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Research Article

SYNTHESIS AND CHARACTERIZATION OF L-PROLINE POTASSIUM IODIDE CRYSTAL

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ABSTRACT

L-proline is an organic material, potassium iodide is an inorganic material and these two materials were mixed to form a semi-organic material viz. L-proline potassium iodide (LPPI) crystal in this work. Single crystals of L-proline potassium iodide were grown in an aqueous solution with slow evaporation process. LPPI crystals were obtained after the growth period of 35 days. XRD studies revealed the grown LPPI crystal to be crystallizing in a tetragonal structure. The grown LPPI crystal was analyzed for mechanical stability. Dielectric studies of the LPPI crystals were carried out to evaluate the dielectric constant, dielectric loss and AC conductivity. UV-visible-NIR spectral studies were performed in the wavelength range 200-1100 nm, and linear optical properties like transmittance, absorption coefficient and extinction coefficient of the sample were evaluated. Using Kurtz-Perry technique, second order NLO studies of the grown crystal of LPPI were carried out. In order to confirm the functional groups of the prepared sample, FTIR study was taken. EDS study was done to find the weight percent of the elements in the sample. Electronic polarizability and LDT value of LPPI crystal were estimated and the results were analyzed.

Keywords: Semi-organic crystal, Amino acid, Transmittance, Dielectrics, Microhardness, Electronic polarizability.

1. INTRODUCTION

There is a great need for effective nonlinear optical devices in the current technological era to meet daily needs. Amino acids often have an asymmetrical structure that exhibits exceptional NLO properties. As a result, it becomes increasingly important to generate new single crystals made of amino acids [1-3]. Amino acids are building blocks of proteins. Because they include both the proton acceptor amino (-NH2) group and the proton donor carboxyl acid (-COO) group, amino acids are promising materials for NLO applications. Amino acids' dipolar nature displays distinctive physical and chemical characteristics.

Proline $(C_5H_9NO_2)$ is a readily available amino acid that seems to be rigid and directional in biological systems because, unlike other amino acids, its amine group (-NH) is a component of the pyrrolidine ring. Some L-prolinebased crystals such as prolinium picrate, L-proline cadmium chloride monohydrate, prolinium tartrate, Lproline lithium chloride monohydrate, L-proline succinate, L-proline dimercury chloride, etc. have been reported in the literature [4-8]. Uma Devi et al. synthesized a crystal of L-prolinium picrate, employing temperature reduction method and studies like optical, thermal, SHG, electrical studies of the grown crystal were carried out and analyzed [9]. Nucleation kinetics, growth and analysis of structural, optical, dielectric and mechanical properties of nonlinear optical material Lproline manganese chloride was successfully grown by Anbuselvi et al. [10] from its aqueous solution by slow evaporation technique. Synthesis, crystal growth, structure as well as characterization of a novel semiorganic and nonlinear optical L-proline lithium bromide monohydrate single crystal were carried out by Sathiskumar et al. [11]. From the literature survey, it is figured out that the growth and studies of L-proline

potassium iodide crystals have not been reported in the journals so far. Hence L-proline potassium iodide (LPPI) crystals have been grown and studied in this work.

2. MATERIAL AND METHODS

2.1. Material

AR grade chemicals like L-proline and potassium iodide were purchased commercially from Merck India and the purity of the chemicals is 99.5%. The chemicals were used as purchased for synthesis and crystal growth.

2.2. Crystal growth

The purchased chemicals L-proline and potassium iodide were taken in a 1:1 molar ratio and dissolved in deionized water and the saturated solution was prepared at 40°C. The saturated solution is the solution that does not dissolve any more solute and the solution was stirred for about 2 hours using a hot-plate magnetic stirrer. The L proline potassium iodide compound was formed as per the following equation.

 $C_5H_9NO_2$ (L-Proline) + KI (potassium iodide) $\rightarrow C_5H_9NO_2.KI$

L-Proline potassium iodide

Then it was filtered to avoid unwanted things like dust and un-dissolved materials. To obtain the seed crystals the filtered solution was collected in a glass dish. The recrystallization of the seed crystals was carried out twice to improve the purity of the sample and this process took about ten days. Seed-immersion aqueous solution method was adopted so as to grow the bigger-sized bulk crystals. Again, the saturated solution of the sample was prepared, stirred well and filtered. After three days, the solution was formed into a supersaturated solution. Some good-quality seed crystals of L-proline potassium iodide (LPPI) were immersed in the supersaturated solution in a beaker covered with a perforated foil. The beaker was kept in a vibration-free place and it took about 35 days to harvest some big-sized crystals of LPPI. One such harvested crystal of LPPI is presented in figure 1. It is seen that the grown crystal of LPPI is colourless, transparent and non-hygroscopic. The size of the crystal of LPPI is observed to be $16 \times 10 \times 7 \text{ mm}^3$.



Fig. 1: Grown crystal of LPPI

3. RESULTS AND DISCUSSION

3.1. Single-crystal X-ray diffraction data

X-ray diffraction (XRD) method is used to find the lattice parameters and crystal structure. There are two XRD methods, namely the powder XRD method and single crystal XRD method to find the crystal structure. Since the sample is a single crystal, single crystal XRD method was adopted to ascertain the crystal structure. Single crystal X-ray diffractometer collects crystallographic data required for structure determination. The grown LPPI crystal was subjected to single crystal X-ray diffraction study at room temperature with MoK_{α} radiation (λ = 0.71073Å) using Bruker-Nonius MACH3/CAD4 diffractometer and the structural data were obtained. The obtained single-crystal XRD data for L-proline potassium iodide (LPPI) crystal is provided in table 1. The data obtained showed that LPPI crystal belongs to the tetragonal crystal system. For comparison purposes, the lattice parameters of L-proline crystal are given in the same table. When we compare the data, the crystal structure of L-proline and L-proline potassium iodide crystals are different. It is observed that potassium iodide crystal crystallizes in cubic structure and L-proline crystal crystallizes in orthorhombic structure, but L-proline iodide crystal crystallizes in tetragonal potassium structure.

Table 1: Single-crystal XRD data of LPPI crystal

Sampla	Parameters (Å)			Unit Cell	M 0	Rº.	~ ^0
Sample	a	b	С	Volume $(\text{Å})^3$	u	Р	Ŷ
L-proline hydrate crystal [12]	11.550	9.020	5.200	541.74	90	90	90
L-proline potassium iodide(LPPI) crystal	4.745(2)	4.745(4)	6.721(2)	151.33(3)	90	90	90

3.2. UV-visible spectral study

In UV-visible spectroscopy, the electrons involved are usually the valence or the bonding electrons, which can be excited by absorption of UV or visible or nearinfrared (NIR) radiation. The quantity of absorption is dependent on the wavelength of the radiation and the structure of the compound. The radiation absorption is due to the subtraction of energy from the radiation beam when electrons in orbitals of lower energy are excited into orbitals of higher energy. After the sample absorbs a portion of the incident radiation, the remainder is transmitted on to the detector. This remainder radiation is changed into an electrical signal that exhibits itself after amplification. The transmission spectrum shows what percentage of the incoming light can make it through the sample. UV-visible spectrum yields information relating to the structure of the molecule for the reason that absorption of UV and visible light entails the σ and π orbital electrons promoted from the ground state to higher states [13]. The UV-visible spectrum of LPPI crystal was recorded using Perkin Elmer Lamda 35 UV-visible spectrophotometer in the wave length range 190-800 nm and the spectrum is shown in fig. 2.



Fig. 2: UV-visible absorbance spectrum of LPPI crystal

From the UV-visible absorbance spectrum, it is observed that the sample has low absorbance in the visible region, and hence it has a wide optical transmission window. Near the absorption edge, the UV cut-off wavelength value is 257 nm for LPPI crystal. Using the formula $E_g = 1240 / \lambda$ the optical bandgap of the sample is determined (here λ is UV cut-off

wavelength) and the obtained value of bandgap (E_g) is 4.825 eV. The transmittance (T) values of LPPI crystal are arrived at using the relation T = (1 / 10^A), where A indicates the absorbance of the sample. The transmittance spectrum is drawn using the transmittance values, and presented in fig. 3.



Fig. 3: Optical transmittance spectrum of LPPI crystal

The linear absorption coefficient (α) of the LPPI crystal was calculated using the following expression:-

$$\alpha = \frac{2.303}{t} \log\left(\frac{1}{T}\right),$$

where t is the sample thickness.

The plot of absorption coefficient versus optical energy for the sample is shown in figure 4. The result indicates that the absorption coefficient of the sample is low in the visible region and is high at the optical bandgap at E_g = 4.83 eV. The dependence of the optical absorption coefficient on photon energy is used to study the band structure and the type of transition electrons. The optical bandgap and the linear absorption coefficient (α) near the absorption edge is given by

$$\alpha = \frac{A(hv - Eg)^n}{hv}$$

where E_g denotes the optical bandgap of the crystal and A is a constant. For a direct transition, n = 1/2. The plot of $(\alpha h \upsilon)^2$ versus $h \upsilon$ (Tauc's plot) is shown in figure 5. The bandgap was assessed by extrapolating the linear part to the energy axis and its value is found to be 4.83 eV for LPPI crystal [14, 15].

It is possible to derive the extinction coefficient (K) of the LPPI crystal sample from the following relation:-

$$K = \frac{\lambda \alpha}{4\pi}$$

where the wavelength of light is λ and it can also be termed as the linear attenuation coefficient that is a measure of how easily a material permits penetration by a beam of light. If this quantity is less, it is better for NLO crystals [16]. Since the extinction coefficient depends on the linear absorption coefficient, a plot of the extinction coefficient versus absorption coefficient for LPPI crystal is drawn and shown in fig. 6. The result indicates that the extinction coefficient varies linearly with the absorption coefficient up to the cut-off wavelength and then decreases.



Fig. 4: Plot of linear absorption coefficient versus optical energy for LPPI crystal



Fig. 5: Tauc's plot for LPPI crystal



Fig. 6: Plot of extinction coefficient (K) versus absorption coefficient (α) for LPPI crystal

3.3. FTIR study

In Fourier Transform Infrared (FTIR) spectral study, the spectrum is recorded in the time domain with Fourier transformation logic and then changed into the frequency domain. Here, KBr pellet method was adopted and in this method, potassium Bromide (KBr) is milled with the sample and compressed into a thin pellet. Since KBr is transparent, it forms the pellet [17]. In the present work, an FTIR spectrometer (Model: Perkin-Elmer make) was used to record the FTIR spectrum of LPPI crystal in the wavenumber range 4000-400 cm⁻¹, and the recorded spectrum is presented in fig. 7.



Fig. 7: FTIR spectrum of L-proline potassium iodide crystal

The spectrum shows the prominent absorption bands and the characteristic peaks are identified and assigned to various functional groups. The absorption band at 3425 cm⁻¹ is assigned to NH_2^+ stretching vibration and OH stretching of COOH. The peak at 1619 cm⁻¹ indicates the NH_2^+ bending and asymmetric COO⁻ stretching vibrations. The absorption peak at 1435 corresponds to symmetric COO⁻ stretching vibration. The peak observed at 1036 cm⁻¹ is due to C-N stretching. The infrared absorption peak at 881 cm⁻¹ is assigned with a metal-oxygen bond of the sample. The FTIR assignments are given by the literature [18, 19]. The vibration frequencies and their assignments are given in table 2.

Table 2: FTIR assignments to the absorptionpeaks/bands for LPPI crystalline sample

Absorption peaks/bands (cm ⁻¹)	Assignments
3425	$\mathrm{NH_2}^+$ stretching and OH
3723	stretching of COOH
1610	NH_2^+ bending and
1619	asymmetric COO ⁻ stretching
1435	Symmetric COO ⁻ stretching
1036	C-N stretching
881	Metal-oxygen bond

3.4. EDS Spectral Study

Energy dispersive spectroscopy (EDS or EDAX) uses the X-ray spectrum emitted by a solid sample which is bombarded with an intensive beam of electrons. It is possible, by using this method, to detect all the elements having atomic number from 10 to 92. Quantitative analysis entails measuring line intensities for each element in the sample and the same elements in calibration standards of known composition. The scanning electron microscope (SEM) with an EDS facility can be used for recording the EDS spectrum of the sample. In this work, the EDS spectrum of LPPI crystal was recorded with an EDS spectrometer (EDAX-INCA, Oxford Instruments, UK) and it is shown in figure 8. It is confirmed from the results that LPPI crystal contains the elements like C, O, N, K and I. Table 3 provides the weight percent and atomic percent of the elements in the sample. Atomic percent is determined by the number of atoms in the sample and the weight percent is based on the mass or atomic weight of the elements. The atomic percent can be converted into the weight per cent of elements and vice

versa. It is to be mentioned here that the hydrogen element in the sample cannot be detected by EDS spectroscopy.



Fig. 8: EDS spectrum of LPPI crystal

Table 3: Weight percentage and atomicpercentage of elements in LPPI crystal

Element	Weight percent	Atomic percent
Carbon (C)	8.33	28.39
Nitrogen (N)	4.46	13.02
Oxygen (O)	5.35	13.79
Potassium (K)	15.56	16.27
Iodine (I)	56.52	18.22

3.5. Electronic polarizability, Penn gap energy, and Fermi energy

Polarizability arises due to the charge separation when an electric field is applied to a dielectric material. It is defined from the relation dipole moment $(\mu) = \alpha E$ where α is the polarizability and E stands for the applied electric field. It is known that polarizability is responsible for the dielectric constant and refractive index at high frequencies. It depends on many factors like valence electron plasma energy, Penn gap, Fermi energy, etc. The plasma energy is estimated using the following expression:-

$E_v = 28.8 [(Z' \times \rho) / M]^{1/2}$

where Z' stands for the number of valence electrons of L-proline potassium iodide (LPPI) crystal, ρ is the density of the crystal and M is the molecular weight. For LPPI crystal, M = 281.14 g mol⁻¹, ρ = 3.083 g/cc, Z'= 54. Penn gap energy can be determined using E_p = E_v (ϵ '- 1)^{-1/2}, where ϵ ' is the dielectric constant at 1 MHz [20, 21]. Fermi energy is the kinetic energy of the particles in the highest occupied state and it is determined using the equation $E_F = 0.2948 \text{ x } E_v^{4/3}$. The calculated values of plasma energy, Penn gap energy and Fermi energy of LPPI crystal are given in table 4. Using the values of E_p , E_F and E_v , the electronic polarizability of the LPPI crystal can be estimated by the following relation [27]

 $\alpha = [(E_v^2 S) / (E_v S + 3E_p^2)] \times (M/\rho) \times 0.396 \times 10^{-24},$ where S = 1- (Ep/4EF) + 1/3 (Ep/4EF)2. Here, S is a constant depending on a material [22, 23], and this method of estimation is known as Penn analysis. By this analysis, the estimated value of electronic polarizability of LPPI crystal is 1.993 x 10⁻²³ cm³.

The Electronic polarizability of the sample can also be determined using the Clausius-Mossotti relation and the expression is given below.

 $\alpha = (3M/4\pi N\rho) \left[(\epsilon - 1) / (\epsilon + 2) \right]$

where N is the Avogadro's number and the obtained value of electronic polarizability is 1.947×10^{-23} cm³. From both methods, the value of the electronic polarizability of LPPI crystal is almost the same. The value of electronic polarizability can be used to develop the three-dimensional assessment of molecular stacking in the crystal.

Table 4: Values of plasma energy, penn gapenergy and fermi energy for LPPI crystal

	<u> </u>
Energy parame	eters Values
Plasma energ	y 22.162 eV
Penn gap ener	gy 13.961 eV
Fermi energy	9.824 eV

3.6. Dielectric constant, dielectric loss and AC conductivity

An LCR meter was used at different frequencies and temperatures to measure dielectric characteristics like dielectric constant and dielectric loss of LPPI crystal. The polished single crystal of LPPI was electrode on either side with a graphite coating to make it behave like a parallel plate capacitor. Measurements were done two times to ascertain the correctness of the observed results. The dielectric constant of the crystal was calculated using the relation $\epsilon_r = C/C_o$, where C is the capacitance of the capacitor in the presence of the crystal and C_o is the capacitance in air. By measuring the dielectric constant as well as the dielectric loss as a function of frequency and temperature, ideas of

electrical processes that are taking place in materials can be obtained. The variations of the dielectric constant and the dielectric loss for LPPI crystal with frequency at different temperatures are shown in figs. 9 and 10. From the data, the dielectric parameters are observed to decrease with an increase in frequency. The high values of the dielectric constant at low frequencies may be due to the presence of space charge polarization [24].



Fig. 9: Frequency dependence of dielectric constant with frequency for LPPI crystal at different temperatures



Fig. 10: Frequency dependence of dielectric loss with frequency for LPPI crystal at different temperatures

It is noticed that the dielectric parameters increase when the temperature of the sample increases. By Miller's rule, the lower value of the dielectric constant at higher frequencies is a suitable parameter for enhancing the SHG coefficient. The low value of the dielectric loss at high frequency reveals the high optical quality of the crystal with a low number of defects, which is the desirable property for NLO applications [25].

The AC conductivity (σ_{ac}) of LPPI crystal was determined using the relation $\sigma_{ac} = 2\pi f \varepsilon_0 \varepsilon_r$ tan δ , where f stands for the frequency of the AC supply, ε_{o} stands for the permittivity of free space or vacuum (8.852 $\times 10^{-12}$ F/m), ε_r for the relative permittivity or dielectric constant and tan δ for the dielectric loss. The values of AC conductivity of LPPI crystal are given in figure 11. From the results, it is found that AC conductivity increases with the increase of temperature of the sample. This is due to the excitation of charged carriers from the valence band to the conduction band when the temperature is increased. For many substances, as the temperature increases, more and more defects are produced, which in turn, increase the conductivity. The defect concentration will increase exponentially with temperature, and consequently, the electrical conduction also increases [26]. It is noticed that the AC conductivity of the grown LPPI crystal obeys the Arrhenius relation as given by $\sigma_{ac} = \sigma_{o} \exp(-E / kT)$ where σ_0 is the pre-exponential factor, E is the activation energy for the AC conduction process and k is the Boltzmann's constant [27].



Fig. 11: Frequency dependence of AC conductivity with frequency for LPPI crystal at different temperatures

3.7. Measurement of SHG efficiency

At high intense laser fields (E), the susceptibility becomes field-dependent, and therefore, the nonlinear response is expressed by writing the induced polarization as

 $\mathbf{P} = \boldsymbol{\varepsilon}_{0} \boldsymbol{\mathcal{X}}^{(1)} \mathbf{E} + \boldsymbol{\mathcal{X}}^{(2)} \mathbf{E} \cdot \mathbf{E} + \boldsymbol{\mathcal{X}}^{(3)} \mathbf{E} \cdot \mathbf{E} \cdot \mathbf{E} + \dots$

In the above expression, $\boldsymbol{\mathcal{X}}^{(l)}$ is the linear term responsible for material's linear optical properties like refractive index, dispersion, birefringence, and absorption. $\pmb{\mathcal{X}}^{(2)}$ is the quadratic term that describes second order NLO effects like second harmonic generation (SHG) in non-centrosymmetric materials. $\boldsymbol{\mathcal{X}}^{\scriptscriptstyle{(3)}}$ is the cubic term responsible for third harmonic generation, stimulated Raman scattering, phase conjugation and optical bistability. In this work, measurement of SHG efficiency for LPPI crystal was carried out by Kurtz and Perry test [28]. The powdered sample was illuminated by the Nd:YAG laser making use of the first harmonics output of 1064 nm having a pulse width of 8 ns and a repetition rate of 10 Hz. Here, potassium dihydrogen phosphate (KDP) sample was used as the reference material. The emission of green laser light indicates that the LPPI crystalline sample is a second-order NLO material. The obtained value of relative SHG efficiency of LPPI crystal is 1.7 times that of the KDP sample. It is to be stated here that the particle size of both LPPI and KDP samples was maintained at 150-175 µm. For comparison purposes, the values of SHG efficiency of some of the L-prolinebased crystals are given in table 5.

Table 5: Values of SHG efficiency of some L-proline based crystals

NLO crystal name	Relative SHG efficiency (Reference sample: KDP)
Bis-L-proline cadmium iodide [17]	2
L-proline lithium chloride [29]	0.2
L-proline lithium bromide [30]	0
L-proline cadmium chloride [31]	2
L-proline potassium iodide (present work)	1.7

3.8. Mechanical properties

The micro hardness of the sample was assessed by using the Vickers micro hardness tester. In this experiment, a pyramidal indenter was employed. By applying loads, measurement of the average diagonal indentation length (d) was taken and using these values, the Vickers micro hardness (H_v) was found using the relation

$$H_v = 1.8544 \text{ x P} / d^2$$
,

Where, P is the indentation load. The plots of micro hardness or average diagonal indentation length versus indentation load for LPPI crystal are shown in figure 12. It is observed that the hardness increases with an increase of the applied load up to 80 g and, then it decreases. It is seen that when the load is applied beyond 80 g, a crack is formed on the surface of the crystalline sample. The increasing trend of hardness is due to the reverse indentation size effect and the decreasing trend is due to the normal indentation size effect [32, 33].



Fig. 12: Plots of microhardness number (H_v) or average diagonal indentation length (d) versus applied load for LPPI crystal

Meyer gave a relation between the load (P) and average diagonal indentation length (d) as $P = k_1 d^n$, where k_1 is the constant depending on the material and, 'n' is Meyer's index or work hardening coefficient. Upon taking logarithm on both sides of the above relation, we get an equation of the straight line and, hence the value of work hardening coefficient (n) can be obtained [34]. The plot of log (P) against log (d) for LPPI crystal is shown in fig. 13 and from this fig., the value of work hardening coefficient of the LPPI crystal is obtained to be 2.852. According to Onitsch and Hanneman, for hard materials the value of work hardening coefficient (n) should lie between 1 and 1.6 and for soft materials it should be above 1.6. Hence, LPPI crystal belongs to the softer material category [35].



Fig. 13: Plot of Log (P) versus log (d) for the grown LPPI crystal

Toughness measures the relative degree of resistance to impact without any fracture in the material. An equilibrium relation for a well-developed crack extending under the centre loading condition is given by the fracture mechanics of the indentation process. As a result of indentation, there are two types of cracks namely, radial-median and Palmqvist cracks. The following formula for fracture toughness depends on the nature of cracks exhibited by the crystal. The fracture toughness (K_c) for the median type of crack system is given by:

$$K_c = \frac{P}{\beta_o c^{3/2}} ,$$

where P is the applied load, c is the crack length of indentation, $\beta_0 = 7$ for Vickers indenter. Since the crack is formed on the surface of the crystal at 80 g, P = 80 g is taken into account. The calculated fracture toughness of LPPI crystal is 0.084 g/(μ m)^{3/2}. Brittleness is also a significant property of the crystal, and it determines the fracture without any appreciable deformation. It is expressed in terms of brittleness index (B_i), given by $B_i = \frac{H_v}{K_c}$, where H_v is the Vickers hardness number.

The value of brittleness of LPPI crystal is derived as 0.768 $\mu m^{-1/2}$. Other mechanical properties of the grown LPPI crystal, such as yield strength and the stiffness constant, were determined using the values of microhardness. Yield strength is determined using the relation $\sigma_y = (H_v/3)$ and the stiffness constant is determined using the relation $C_{11} = H_v^{7/4}$, where H_v is the microhardness of the material. The estimated values of yield strength and stiffness constant of LPPI crystal are provided in table 6. From the data, it is observed that both yield strength and stiffness constant increase with the increase of the applied load for sample up to 80 g and then these values decrease. When a low load is applied on the sample, it seems that the sample is tightened due to an increase of bond strength and hence the mechanical properties like hardness, yield strength and stiffness constant increase with further increase of applied load up to 80 g [36].

Table 6: Values of yield strength and stiffnessconstant for LPPI crystal

Sample	Indentation load (g)	Yield strength x 10 ⁶ (pascal)	Stiffness constant (pascal)
LPPI - crystal -	20	93.426	6.07136E+14
	40	115.966	8.86228E+14
	60	154.186	1.45896E+15
	80	183.260	1.97392E+15
	100	145.041	1.31089E+15

3.9. Measurement of laser damage threshold value

Laser damage threshold (LDT) is an important parameter for NLO crystals and this value is the limiting factor in the development of laser systems and NLO devices. In optical materials, laser damage is a phenomenon including the interaction of high-power laser radiation with matter and different physical, chemical, mechanical, optical and, other aspects of materials that come into play. It is known that the harmonic conversion efficiency is proportional to the power density of the laser beam. Therefore, if we increase the power to increase the efficiency, it often leads to the breakdown of the material, catastrophically damaging the crystal. It is then useful to prescribe the maximum permissible power for a particular crystal, defined as damage threshold. The experimental set-up used for the measurement of laser damage of the sample consists of a Q-switched Nd:YAG laser having a wavelength of 1064 nm and a pulse width of 10 ns. An attenuator was used to control the energy of laser pulses and the occurrence of single pulse damage was detected by monitoring the fall of transmitted intensity as detected by a fast PIN type Si photodiode. The value of LDT was calculated using the equation $P = E/\pi \tau r^{2}$, where E is the input energy in mJ/pulse, τ is the pulse

width, and r is the radius of the laser spot. The estimated value of LDT for LPPI crystal is 2.14 GW/cm^2 . Since this value of LDT is high, the grown crystal of LPPI could be used for NLO applications [37, 38].

4. CONCLUSION

The Aqueous solution growth method was adopted to grow the single crystals of L-proline potassium iodide (LPPI) and the sample crystal is colourless, transparent and non-hygroscopic. The crystal structure of the crystalline LPPI sample belongs to the tetragonal structure. Measurements of Dielectric properties like dielectric constant and dielectric loss of the sample were taken at various frequencies and temperatures and AC conductivity was arrived at. The transmittance for the sample is found to be about 80%, and using values of transmittance the linear optical parameters like the absorption coefficient, the extinction coefficient, and the absorbance were estimated. Using Tauc's plot, the optical band gap of the LPPI crystal was found to be 4.83 eV. By the EDS method, the elements, namely C, O, N, K and I in the grown crystal of LPPI, could be identified. The chemical groups of the sample were found by FTIR analysis. By theoretical analysis, the value of electronic polarizability of LPPI crystal is found to be 1.993 x 10⁻²³ cm³ and Penn gap energy, plasma energy, Fermi energy of LPPI crystal were evaluated. By Vickers hardness method, the mechanical parameters like hardness, work hardening coefficient, stiffness constant, yield strength, fracture toughness and brittleness index of LPPI crystal have been estimated. The obtained value of LDT for LPPI crystal is 2.14 GW/cm². By the Kurtz-Perry method, the value of relative SHG efficiency of LPPI crystal is 1.7 times that of KDP sample, and, since this value is higher than most of L-proline-based crystals, LPPI crystal could be useful for laser, optoelectronic and NLO applications.

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