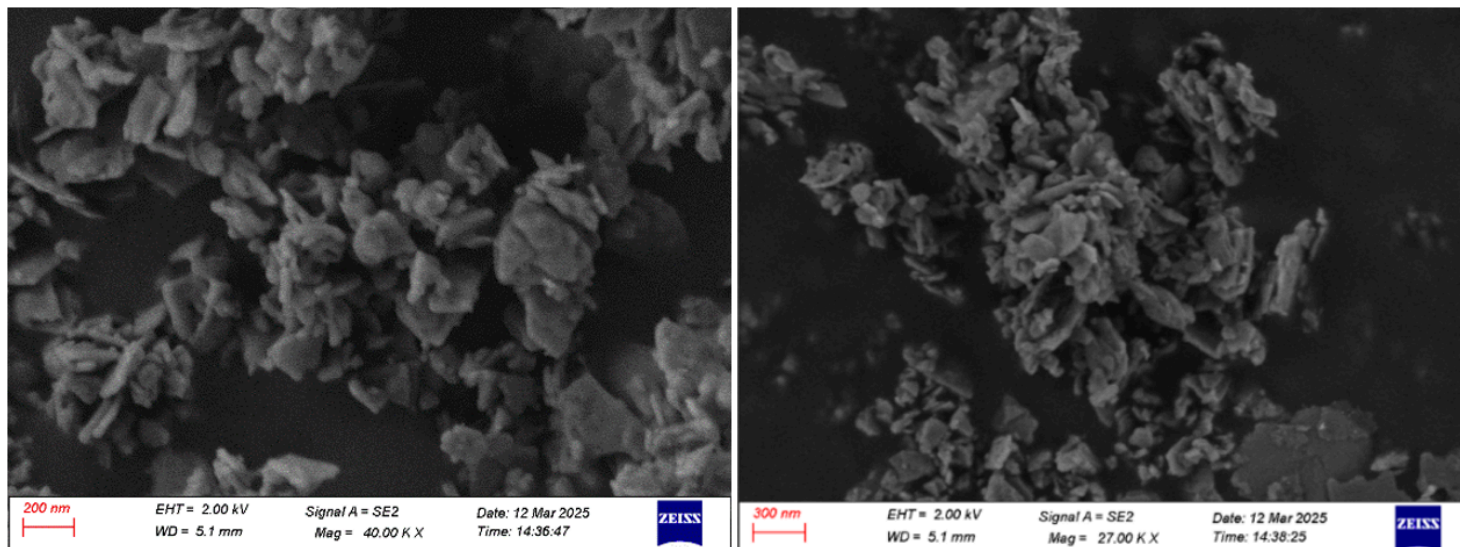


Figure 2

FESEM images of  $\text{Y}_2\text{O}_3$  nanoparticles

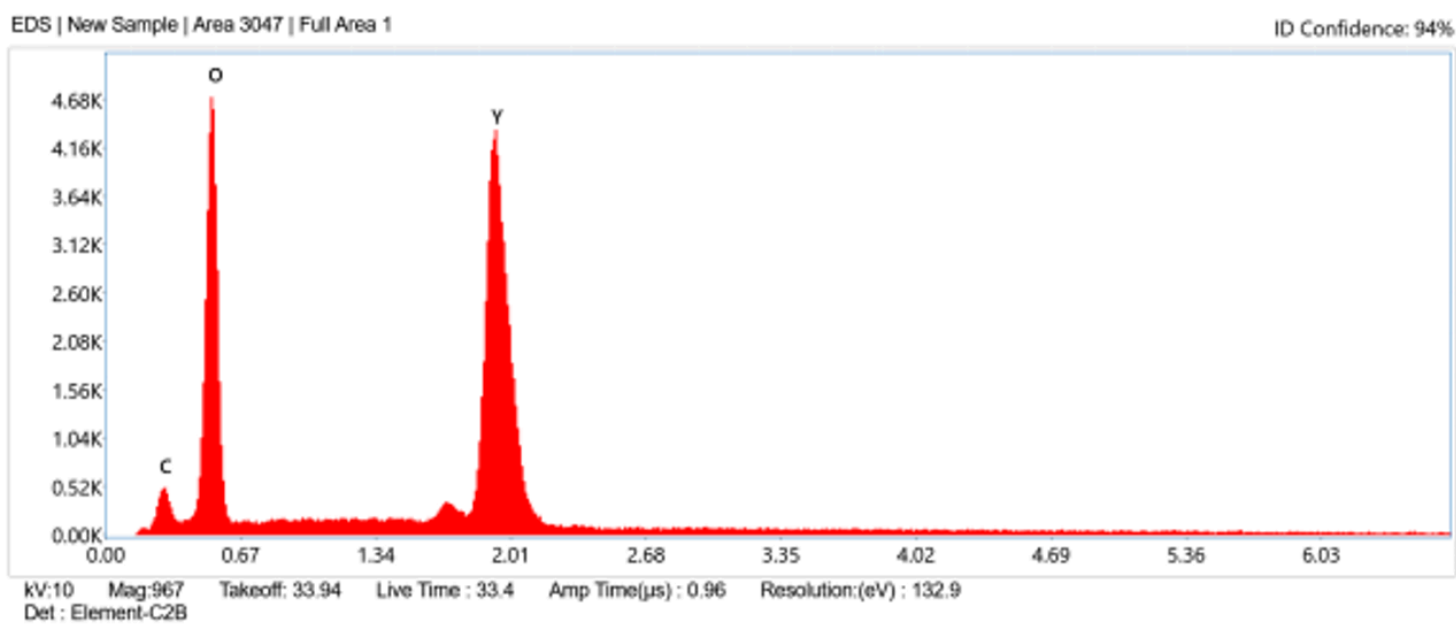


Figure 3

EDAX pattern of  $\text{Y}_2\text{O}_3$  nanoparticles

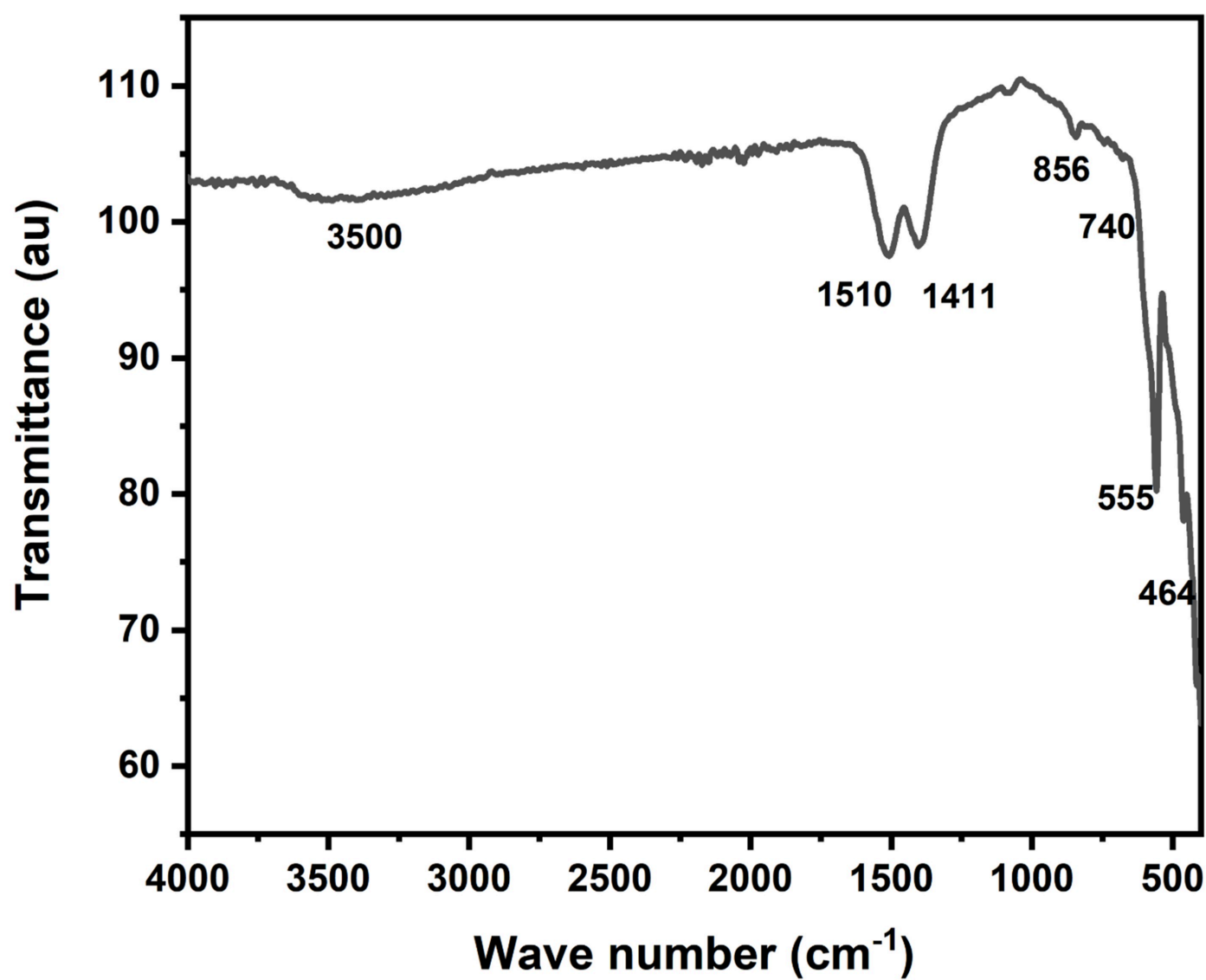


Figure 4

FTIR spectrum of the synthesised Y<sub>2</sub>O<sub>3</sub> nanoparticles

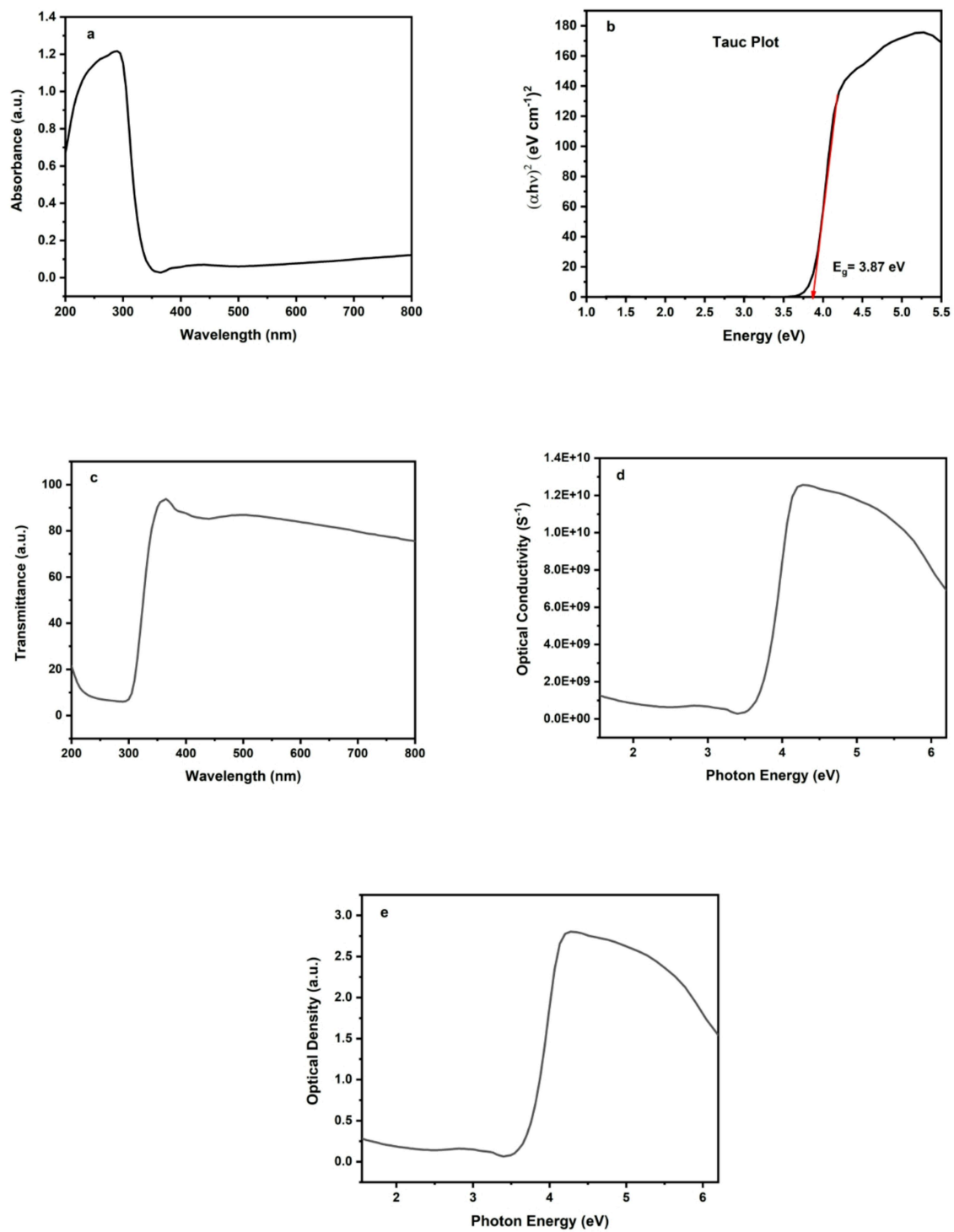


**Figure 5**

a) UV absorption spectrum, 5b) Tauc plot, 5c) transmittance spectrum, 5d) optical conductivity and 5e) optical density of  $\text{Y}_2\text{O}_3$  nanoparticles

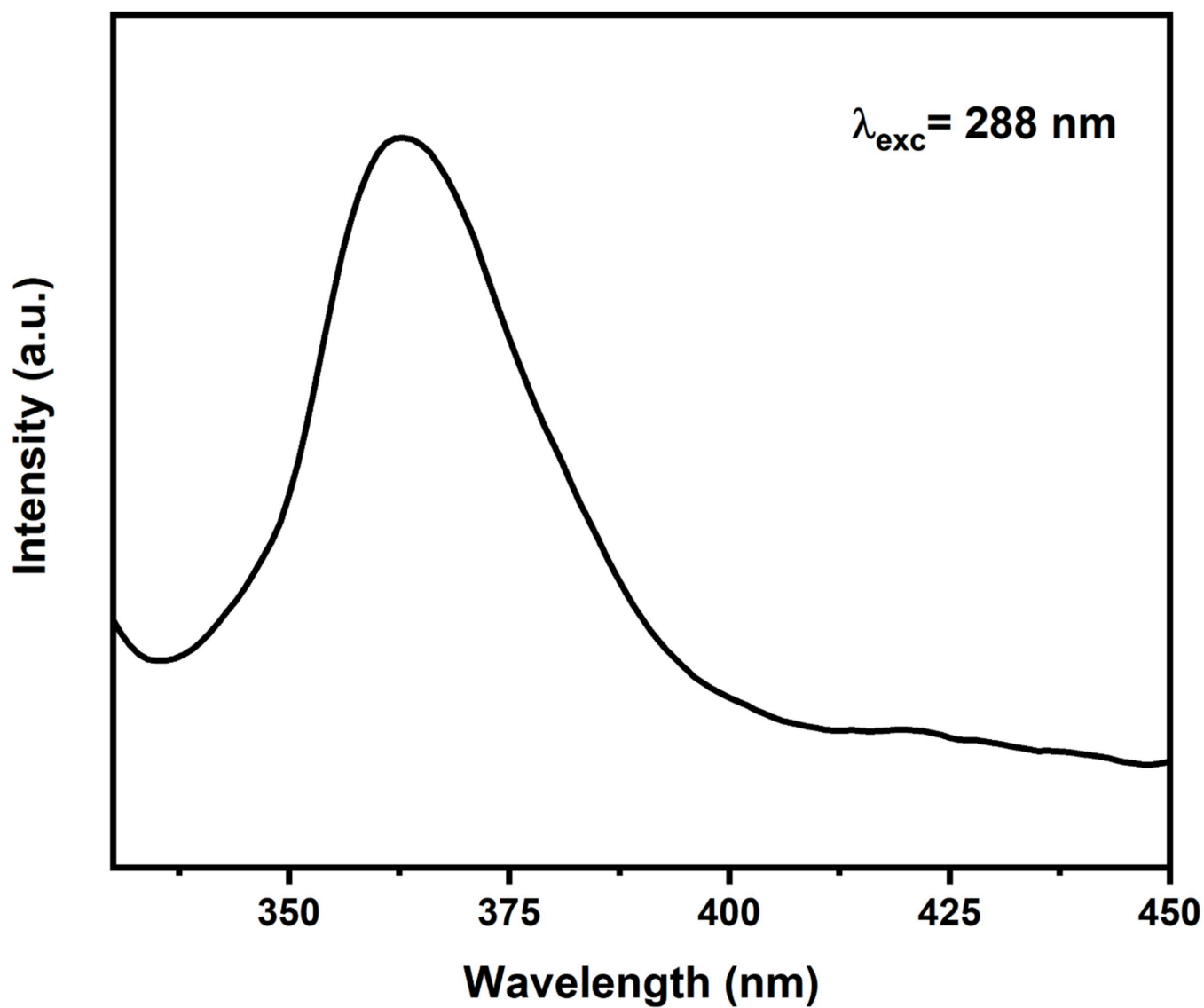


Figure 6

Emission spectrum of  $\text{Y}_2\text{O}_3$  nanoparticles

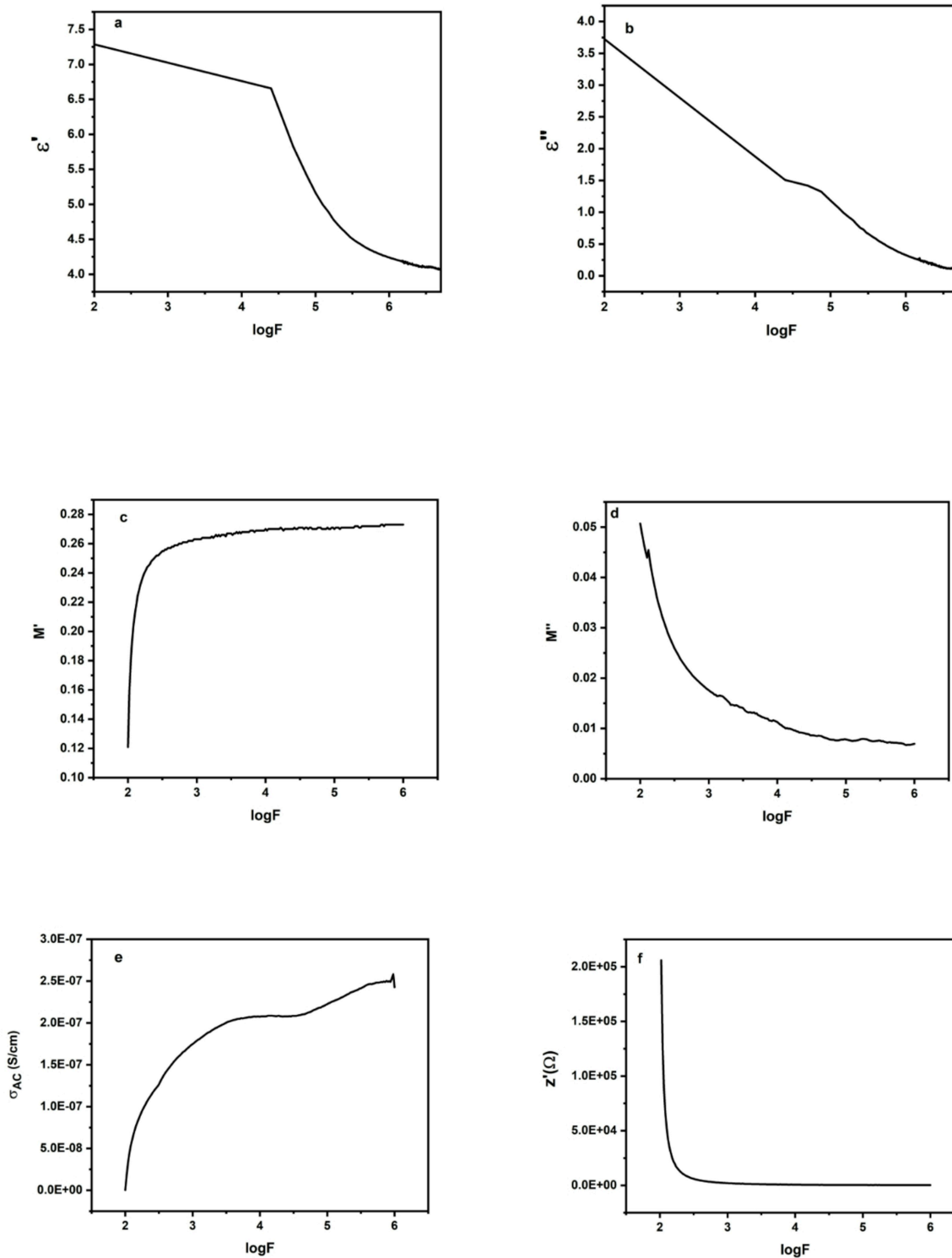


**Figure 7**

a) Dielectric constant b) loss factor c) real part of complex electric modulus d) imaginary part of complex electric modulus e) AC conductivity f) real part of impedance of  $Y_2O_3$  nanoparticles

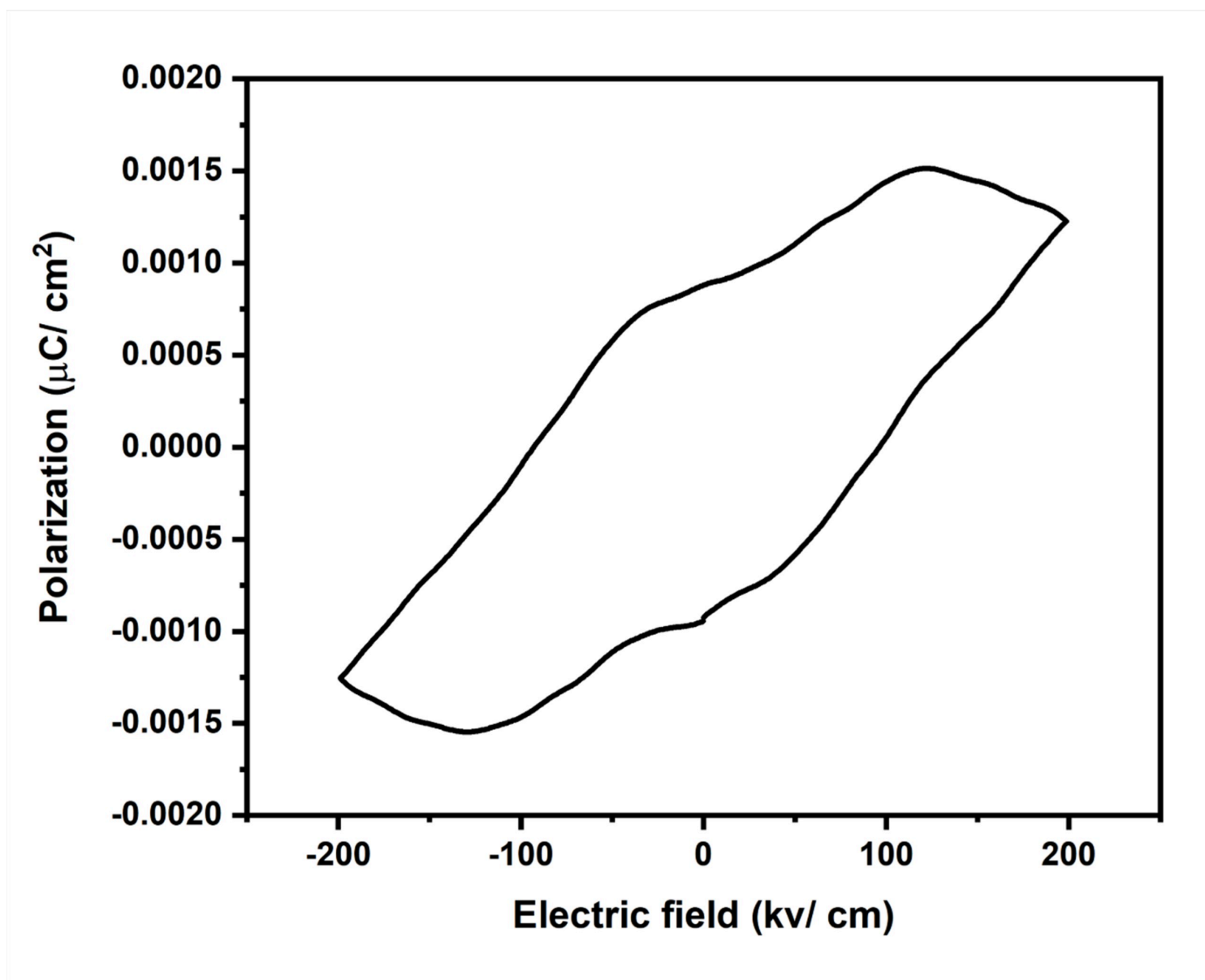


Figure 8

P-E hysteresis loop of the synthesized  $\text{Y}_2\text{O}_3$  nanoparticles