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Structural, Optical and Ftir Studies of Baso₄ Nano Particles.

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ABSTRACT

Precipitation of nano particles is an important production procedure in industry to receive nano materials that are widely used in many fields. The product properties are strongly dependent on the properties of the particles i.e., average size, size distribution and morphology. The specific properties and applications of barium sulphate nano particles have attracted intensive investigation. There are numerous tedious techniques for synthesis of nano particles. The BaSO₄ nano particles were prepared successfully by direct chemical precipitate method at room temperature. The products were characterized through X-ray diffraction (XRD), Optical and Fourier Transform Infrared Spectroscopy (FTIR) techniques.

KEYWORDS Barium Sulphate, Ordinary chemical precipitation, XRD, optical study.

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1. INTRODUCTION

A major trend in research and development has been the shift of interest towards tiny particles. This can be summarized under the general term “nanotechnology”. In the engineering and materials science community, the term “ultra fine particles” and “submicron particles” were used before “nanoparticles” came into being. Nowadays, three main notations for nanoparticles are being used: nanoparticle, nanocrystal and nanocluster¹. The synthesis of inorganic materials with nanometer size, controlled surface properties and controlled morphology attract increasing interest recently due to its significant applications in various fields. Barium sulphate, which is commonly referred to as barite, is desirable for several uses on account of its high specific gravity, opaqueness to X-rays, inertness and whiteness. It has been pan optically utilized in industrial applications such as paper coatings, filler in plastics and pigments in paint. They may also apply in the studies of biomineralization, molecular recognition, and pharmaceutical formulations. Rather than it is a very good thermo luminescence material, which is used in radiation dosimeter purposes²⁻⁷. Barium sulfate (BaSO_4) is used clinically as a contrast agent for gastrointestinal radiography and as a radiopacifer in acrylic bone cement due to exhibiting high X-ray attenuation, insolubility, and biocompatibility⁸⁻⁹. BaSO_4 exhibits a broad range of high attenuation due to a K-absorption edge at 37 keV, which is at the lower end of the photon energy range utilized by many commercial preclinical and clinical imaging instruments. In the present study, BaSO_4 nanoparticles were synthesized using by chemical precipitation method. The precipitated BaSO_4 nanoparticles were characterized using XRD, Optical and FTIR studies.

2. MATERIALS AND METHODS

The raw materials used in the study were Barium Nitrate ($\text{Ba}(\text{NO}_3)_2$), Ammonium Sulphate ($(\text{NH}_4)_2\text{SO}_4$), Stearic Acid ($\text{C}_{18}\text{H}_{36}\text{O}_2$). These chemicals were used directly without any further purification. The double distilled water was used as a solvent. Three solutions are prepared namely, solution A, B, C. The following experimental procedure of three solution are given below:

Solution A: 0.1 M of Ammonium Sulphate ($(\text{NH}_4)_2\text{SO}_4$) was mixed with 50 ml of distilled water.

Solution B: 0.1 M of Barium Nitrate ($\text{Ba}(\text{NO}_3)_2$) was mixed with 50 ml of distilled water.

Solution C: 0.1 M of Stearic Acid ($\text{C}_{18}\text{H}_{36}\text{O}_2$) was dissolved in 20ml of ethyl alcohol.

Approach I: Solution A was directly dropped into solution B while stirring at room temperature with dispersant at strong magnetic stirring.

Approach II: The stearic acid was added drop wise into the mixed solution. The steady drop rate was 20 drops per min.

After stirring the solution were kept 30 min for allowing the precipitate to settle. Precipitates were then separated, centrifuged and rinsed with doubly distilled water. After the last centrifugation sediments particles were dried in the microwave oven. The products were slightly grinded for analysis.

3. RESULTS AND DISCUSSION

3.1 Powder X-Ray Diffraction Study

X-Ray diffraction study was effectively used to identify the crystal structure and determine the particle size. Fig.1. Shows the typical XRD pattern of BaSO₄ particles prepared through direct precipitation techniques. Barium sulphate nano particles have the orthorhombic structure with the lattice constant $a = 7.154\text{\AA}$, $b = 8.899\text{\AA}$, $c = 5.454\text{\AA}$ which is in good agreement with the reported data (PC PDF card no. PDF# 897357). The crystalline size was calculated using the Debye-Scherrer's formula. The average particle size of the BaSO₄ have been calculated by

$$\bar{r} = K \lambda / \beta \cos \theta$$

Where \bar{r} - the average diameter

K- the shape factor

λ – the X-ray wavelength

β - the width of the peak

θ - Bragg's diffraction angle

The crystalline sizes of the sample are estimated from the line width of the (231) XRD peaks. The average particle size was calculated as 61 nm for BaSO₄ nano particles.

3.2 Optical Study

The prepared sample of BaSO₄ nano particles characterized by UV-VIS spectroscopy. The optical spectrum of BaSO₄ nano particles recorded from the range between 190- 1100 nm. In this work a BaSO₄ nano particles was prepared at room temperature. The maximum transmission was observed at 84%. From figure 2, the band gap BaSO₄ nano particles is 6.53eV. A small band position appeared at 1084 nm. It may be due to the presence of impurities.

3.3 Ftir Study

Figure 3 shows the FTIR spectrum of BaSO₄ nano particles. The sulphate group has 4 fundamental vibrational modes. One non degenerate (ν_1), one doubly degenerate (ν_2) and two triply degenerate (ν_3 and ν_4). The peaks at 470cm^{-1} corresponds to symmetrically bending ν_2 vibrational mode. The absorption peaks appeared at 3440cm^{-1} and 1632cm^{-1} are due to stretching and deformation of absorbed water molecule. The peak at 1043cm^{-1} of BaSO₄ is present. The peaks

appeared at around 2081cm^{-1} is overtones and combination bands of the sulphur-oxygen stretching and bending vibrations.

4. CONCLUSIONS

The BaSO_4 nano particles were prepared successfully by direct precipitate method. XRD analysis study confirms that the synthesized BaSO_4 is in orthorhombic structure. The maximum transmission and band gap calculated from the UV-visible spectrum. The functional groups of BaSO_4 nano particles are identified by FT-IR study.

5. REFERENCES

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Fig.1 Powder XRD pattern of BaSO_4 nano particles

Fig.2 Optical spectrum of BaSO_4 nano particles

Fig.3 FTIR spectrum of BaSO_4 nano particles

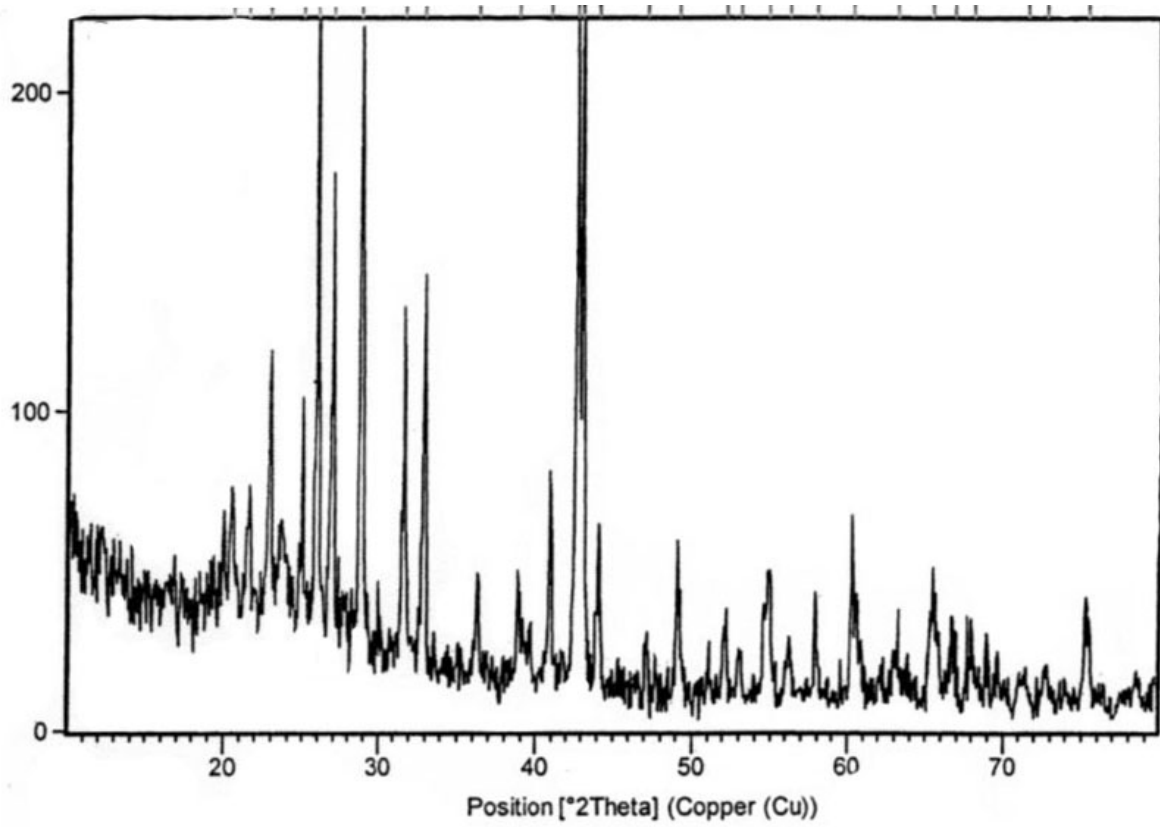


Fig1. Powder XRD of BaSO₄ nano particles

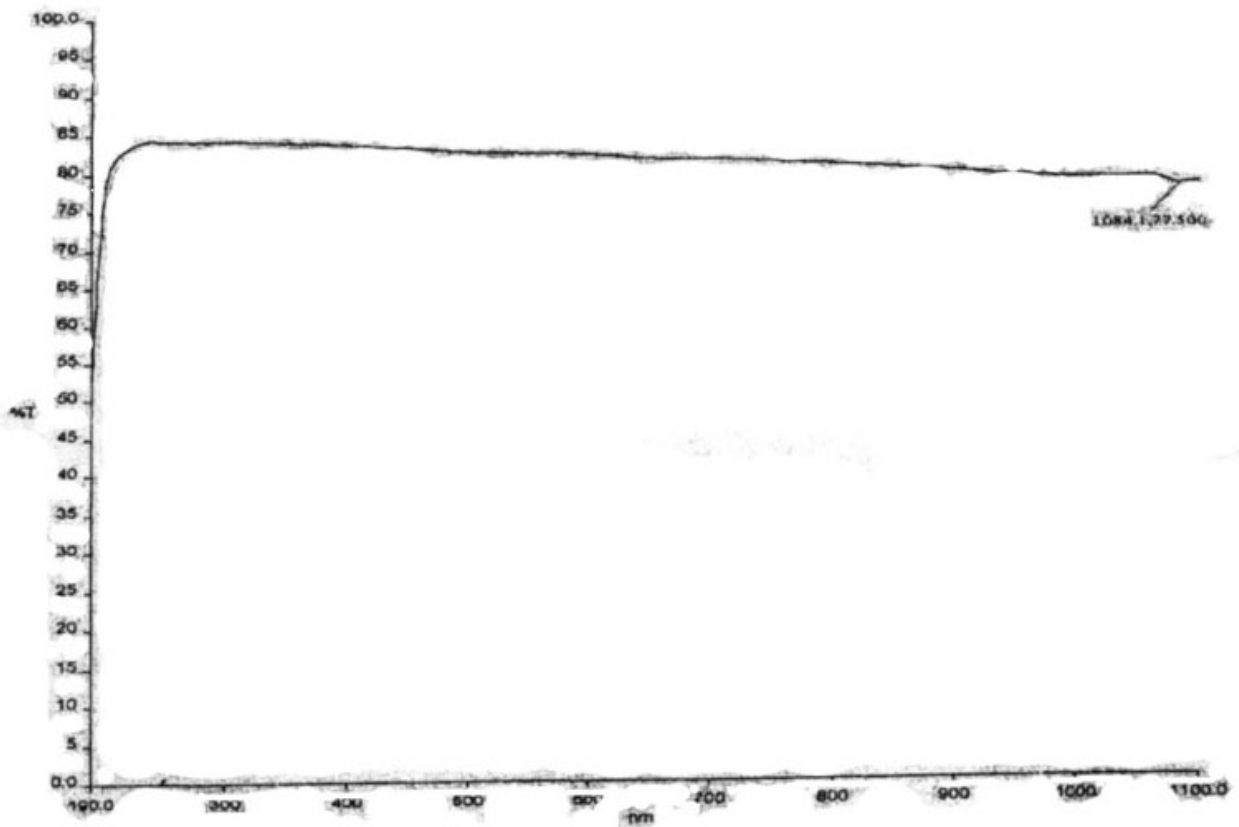


Fig 2. Optical spectrum of barium sulphate nano particles

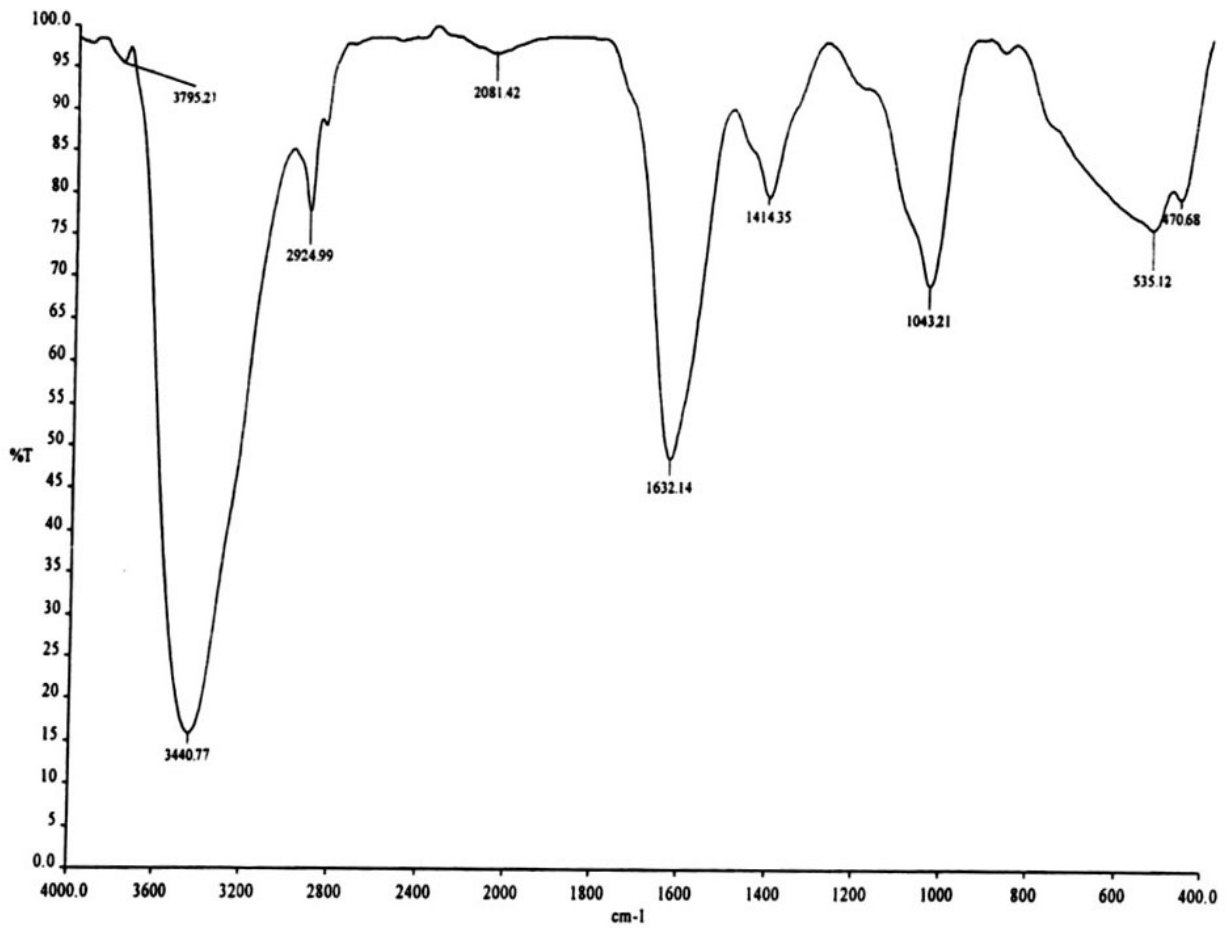


Fig 3. FTIR studies of barium sulphate nano particles