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GROWTH AND STUDIES OF PURE AND PICRIC ACID -DOPED UREA SUCCINIC ACID SINGLE CRYSTALS

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ABSTRACT

Pure and picric acid doped urea succinic acid (USA) crystals were grown from aqueous solution by slow solvent evaporation technique at room temperature. X-ray diffraction studies have confirmed the crystal structure and crystallinity of the grown crystals. Nonlinear optical behavior of pure and picric acid doped USA crystals have been studied for the first time by Kurtz-Perry powder technique. UV-Vis-NIR absorption and transmission spectra were measured and the cut-off wavelength, band gap energy and refractive index of the grown crystals were determined. Micro hardness analysis carried out on the material and the value of Work hardening coefficient (n) and elastic stiffness constant (C_{11}) were calculated. The thermal stability and the trend of decomposition of grown crystals were analyzed by TG/DTA analyses. The dielectric studies were carried and AC conductivity of grown crystals was determined. The vibrational frequencies of various functional groups have been derived from FTIR spectrum.

Keywords: A1. Growth from solution; A2. Characterization; B1. Nonlinear optics.

1 .INTRODUCTION

There is currently a considerable effort to develop new organic materials with large second-order nonlinear optical (NLO) susceptibilities because of their potential applications in optical signal processing and frequency conversion Urea is one of the organic crystals that have been put to practical uses. It has larger nonlinear optical coefficients, a high degree of birefringence and relatively high laser damage threshold. Since urea transparency range extends to 200 nm in the short wavelength limit, it is well known for frequency conversion devices such as second and fifth harmonic generation [8] and it is used as the first organic optical parametric oscillator. The powder second-harmonic generation (SHG) efficiency is 2.5 times that of ADP and the d_{14} nonlinear coefficient is 2.5 ± 0.2 times that of d_{36} of ADP. In spite of versatile applications urea has some undesirable mechanical and chemical properties, i.e., mechanically soft and hygroscopic in nature. As a result of its hygroscopic nature, urea cannot be exposed to normal atmosphere and for practical applications it is being used by immersing it in an index-matching fluid with compatible chemical and optical characteristics

2. EXPERIMENTAL PROCEDURES

Synthesis and solubility*:* Selection of suitable solvents for the growth of good quality single crystals is very important. High-purity Analytical Reagent (AR) grade urea, succinic acid and picric acid along with demineralized water were used for the synthesis and growth process. Pure USA salt was synthesized by stoichiometric incorporation of urea and succinic acid in the molar ratio 1:1. The component salts were very well dissolved in demineralized water and it was thoroughly mixed using a magnetic stirrer and the mixture was heated at 40 °C till a white crystalline salt of USA was obtained. Temperature was maintained at 40 °C to avoid decomposition. The pure USA crystal was colourless, but the doped crystals were yellow mixed white in colour. Morphological changes have been observed between pure and doped USA crystals. The grown crystals are displayed in the photograph 2 (a) to 2 (d). Dimensions of pure and doped USA crystals are 12 × 8×7, 12× 6 × 3, 16 × 5 × 3 and 24 × 4.5 × 2 mm^3 for pure and 0.5 mole %, 1 mole % and 1.5 mole % of picric acid-doped USA crystals respectively.

3. RESULTS AND DISCUSSION

Single crystal X-ray diffraction analysis for grown pure and picric acid-doped USA crystals have been carried out to identify the structure and lattice parameters using an ENRAF NONIUS CAD4-F X-ray diffractometer with graphite monochromatic MoK∝ ($\lambda = 0.71069$ Å). From the study, it was observed that pure and picric acid-doped USA crystals crystallize in monoclinic structure with space group $P2_1/c$ and the calculated unit cell parameters are listed in 1. The higher energy electronic transition is promotion of an electron from a π bonding molecular orbital into a π* antibonding molecular orbital, known as π-π* transition (ligand π-π* transition). This means that only compounds with π electron and non-bonding electrons can produce UV-Vis-spectra.

Table 1: The values of cut-off wavelength, band gap energy and refractive index for pure and doped USA crystals

Samples	**Cut-off Wavelength** (nm)	**Band gap energy** (eV)	**Refractive index**
Pure USA crystal	240	5.1	1.93
USA + Picric acid (0. 5 mole %)	250	4.96	2.006
USA + Picric acid (1 mole %)	252	4.92	2.01
USA + Picric acid (1. 5 mole %)	255	4.86	2.02

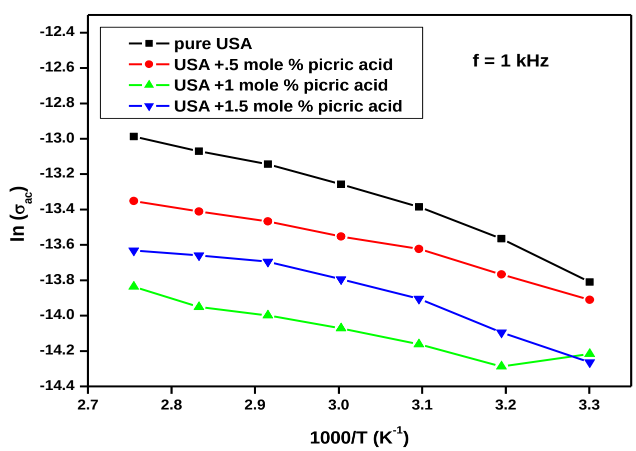

Figure 1: Plot of ln (σ_{ac}) versus (1000/T) for pure and doped USA

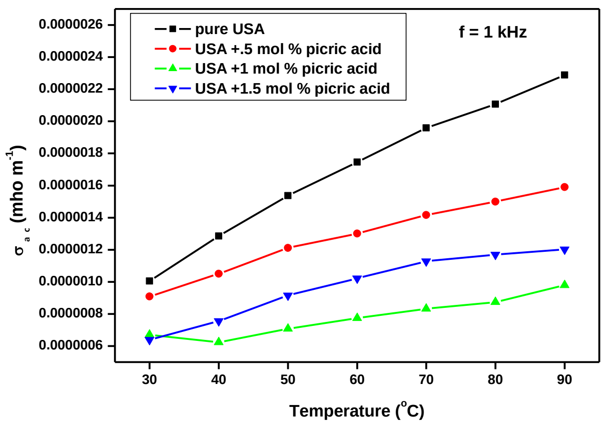

Figure 2: Plot of AC conductivity verses temperature for pure and doped USA

4. CONCLUSION

Pure and picric acid-doped USA single crystals have been grown by slow evaporation technique at room temperature. The grown crystals are observed to be transparent and well-defined external appearance. The crystal systems and the unit cell parameters of the grown crystals were identified from single crystal X-ray diffraction analysis. The crystalline nature of the grown crystals was confirmed by powder X-ray diffraction and the diffraction peaks were indexed. FTIR studies revealed the presence of different vibrational bands. When urea succinic acid crystals are doped with picric acid, it is observed that SHG efficiency relative to that of KDP increases. Thermal stabilities of pure and doped USA crystals were studied by TG/DTA analysis. The optical characteristics were assessed by UV spectral analysis and it indicates the transmission in the visible region. The dielectric studies were carried out, and the variations of dielectric constant and dielectric loss with temperature have been studied. The AC conductivity measurements were made and activation energy values were calculated.

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