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Spectroscopic, Mechanical and Optical Studies of L-Valine Picrate (LVP) Single Crystal

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Abstract: L-Valine Picrate (LVP) single crystal was grown for the aqueous solution. The grown crystal was characterized by single crystal XRD studies to confirm the crystal structure. Functional groups present in the sample were analyzed using FT-IR spectrum. The UV- Visible spectrum of LVP was recorded in the wavelength region from 200 nm to 1100 nm and the evaluated band gap is 2.33 eV. The mechanical properties of the grown crystals have been studied using Vickers micro hardness tester. This crystal can be a suitable material for the optoelectronic devices like LED and Laser diodes.

Keywords: LVP, monoclinic, space group $P2_1$, UV-Visible spectrum, Band gap

1. Introduction

Nowadays NLO materials are having potential applications in the area of telecommunication and optical storage devices [1].Amino acid crystals are potential candidates for optical second harmonic generation because all amino acids except glycine contain chiral carbon atom and crystallize in non-centrosymmetric space groups. The nonlinear susceptibility of an organic material would be larger when it has donor - acceptor conjugate or molecular system. Organic π-conjugated systems are interesting because they exhibit large molecular quadratic hyperpolarizabilities, scope for altering the properties by changing electron donor and electron acceptor moieties at their two ends [2]. Picric acid, as an electron acceptor, forms charge transfer molecular complexes with number of electron donor compounds through electrostatic or hydrogen bonding interactions. There are numerous studies which analyze the formation of picric compounds with amino acids like L-valine, L-glycine, L-asparagine and L-proline [3-5]. The aim of the present communication is to study the growth, physical and chemical properties of L-Valine Picrate crystals that may find wide applications inoptoelectronic devices.

2. Growth of L-valine picrate (LVP) crystals

LVP was synthesized by the reaction between the equimolar picric acid and the aminoacid, L-valine. The reactants were thoroughly dissolved in double distilled water and stirred well using a temperature controlled magnetic stirrer at 45°C to yield a homogeneous mixture of solution. Then the solution was allowed to evaporate at room temperature, which yielded yellow crystalline salt of LVP after 20 days. The process of recrystallization was carried out to purify the synthesized salt. The photograph of the harvested crystals are shown in figure 1.

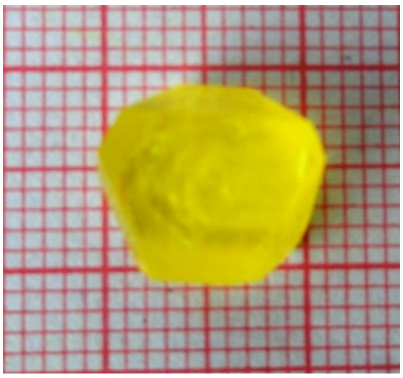

Figure 1. Photograph of LVP single crystal

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3. Single Crystal XRD Analysis

The grown crystals were subjected to single crystal X-ray diffraction studies using an ENRAF NONIUS CAD4 automatic X-ray diffractometer with MoKα (λ=0.7170 Å) to determine the cell parameters. The crystal exhibits a monoclinic system with space group $P2_1$ with cell parameters

a= 9.974 Å

b=6.263 Å

c=12.635 Å

β=110.37 Å

Calculated volume of the unit cell =789.272 $Å^3$.

4. FT-IR analysis of LVP

Functional groups present in the sample were analyzed using FT-IR spectrum. The Fourier transform infrared spectral analysis of LVP was carried out between 400cm^{-1} and 4000 cm^{-1} by recording the FT-IR spectrum using Perkin Elmer spectrophotometer by KBr pellet technique and is shown in Figure 2. From Table 1, assignments, the formation of all the functional groups could be confirmed.

1630	NH_3^+ asymmetric deformation
1536	NH_3^+ symmetric deformation
1338	(NO_2) symmetric stretching
1285	phenolic C–O stretching
1059	C–C stretching
900	$[NH_3]^+$ rocking; C–C stretching
701	CH_3 rocking
541	NO_2 rocking

5. UV-Visible Spectral Analysis of LVP

The UV-Visible spectrum for LVP was recorded in the wavelength region from 200 nm to 1100 nm with the resolution of 1nm using Perkin Elmer Lambda 35 spectrophotometer and is shown in Figure 3. The material is found to be transparent to all radiations in the wavelength range 200–1100 nm.

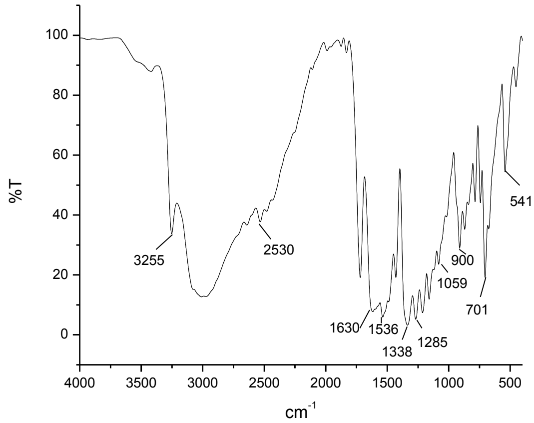

Figure 2. FTIR spectra of LVP single crystal

The absence of absorption in the visible region clearly indicates that LVP crystals can be used as window material in optical instruments. The higher percentage of transmission in the visible region clearly depicts the intrinsic property of the compound and the crystal is free from any defects. The lower cut off wavelength is 512 nm. Excellent optical transmittance with the lower cut-off wavelength at 512 nm makes it as a potential material for device fabrication.

6. Optical Band Gap of LVP

Optical materials are becoming increasingly important in communications where an entire network of optical fibers, LEDs, laser and detectors has already been installed for transmission of voice and data. Optical disk recordings with semiconductor laser playback are replacing the conventional piezoelectric pickups. Solar cells are now common components in toys, calculators and other consumer electronics. The dependence of optical absorption coefficient with the photon energy helps to study the band structure and the type of transition of electrons.

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The absorption coefficient (α) were determined using Beer's law

$$\alpha = \frac{2.3036 \log\left(\frac{1}{T}\right)}{d}$$

where, t-thickness of the sample cell, T-transmittance.

A graph is plotted between the Photon energy (E) in eV and $(\alpha h\nu)^{1/2}$ and the linear region of the curve were extrapolated to find the x-intercept which gives the Band gap of the compound. From the band gap value, the optical property of the crystal can be justified. The band gap curve is shown in Figure 4 and the band gap evaluated is 2.33 eV. As a consequence of wide band gap, this crystal can be a suitable material for the optoelectronic devices like LED and Laser diodes.

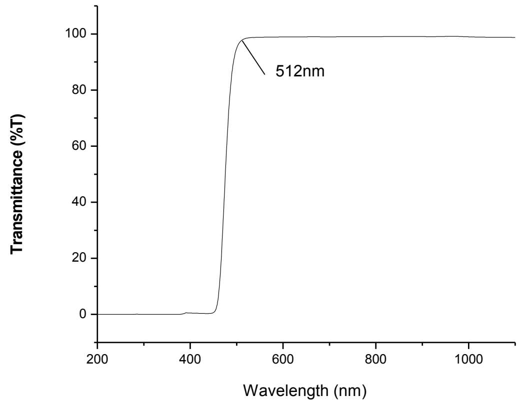

Figure 3. UV spectra of LVP crystals

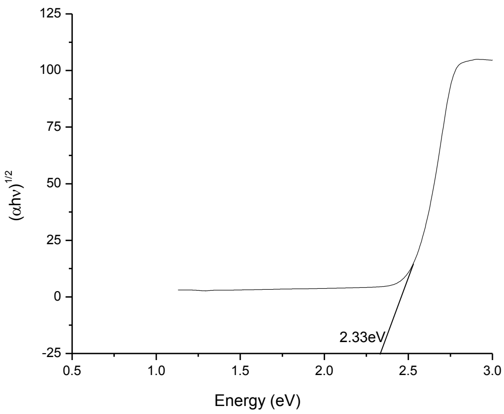

Figure 4. Bandgap curve for LVP crystals

7. Vicker's Micro Hardness Analysis of LVP

Micro hardness is primarily used to study the mechanical strength of a material. Selected smooth surfaces of the LVP crystals were subjected to static indentation test at room temperature with a constant indentation time of 15 s.

Indentations were made with a Leitz microhardness tester on the surfaces by varying the load from 25 g to 100 g. Vicker's micro hardness number have been calculated using

$$H_v = 1.8544\ P/d^2\ kg/mm^2$$

where P is the applied load and d is the mean diagonal length of the indenter impression. Vickers micro hardness plot as a function of the applied load is shown in Figure 5.

It is evident from the plot that the micro hardness value of LVP increases with increasing load, which confirms the high mechanical strength of the crystal.

The value of the work hardening coefficient n was estimated from the plot of log P versus log d (Figure 6). A linear graph was observed with the slope of 4.09 which also confirms the mechanical strength of the crystal. According to Onitsch and Hanneman 'n' should be between 1 and 1.6 for hard materials and above 1.6 for softer ones. Hence LVP belongs to soft category.

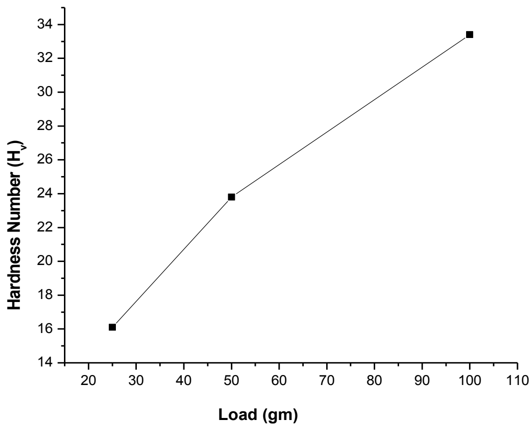

Figure 5. Hardness curve for LVP crystal

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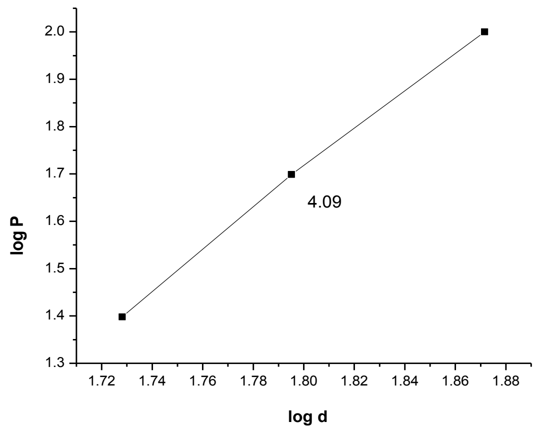

Figure 6. Work hardening Coefficient curve for LVP crystal

8. Conclusion

L-Valine Picrate (LVP) single crystal was grown for the aqueous solution. The grown crystal was characterized by single crystal XRD studies to confirm the crystal structure. The crystal exhibits a monoclinic system with space group $P2_1$. Functional groups present in the sample were analyzed using FT-IR spectrum. The UV- Visible spectrum of LVP was recorded in the wavelength region from 200 nm to 1100 nm and the evaluated band gap is 2.33 eV. The mechanical properties of the grown crystals have been studied using Vickers micro hardness tester. According to Onitsch and Hanneman 'n' should be between 1 and 1.6 for hard materials and above 1.6 for softer ones. Hence LVP belongs to soft category. This crystal can be a suitable material for the optoelectronic devices like LED and Laser diodes.

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