



Growth, structural, spectral, optical and electrical properties of 2-aminophenol single crystals



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ABSTRACT

Good quality single crystals of 2-aminophenol were grown by slow evaporation solution growth technique at room temperature. Crystal structure and crystalline nature was determined by X-ray diffraction studies. Presence of functional groups in the crystal was confirmed by FT-IR analysis. UV transmittance study shows the large transmittance in the entire visible region. Dielectric constant and loss for the crystals were taken at different temperature. Photoconductivity study exhibits positive nature of the grown crystal. DC conductivity studies were also carried out for the grown crystal.

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1. Introduction

In recent years research on nonlinear optical materials have gained considerable attention due to their potential applications in optical communications, image processing, data storage, optical modulators and optical switches [1–4]. While comparing inorganic counter parts organic material possess large second order non-linearity ($\chi^{(2)}$), fast response time, ease of synthesis and device fabrication [5,6]. Because they are formed by weak van der Waals and hydrogen bonds. Now a days there is a considerable interest on the synthesis of new organic non linear properties. 2-Aminophenol is a organic material having molecular weight of 109.13 and belongs to the orthorhombic system. Previously its structure was reported by several workers [7–9]. But there is no significant studies are available for this material. In the present work we take initiation for growing 2-aminophenol crystals by slow evaporation solution growth technique at room temperature and their structural, spectral, optical and electrical properties were reported.

2. Experimental procedure

2.1. Crystal growth

Commercially available 2-aminophenol (Merck) was dissolved in acetone and stirred well for about 1 h using magnetic stirrer. The saturated solution was filtered twice using Whatman (No. 42 grade)

filter paper. Then the solution was transferred to 250 ml beaker for evaporation. To control evaporation of the solvent top of the beaker was covered by thin plastic sheet. After two weeks optically good quality crystals were obtained from the mother solution. Quality of the crystals are presented in Fig. 1.

3. Result and discussion

3.1. X-ray diffraction studies

Grown 2-aminophenol single crystals were subjected to single crystal XRD analysis using ENRAF NONIUS CAD-4 X-ray diffractometer with Moka ($\lambda = 0.7107 \text{ \AA}$). From the result it is concluded that grown crystal belongs to orthorhombic system with centrosymmetric space group Pbca and the lattice parameter values are $a \text{ (\AA)} = 7.253$, $b \text{ (\AA)} = 7.833$, $c \text{ (\AA)} = 19.641$, $\alpha = \beta = \gamma = 90^\circ$ and $V \text{ (\AA}^3\text{)} = 1116$. These parameters reveal good agreement with earlier reported values [7]. Crystals were finely crushed and subjected to powder XRD analysis using Bruker AXS D8 advance powder diffractometer with Cu, wavelength 1.5406 \AA were used. The sample was scanned in the reflection mode in the 2θ range $5\text{--}80^\circ$. The recorded spectrum is shown in Fig. 2. Sharp and well defined Bragg's peaks confirm the crystalline nature of the crystal. It is interesting to note that while comparing other phenol crystals 2-aminophenol shows very high crystalline nature [3,10].

3.2. FT-IR analysis

The FT-IR spectrum of 2-aminophenol crystals is studied through PerkinElmer FTIR spectrometer using KBr pellet technique

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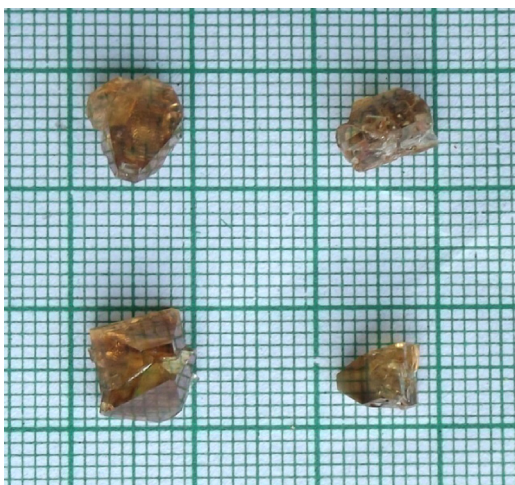


Fig. 1. As grown crystals of 2-aminophenol.

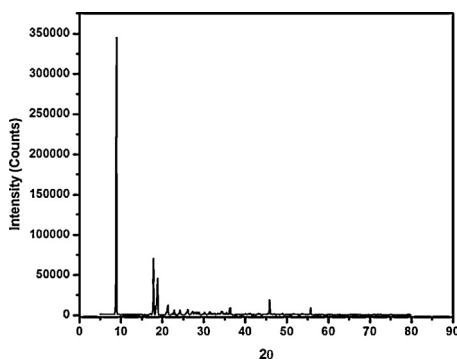


Fig. 2. Powder XRD pattern of 2-aminophenol.

and the resulting spectrum is shown in Fig. 3. The band observed at $3375\text{--}3298\text{ cm}^{-1}$ were assigned to OH and NH_2 symmetric and asymmetric stretching vibrations. Peak at 3046 cm^{-1} is due to aromatic C–H stretch. The skeletal vibrations of the ring could be assigned to 1457 , 1506 and 1599 cm^{-1} . The peaks at 734 , 838 and 898 cm^{-1} are due to C–H out of plane bending vibration. C=C out of plane bending vibration could be assigned to 482 cm^{-1} . Vibration at 1073 cm^{-1} is assigned to C–N stretching vibration. The symmetric and asymmetric stretching of CH_2 is found at $2843\text{--}2953\text{ cm}^{-1}$.

3.3. Optical transmittance studies

Optical transmittance studies for the grown crystals were recorded using a PerkinElmer lambda 35 spectrometer in the range $200\text{--}1100\text{ nm}$. Recorded optical transmittance spectrum is shown in Fig. 4. It is noted from the figure that absorption decreases around 340 nm which leads transparency upto 1100 nm . Absence of

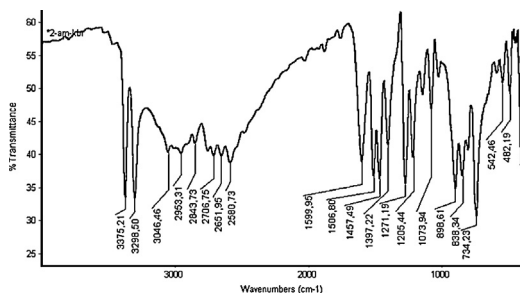


Fig. 3. FT-IR spectrum of 2-aminophenol.

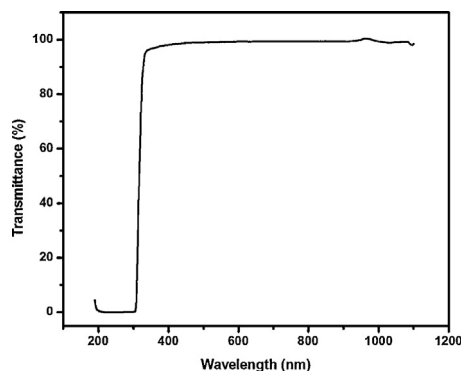


Fig. 4. Optical transmittance spectrum of 2-aminophenol.

absorption and transparency in the visible region illustrate the suitability of 2-aminophenol crystal in the visible region [11]. Optical band gap was found to be 3.89 eV (Fig. 5). Materials with high band gap could possess high laser damage threshold [12].

3.4. Dielectric studies

Dielectric studies for the grown crystals were carried out in the frequency range from 50 Hz to 5 MHz using Hioki LCR meter (3532-50). Cut and polished crystals were used for the measurement. The dielectric constant of the crystal was calculated by the given formula

$$\epsilon_r = \frac{Cd}{\epsilon_0 A} \quad (1)$$

where C is the capacitance of the crystal, d is the thickness of the crystal, ϵ_0 is the free space permittivity and A is the cross sectional area of the sample. Fig. 6a shows the dielectric constant vs frequency for the grown crystal. The dielectric constant is very low at high frequency and decreases slowly at higher frequencies and finally attains a constant value at very high frequencies (above 1 MHz). It may be due to all four polarizations namely electronic, ionic, space charge and orientation. Out of these polarizations space charge polarization is mainly dependent upon the purity of the sample. Hence high value of dielectric constant at low frequency is attributed to space charge polarization [13,14]. Fig. 6b shows dielectric loss with respect to frequency. The dielectric loss is very low at high frequency. This low value suggests that sample possesses enhanced optical quality for nonlinear device applications.

3.5. Photoconductivity

Photoconductivity measurement for the grown crystals were taken at room temperature using Keithley 6517B electrometer. Crystals were cut and polished in a regular shape and used for the

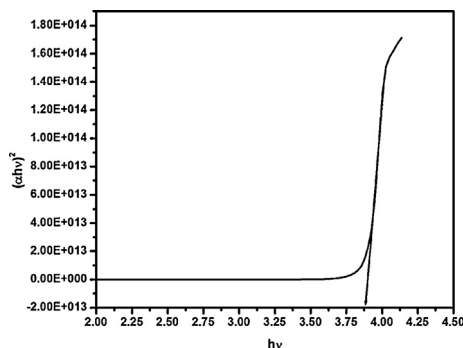


Fig. 5. $(\alpha h\nu)^2$ vs $h\nu$.

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