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Effect of L-Valine on the Growth and Characterization of Potassium Bromide Crystal

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ABSTRACT

Nonlinear optical single crystals of L-Valine doped Potassium Bromide (LVPB) were grown by synthesization of KBr doped with L-Valine by dissolving it with the solvent as water. At room temperature, good optical crystals of clear transparency were harvested by solution growth slow evaporation technique. Using a computer program, powder XRD analysis confirms the grown crystal from the calculation of 2theta and hkl values. Available functional groups in the LVPB grown crystal was exposed by FTIR analysis which confirms the inclusion of L-Valine. The thermal stability of grown LVPB was found to be noted as 225°C from the TGA-DSC studies. The absorption and transmission spectra of UV-Vis-NIR reveal the optical transparency of the crystal which leads to an idea to fabricate the optical devices.

1. Introduction

Researchers attention was recently attracted towards the potential applications of NLO crystals which plays a vital role in high-speed data transfer, optical storage, optoelectronics, optical communication, etc., For the past few years, the investigation was focused on inorganic crystals for their SHG behavior(1-3). Now a day's semi-organic material attracts much interest in compared with organic or inorganic material due to their enhanced NLO behavior. The special behavior of the semi-organic crystals was due to the following features (i) donor and acceptor dipolar structure (ii) delocalized π-electron (iii) the organic ligand bonded with metal ions, a wider range of transparency, thermal-chemical and mechanical stability, etc.,(4-8). The dipole nature and presence of zwitterions made a foundation to concentrate on amino acid crystal growth with enriched NLO behavior. The present study gives the synthesis and growth of single crystals of LVPB with the following characterization studies such as UV-Vis-NIR, FTIR, XRD, and TGA-DSC.

2. Experimental Procedure

2.1. Synthesis

Single crystal of LVPB was grown by doping L-Valine in Potassium Bromide. LVPB salt was synthesized by taking 6.78gram of potassium bromide with an inclusion of 0.885gram of L-Valine. The above said two salts were taken and dissolved in deionized water, because of its easily soluble nature in water. The estimated amount of chemicals were stirred well using a magnetic stirrer for an hour after dissolving it in deionized water. The compound of LVPB was formed as shown in the fig.1 and repeatedly crystallized for the good purity harvest.

Fig.1 Morphology of LVPB

2.2.Measurements

UV-Vis-NIR spectrum was recorded by double beam UV-Visible spectrophotometer for the LVPB crystal. PERKIN ELMER Fourier Transform Infra Red spectrometer using KBr pellets between the range 4000-400cm^{-1} was used to record the FTIR spectrum. X-ray powder diffraction pattern was observed by RICH SEIFERT X-ray diffractometer. Perkin Elmer Pyres Diamond analyzer traced the thermograms from room temperature to 1200°C in the nitrogen atmosphere at a heating rate of 10K/min.

3. Results and Discussion

3.1.UV-Vis-NIR Analysis

Electronic energy level transitions in a compound will be predicted by UV-Vis-NIR spectral analysis (9). The potential NLO material identification is primarily done by UV-Vis-NIR transmission spectra which one is a key factor. If the material has wider transparency without any absorption at the fundamental wavelength and second harmonic wavelength then it will be concluded that it is a quality NLO material. Molecular structure information is also useful to know about the absorption of visible and UV light which involves the excitement of electrons in the π and σ orbital from the lower to higher states (10-11).The optical enrichment of LVPB crystal was determined using a VARIAN CARY 5E UV-Vis-NIR spectrophotometer within a wavelength region of 190-1100 nm. At 225nm the lower cut-off wavelength was observed and the grown crystal shows good transmittance ranges between 225nm to 1100nm. Suitability of the grown crystals for a second harmonic generation was confirmed from the visible range transmission (12).

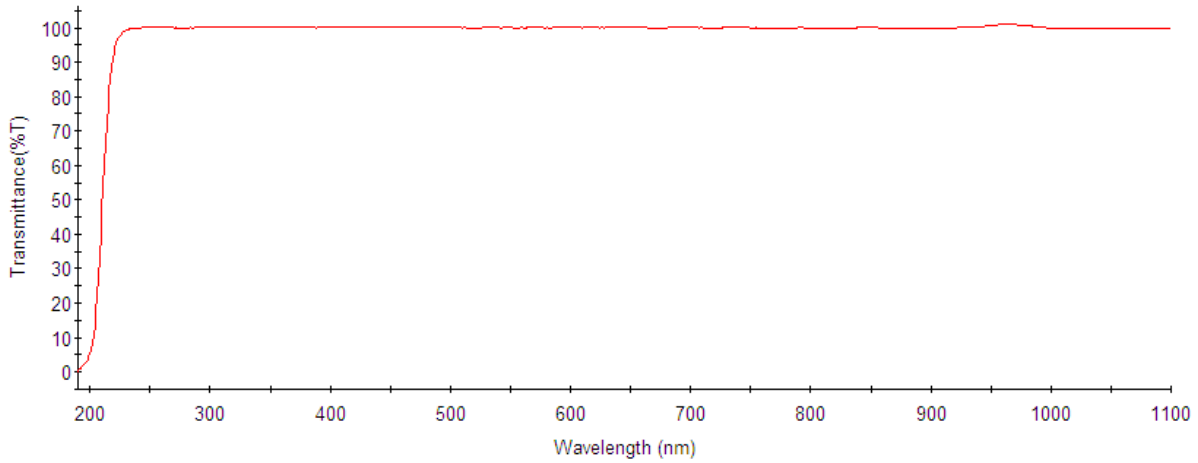

Fig.2.The UV-visible transmittance spectrum of LVPB

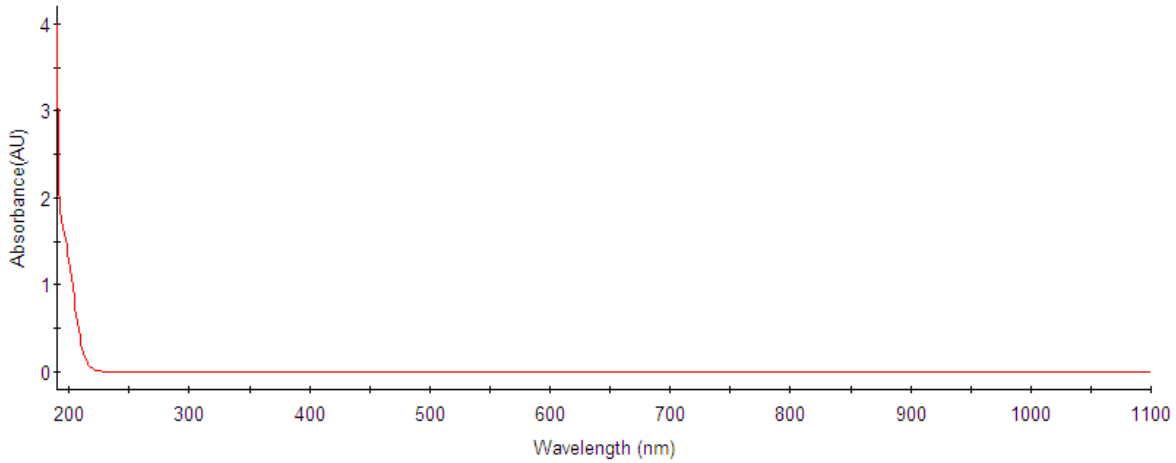

Fig.3.The UV-visible Absorbance spectrum of LVPB

3.2. FTIR Spectral Studies

LVPB crystal's Fourier transform infrared spectrum was recorded using Perkin Elmer Fourier transform infrared spectrometer by utilizing KBr pellets in the range between 4000-400cm^{-1} shown in figure.4.Table.1 gives the tabulated tentative assignments of L-Valine which confirms the inclusion of L-Valine on Potassium Bromide. The zwitterionic nature of the grown crystals was verified with the presence of $COO^-$and NH_3^+ groups.

Table 1: FT-IR spectrum of LVPB

Observed FTIR Frequencies	Assignments
2208	C-H Symmetric Stretching
2146	Combination band of NH_3^+ bending vibration.
2083	NH_3^+ degenerative deformation and NH_3+ torsion.
1602	COO^- symmetric vibration.
1552	NH_3^+ symmetric deformation.
1145	NH_3^+ rocking.
1132	CH_2 wagging.
1119	Symmetric C-O-C stretching.
983	C-C Stretching.
617	Liberation of H_2O

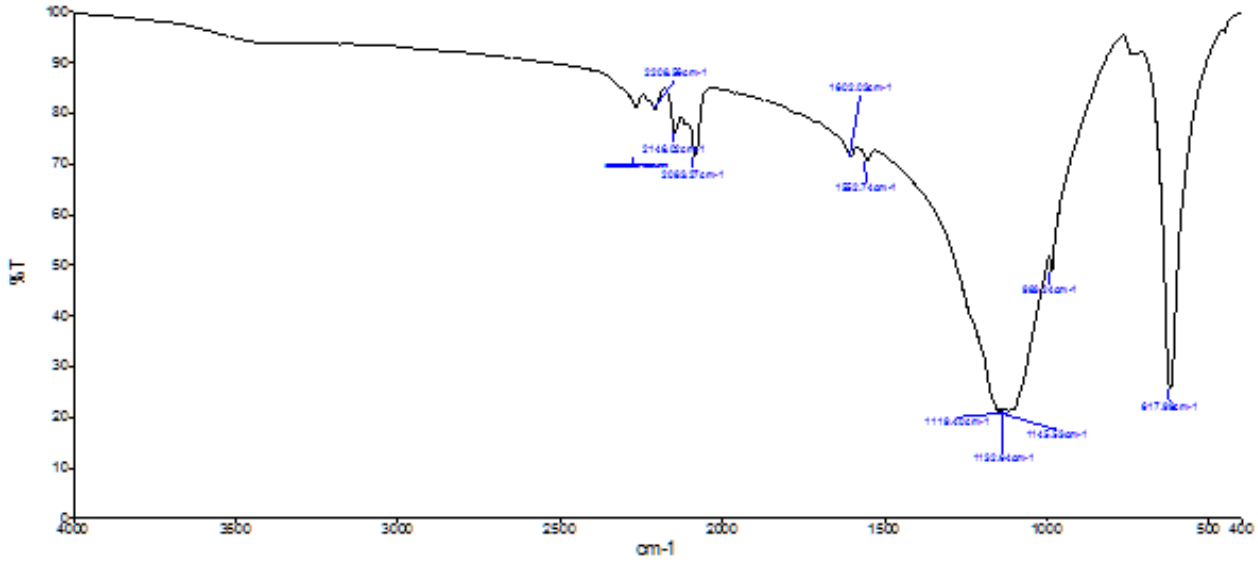

Fig.4.The FT-IR spectrum of LVPB

3.3. Thermal Analysis

Thermal stability information of the grown LVPB crystal was recorded by thermal analysis. In the field of fabrication technology, TGA-DSC plays a vital role in the determination of thermal stability which will help to fabricate under heat generation while shaping the crystals. The TGA-DSC curves of LTPB are shown in the fig.5. Starting of decomposition of the grown crystal was found to be observed at 225°C and the included L-Valine completely decomposed at 300°C. CO_2 and NH_3 liberation took the sole responsibility for weight loss. Formation of the endothermic peak from 225°C to 300°C in the DSC spectrum also confirms the decomposition of L-Valine. Then it was understood that the residue is due to the potassium bromide.

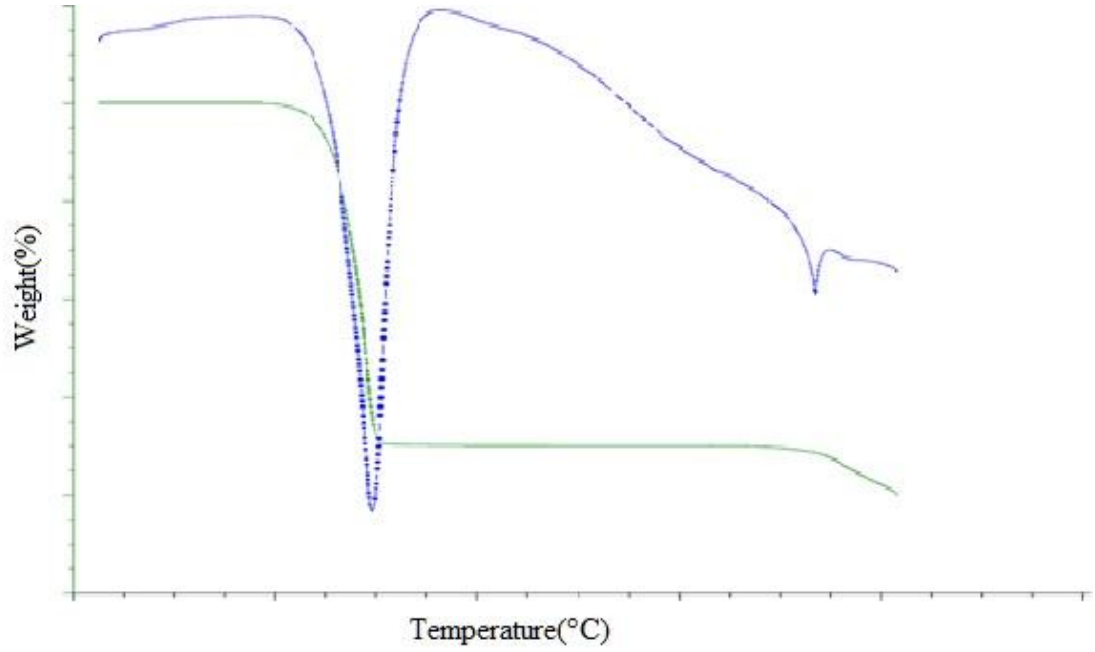

Fig.5.The TG/DSC spectrum of LVPB

3.4.Powder XRD Analysis

Reflection plane identification was done by submitting the grown LVPB crystal to powder X-ray diffraction. The grown crystal was crushed into fine particles with uniform size and made to expose in the path of X-rays. Fig.5shows the powder X-ray diffraction of LVPB crystal. Using the INDEXING SOFTWARE package the reflections observed in the diffraction pattern were indexed. Obtained 2θ,d-spacing, and hkl values were tabulated in Table-2. Thus, from the tabulated values it was found to be in good agreement for the grown crystal with the experimental calculations.

2θ	hkl
25.754	2-1 1
28.416	0 0 2
31.023	1 3 1

Table 2: Powder XRD of LVPB

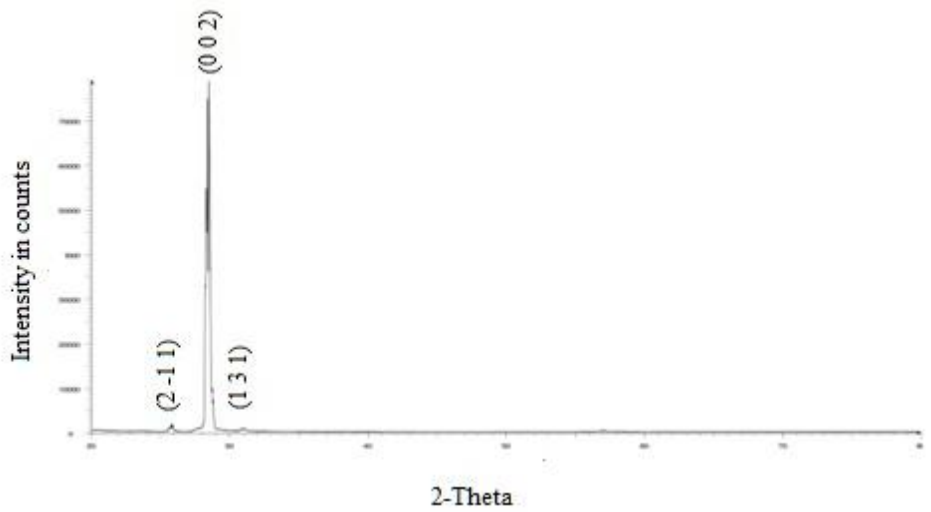

Fig.5.The XRD spectrum of LVPB

4. Conclusion

Adopting slow evaporation solution growth technique L-Valine Potassium Bromide transparent single crystal was grown at room temperature from a saturated solution. LVPB single crystal was characterized by X-ray diffraction and the inclusion was confirmed from the reported values. The optical studies confirmed that the grown LVPB crystal has very wide transparency range in the UV and visible spectral region with a lower cut off wavelength at 225nm. Presence of functional groups and the molecular modes of vibration were identified from FTIR analysis. The TGA-DSC analysis fixed the thermal stability of the LVPB crystal as 225°C which frames an idea about the device fabrications with an operating temperature within 225°C.

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