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Journals:


Growth and Characterization of high quality doped nonlinear optical crystals of L-Alanine Magnesium Chloride (LAMC)

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Abstract

Amino acids exhibit excellent nonlinear optical and electro optical properties. L-alanine magnesium chloride belongs to the amino acid group and has been grown by the slow evaporation solution growth technique (SEST) at room temperature. The grown crystals have been characterized by UV-vis-NIR spectroscopy; powder X-ray diffraction and Fourier transform infrared (FTIR) Spectroscopy. Second harmonic generation (SHG) efficiency of the grown crystal has been measured by Kurtz perry powder technique. The SHG efficiency of LAMC is found to be 0.3 times that of potassium dihydrogen orthophosphate (KDP).

1. Introduction:

In recent years, the need of nonlinear optical materials is much more than other materials because of their applications in Optoelectronics and Photonics [1, 2]. With rapid progress in crystal growth technology, crystals having attractive NLO properties are being discovered. Organic materials are attractive due to their nonlinearities, ultra fast response time and relative ease of device processing. Amino acid family crystals have over the years been subjected to extensive investigation by several researchers for their non-linear optical (NLO) properties [3–6]. Nonlinear optical crystal capable of generating second harmonic frequency plays an important role in the domain of optoelectronics and photonics. NLO crystals with high frequency conversion second harmonic efficiencies and transparent in the visible and ultraviolet ranges are required for numerous device applications. Most of the organic NLO crystals are constituted by weak Vander walls and hydrogen bonds with conjugated $\pi$ electrons [7]. In these respect amino acids are interesting materials for NLO applications [8].
Organic crystals are having some special properties of large optical nonlinearity and low cutoff wavelength in UV-region; therefore the organic NLO crystals are used in optical devices. However, the organic crystals have certain limitations such as poor mechanical and thermal stability. To overcome these problems, the combination of organic and inorganic hybrid compounds leads to find a new class of materials called semi organic materials having large optical nonlinearity, higher mechanical strength and chemical stability.

A survey of literature shows some complexes of L-alanine with inorganic salts such as LA acetate, LA cadmiumchloride, LA sodiumnitrate, Thiourea L-alanine acetate were reported(9-11). In this paper, we report the growth of L-alanine magnesium chloride (LAMC) by SEST. The title compound was characterized by various techniques.

2. Experimental:

Commercially available AR grades L-alanine and magnesium chloride were taken in the ratio 1:1 to synthesize LAMC. The calculated amount of reactants were thoroughly dissolved into double distilled water and stirred well for about 2h using a magnetic stirrer to obtain a homogeneous mixer. The solution was filtered using Whatmann filter paper to remove the suspended impurities. The filtered solution was taken in a beaker and covered by a perforated sheet. The solution was left undisturbed for evaporation at room temperature. After a span of period of 36 days, LAMC crystal of dimension (13mm×6mm×2mm) was harvested. The grown crystal is shown in figure 1.

Figure 1. As grown Crystal of LAMC
3. Characterization:

3.1. UV-Visible spectral analysis:

![UV–Vis spectrum of LAMC single crystal.]

A good optical transmittance is desirable in an NLO crystal. Since the absorptions near the fundamental or the second harmonic of a Nd: YAG laser, will lead to a loss of SHG efficiency, and this has been a specific drawback in many organic crystal. As a matter of fact, many organic NLO materials with high nonlinear coefficients are often coloured and allow considerable absorption in the visible/near-UV region. Since the material requirement is for crystals capable of generating blue light by SHG from diode lasers, the desired lower cutoff in the transmittance analysis is to be between 200 and 400 nm [12].

The UV-vis-NIR transmittance spectrum is shown in figure 2. It was recorded with SHIMADZU UV-2501 IC, UV-Vis spectrometer in the range 190-800 nm. The crystal shows a good transmittance in the visible region. It is observed that there is no significant absorption in the range 190-800nm. As there is no absorption, the crystal is found to be transparent in the visible and near IR region, an essential parameter required for frequency doubling process [13]. This is advantage of the use of amino acids where the absence of strongly conjugated bonds leads to wider transparency ranges in the visible and UV
spectral regions [14]. The lower cutoff at 210nm combined with the very good transparency window makes the material suitable for optoelectronics applications, the generation of the second and third harmonics of the Nd: YAG.

3.2. Powder X-ray diffraction studies:

The fine power of the title compound has been subjected to powder X-ray diffraction analysis and the recorded pattern is shown in figure [1]. The powder sample was scanned in steps of 0.1° for a time interval of 10 seconds over a 2Θ range of 10° to 70°. The sharp and well defined Bragg’s peaks at specified 2Θ angles show the crystalline nature and purity of the crystal. New peaks in the XRD pattern of the grown crystal confirm the incorporation of magnesium chloride in the grown crystals.

![Powder X-ray diffraction pattern for LAMC.](image)

3.3. Single crystal XRD

The single crystal of LAMC has been subjected to single crystal XRD using The lattice parameters determined for LAMC are a = 5.775Å, b = 6.041Å, and c = 12.335Å, & α=β=γ=90° and the cell volume = 431Å³. The structure is confirmed to be orthorhombic with the space group P2₁2₁2₁.

3.4. Fourier Transform Infrared (FTIR) analysis:
The infrared spectrum of the grown crystal has been taken using in the range of 400-4000 cm\(^{-1}\). The Fourier transform infrared (FTIR) spectrum of LAMC is shown in figure 4. The presence of the functional groups in LAMC crystal are identified. The peaks and their assignments are listed in table 1.

![FTIR spectrum of LAMC](image)

**Figure 4.** FTIR spectrum of LAMC

Amino group of absorption bands was noted at 844.82 cm\(^{-1}\). The peak at 2252.86 cm\(^{-1}\) is due to CH\(_3\) stretching. The sharp absorption peak at 2110 cm\(^{-1}\) is due to combination of NH\(^{3+}\) symmetric stretching and torsional oscillation. The peak at 1419.61 cm\(^{-1}\) is due to symmetric stretching of COO\(^{-}\). The peaks at 1149.57 cm\(^{-1}\) and 1234.44 cm\(^{-1}\) is due to NH\(^{3+}\) rocking. The peak at 412.27 cm\(^{-1}\) is due to COO\(^{-}\) rocking. The C-C-N symmetric stretching vibration is confirmed by the presence of peak at 918.12 cm\(^{-1}\). The peak at 1107.14 cm\(^{-1}\) is due C-N stretching. The peak at 1006.84 cm\(^{-1}\) represents C-N stretching. Due to C-CH\(_3\) bending, a strong absorption peak was formed 844.82 cm\(^{-1}\). The peak at 771.53 cm\(^{-1}\) is due to NO\(_3\) stretching. The peak at 648.08 is due to COO\(^{-}\) plane deformation. The peak at 528.5 cm\(^{-1}\) represents torsional oscillation of NH\(^{3+}\).
3.5. Second Harmonic Generation:

The second harmonic generation (SHG) efficiency was determined by the modified version of the powder technique developed by Kurtz and Perry [15] using an Nd: YAG, 10 ns laser with a pulse repetition rate of 10Hz working at 1064 nm. The sample was ground into fine powder and tightly packed in a micro-capillary tube. It was mounted in the path of the laser beam of 3.6mJ pulse energy obtained by splitting the original laser beam. The output light was passed through a monochromator transmitting only the second harmonic (green) light at 532nm. The green light intensity was registered by a photomultiplier tube and converted into an electrical signal. This signal was displayed on the oscilloscope screen.

Potassium dihydrogen orthophosphate (KDP) ground into samples of identical size was used as reference material in the SHG measurements. Conversion efficiency was computed by the ratio of amplitude of the LAMC and LACC sample to that of the KDP signal amplitude recorded for the same input powder. The SHG efficiency of the grown LAMC crystal was found to be 0.3 times higher than that of KDP.

The efficiency of the frequency conversion will vary with the particle size and the orientation of the crystallites in the capillary tube. Hence, higher efficiency may be expected to be achieved with single crystals by optimizing the phase matching (16).

4. Conclusion

LAMC crystal has been grown from aqueous solution by slow evaporation technique at room temperature. The sharp and well defined Bragg’s peaks of powder XRD pattern at specified 2θ angles shows the crystalline nature and purity of the crystal. The lattice parameters of LAMC are determined by single crystal XRD. It belongs to orthorhombic crystal system with the space group P2₁2₁2₁. The FTIR analyses confirm the presence of various functional groups. The lower cutoff wavelength at 210nm and the wide transparency range (190nm–800nm) observed from the UV–Vis spectrum confirms its suitability of the material for SHG applications. SHG studies revealed that LAMC crystals are a promising material for NLO applications.
References


Synthesis, Growth, and Characterization of Nonlinear Optical Crystal:
L-Alanine Lithium Nitrate

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**ABSTRACT**
Nonlinear optical L-Alanine Lithium Nitrate (LALN) single crystal was grown by slow evaporation solution method at room temperature. The title compound was characterized by various methods such as UV-Vis Spectroscopy, powder X-ray diffraction and Fourier Transform infrared (FTIR) Spectroscopy. The grown LALN was found to crystallize in orthorhombic system with space group P2\textsubscript{1}2\textsubscript{1}2\textsubscript{1}. The SHG efficiency of LALN was found to be 0.42 times that of potassium dihydrogen orthophosphate (KDP) and 0.12 times that of urea.

**Keywords**
UV-Vis Spectroscopy, Powder X-ray diffraction, FTIR Spectroscopy.

**Introduction**
Nonlinear optical (NLO) crystals are vital for the development of laser science and technology, because only this kind of materials can change frequency of laser beam and modulate its amplitude and phase. The extensive research of suitable new nonlinear materials is an important task because of their application in telecommunication for efficient signal processing and optical information storage devices. Organic nonlinear optical materials are of current interest for they are being used in advanced optical data processing devices. Amino acids are good materials for NLO application because they contain proton donor carboxyl acids (-COOH) group and the proton acceptor (NH\textsubscript{3}) group. Semi organic materials possess several attractive properties such as high NLO coefficient, high laser damage threshold and wide transparency range, high mechanical strength and thermal stability, which make the materials suitable for second harmonic generation (SHG) and other NLO applications. A series of studies on semiorganic amino acid compounds such as L-arginine phosphate (LAP), L-arginine hydrobromide (L-AHBr), L-histidine tetrafluoroborate (L-HFB), L-arginine hydrochloride (L-ACHCl), L-alanine acetate (L-AA), and glycine sodium nitrate (GSN) as potential NLO crystals have been reported. In this paper, we report the growth of L-alanine Lithium Nitrate (LALN) by SEST method.

**Experimental:**

**Synthesis and crystal growth:**
LALN was synthesized from aqueous solution of L-Alanine and Lithium Nitrate (AR grade) taken in the equimolar ratio. In solution growth technique, the solubility of material in the solvent plays a vital role in growing large-size single crystal. In order to select the proper solvent for growing large-size single crystals, the solubility of LALN in various solvents was studied. The solubility of LALN in organic solvents like acetone, ethanol, and methanol was found to be very less. Water was found to be a better solvent because of the low evaporation rate compared to other organic solvents. The calculated amount of the reactants were thoroughly dissolved in double distilled water and stirred well for about 2 hours using a magnetic stirrer to obtain a homogeneous mixture.

The completely dissolved solution was filtered using filter paper to remove the suspended impurities and then allowed to crystallize by slow evaporation of solvent at 30°C. The crystallization took place in 22 days and high quality transparent crystals of size 2×0.5×1 mm\textsuperscript{3} were harvested.

**Characterization:**

The UV-Vis transmittance spectrum was recorded using a Shimadzu UV-1061 UV –visible spectrometer. The single crystal X-ray diffraction (XRD) analysis of LALN crystal was carried out using a MESSRS ENRAF NONIUS X-ray Diffractometer and its unit cell dimensions were determined. The crystalline quality was found by PAN Analytical Power XRD. Fourier Transform infrared (FTIR) spectrum was recorded by the KBr Pellet technique using SHIMADZU Spectrometer for the range 400–4000 cm\textsuperscript{-1} to confirm the functional groups. The NLO behavior of L-alanine lithium nitrate crystal was tested by Kurtz powder SHG test using Nd:YAG laser (1064 nm).

**UV-Visible Spectral analysis**

![Figure 2. UV-Vis spectra for LALN](image-url)
crystal. The UV cutoff wavelength was around 250nm. This is an advantage of the use of amino acids where the absence of strongly conjugated bonds leads to wider transparency ranges in the visible and UV spectral regions. 

**X-ray diffraction studies:**

The fine power of the title compound has been subjected to powder X-ray diffraction analysis and the recorded pattern is shown in figure [3]. The powder sample was scanned in steps of 1° for a time interval of 10 seconds over a 2θ range of 10° to 70°. The sharp and well defined Bragg’s peaks at specified 2θ angles show the crystalline nature and purity of the crystal. New peaks in the XRD pattern of the grown crystal confirm the incorporation of lithium nitrate in the grown crystals.

**Fourier Transform Infrared (FTIR) analysis**

The infrared spectrum of the grown crystal has been taken having the green emission (λ = 532 nm) with a pulse duration of 6 ns was passed through the powdered sample. The SHG behaviour was confirmed from the output of the laser beam having the green emission (λ = 532 nm). It is a potential material for frequency conversion. The second harmonic generation signal of 4.9 mV for LALN crystal was obtained for an input energy of 3.6Mili Joules/Pulse. But the standard KDP crystal gave an SHG signal of 11.6 mV for the same input energy. Thus, it is observed that the SHG efficiency of the grown LALN single crystal is 0.42 times that of the standard KDP crystal.

**Conclusion**

Nonlinear optical LALN single crystal has been grown by slow evaporation method at room temperature. The sharp and well defined Bragg’s peaks of powdered XRD pattern at specified 2θ angles shows the crystalline nature and purity of the crystal. The lattice parameters of LALN are determined by single crystal XRD. It belongs to orthorhombic crystal system with the space group P2₁2₁2₂. Grown crystals were subjected to FTIR analysis, to confirm the presence of various functional groups in LALN single crystals. The lower cutoff wavelength at 250nm and the wide transparency range (200nm–900nm) was observed from the UV–Vis spectrum confirms its suitability of the material for SHG applications. The NLO property of the grown crystal was also studied by Kurtz–Perry SHG test.

**References**


**Table 1. FTIR Assignment of LALN crystal**

<table>
<thead>
<tr>
<th>LALN crystal</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>3097</td>
<td>NH⁺ asymmetric stretching</td>
</tr>
<tr>
<td>2596</td>
<td>NH⁺ stretching vibration</td>
</tr>
<tr>
<td>2249</td>
<td>Stretching of CH₃ vibration</td>
</tr>
<tr>
<td>2110</td>
<td>Combination of symmetric NH⁺ bending vibration &amp; torsional oscillation</td>
</tr>
<tr>
<td>1508</td>
<td>NH⁺ symmetric bending</td>
</tr>
<tr>
<td>1454</td>
<td>CH₃ bending</td>
</tr>
<tr>
<td>1411</td>
<td>COO⁻ symmetric stretching</td>
</tr>
<tr>
<td>1377</td>
<td>COO⁻ bending vibration</td>
</tr>
<tr>
<td>1303</td>
<td>CH₃ wagging</td>
</tr>
<tr>
<td>1234</td>
<td>CH₄ stretching</td>
</tr>
<tr>
<td>1149</td>
<td>rocking deformation of NH⁺</td>
</tr>
<tr>
<td>1111</td>
<td>rocking deformation of NH₃</td>
</tr>
<tr>
<td>1014</td>
<td>CH₃ rocking</td>
</tr>
<tr>
<td>918</td>
<td>C-C-N symmetric stretching</td>
</tr>
<tr>
<td>848</td>
<td>C-H bending</td>
</tr>
<tr>
<td>771</td>
<td>CH₂ rocking</td>
</tr>
<tr>
<td>648</td>
<td>O-C=O in plane deformation</td>
</tr>
<tr>
<td>536</td>
<td>COO⁻ rocking</td>
</tr>
<tr>
<td>486</td>
<td>COO⁻ rocking</td>
</tr>
</tbody>
</table>

**Second harmonic generation (SHG) studies**

The second harmonic generation behavior of the powdered material was tested using the Kurtz and Perry method. A high intensity Nd:YAG laser (λ = 1064 nm) with a pulse duration of 6 ns was passed through the powdered sample. The SHG behaviour was confirmed from the output of the laser beam having the green emission (λ = 532 nm). It is a potential material for frequency conversion. The second harmonic generation signal of 4.9 mV for LALN crystal was obtained for an input energy of 3.6Mili Joules/Pulse. But the standard KDP crystal gave an SHG signal of 11.6 mV for the same input energy. Thus, it is observed that the SHG efficiency of the grown LALN single crystal is 0.42 times that of the standard KDP crystal.

Nonlinear Optical Properties of Pure L-Alanine Calcium Chloride (LACaCl₂) Single Crystal

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Abstract – A nonlinear optical crystal, L-Alanine Calcium Chloride (LACaCl₂) was grown from aqueous solution by slow solvent evaporation method at room temperature. The grown crystals were characterized for spectral, optical and second order nonlinear optical properties. LACaCl₂ crystallizes in orthorhombic system. The mode of vibrations of different molecular groups present in the crystal was identified by FTIR study. The grown crystals were found to be transparent in the entire visible region. The NLO property of crystal was found using Nd:YAG laser light of wavelength 1064 nm and measured SHG efficiency was 0.42 times that of pure KDP. Vicker’s hardness proves the mechanical stability of the crystal.

Keywords – L-Alanine Calcium Chloride, Powder X-Ray Diffraction, UV-Visible Spectroscopy, FTIR, Vicker’s Hardness.

I. INTRODUCTION

Most of the amino acids and their complexes belong to the family of organic and semi-organic nonlinear optical (NLO) materials that exhibit wide applications in second harmonic generation (SHG), optical storage, optical communication, photonics, electro-optic modulation, optical parametric amplification, optical image processing, [1–6]. Amino acid family crystals have over the years been subjected to extensive investigation by several researchers for their nonlinear optical properties [7–10]. Among the amino acids, L-Alanine is the simplest aceticrystal with a SHG efficiency of about one-third of that of the well known KDP and it is a naturally occurring chiral amino acid with a non-reactive hydrophobic methyl group (CH₃) as a side chain [11–13]. The L-Alanine molecule exists as a zwitterion, where the carboxyl group dissociates and the amino group protonates. Some complexes of L-Alanine have been recently crystallized and various studies have been investigated by many researchers [14–18].

II. EXPERIMENTAL TECHNIQUE

The starting material was synthesized by taking L-Alanine and calcium chloride in a 1:1 stoichiometric ratio. The calculated amount of calcium chloride was first dissolved in deionized water. L-Alanine was then added to the solution. The solution was agitated with a magnetic stirring device for two hours continuously and filtered after complete dissolution of the starting materials. The solution thus prepared was allowed to evaporate at room temperature and allowed to crystallize by slow evaporation of solvent at 32°C. Well-defined single crystals of good transparency were collected in about five weeks. Transparent single crystals of size up to 2×2×1 mm³ were harvested and are shown in Fig.1.

III. CHARACTERIZATION

3.1 UV-Visible spectral analysis:

The UV–Vis-NIR transmittance spectrum is shown in fig 2. It was recorded with SHIMADZU UV-Vis spectrometer in the range 200–800 nm. The crystal shows a good transmittance in the visible region. It is observed that there is no significant absorption in the range 200–800 nm. As there is no absorption, the crystal is found to be transparent in the visible and near IR region, an essential parameter required for frequency doubling process. Thus use of amino acids leads to wider transparency range in the entire visible and UV spectral regions due to the absence of strong conjugated bonds. The lower cutoff at 210 nm combined with the very good transparency window makes the material suitable for optoelectronics applications, and for the generation of second harmonics.

3.2 Powder X-ray diffraction studies:

The fine powder of the title compound has been subjected to powder X-ray diffraction analysis and the recorded pattern is shown in fig 3. The powder sample was scanned in steps of 0.1° for a time interval of 10 seconds over a 20 range of 10° to 70°. The sharp and well defined Bragg’s peaks at specified 20 angles show the crystalline nature and purity of the crystal. New peaks in the XRD
pattern of the grown crystal confirm the incorporation of calcium chloride in the grown crystals.

3.3. Single crystal XRD

The grown crystal LACaCl₂ has been investigated by single crystal XRD and lattice parameters obtained are a=5.768Å, b=6.006Å, and c=12.301Å, & α=β=γ=90° and the cell volume =426.1Å³. The grown crystal crystallized in orthorhombic system with the space group P2₁2₁2₁.

3.4. Fourier Transform Infrared (FTIR) analysis:

The infrared spectrum of the grown crystal has been recorded in the range of 400-4000 cm⁻¹. The Fourier transform infrared (FTIR) spectrum of LACaCl₂ is shown in fig.4. The presence of the functional groups in LACaCl₂ crystal are identified.

![Fig.3. PXRD of LACaCl₂ single crystal](image)

![Fig.4. FTIR spectrum of LACaCl₂ single crystal](image)

Table 1: FTIR bands/peaks and their assignments LACaCl₂ crystal.

<table>
<thead>
<tr>
<th>Wavenumber (cm⁻¹)</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>2511.32</td>
<td>NH₃⁺ asymmetric stretching</td>
</tr>
<tr>
<td>2110.12</td>
<td>Combination of asymmetric NH₃⁺</td>
</tr>
<tr>
<td>1963.53</td>
<td>C=C stretch of COO⁻ vibration</td>
</tr>
<tr>
<td>1616.35</td>
<td>NH₃⁺ bending degenerate mode</td>
</tr>
<tr>
<td>1454.33</td>
<td>CH₃ asymmetric bending</td>
</tr>
<tr>
<td>1415.75</td>
<td>COO⁻ symmetric stretching</td>
</tr>
<tr>
<td>1300.02</td>
<td>C-H and N-H bending</td>
</tr>
<tr>
<td>1234.44,1153.43</td>
<td>NH₃⁺ rocking</td>
</tr>
<tr>
<td>918.12</td>
<td>overtone of torsional oscillation</td>
</tr>
<tr>
<td>844.82</td>
<td>C-H bending</td>
</tr>
</tbody>
</table>

771.53           | CH₁ rocking                         |
648.08           | O-C≡ O in plane deformation         |
536.21           | torsional oscillation of NH₃⁺       |

3.5. Second Harmonic Generation:

The second harmonic generation (SHG) efficiency was determined by the modified version of the powder technique developed by Kurtz and Perry [19] using Nd: YAG, 10 ns laser with a pulse repetition rate of 10Hz working at 1064 nm. The sample was ground into fine powder and tightly packed in a micro-capillary tube. It was mounted in the path of the laser beam of 3.6mJ pulse energy obtained by splitting the original laser beam.

Potassium dihydrogen orthophosphate (KDP) ground into samples of identical size was used as reference material in the SHG measurements. Conversion efficiency was computed by the ratio of amplitude of the LACaCl₂ sample to that of the KDP signal amplitude recorded for the same input power. The SHG efficiency of the grown LACaCl₂ crystal was found to be 0.42 times that of KDP.

3.6. Microhardness Studies:

Microhardness studies have been carried out on pure LACaCl₂ single crystal using a Leitz Wetzlar Vicker’s microhardness tester. The static indentations were made at room temperature with a constant indentation time of 10 s for all the loads. The hardness was calculated using the relation Hᵥ=1.8544P/d² kg/mm², where p is a load and d is the diagonal length of the indentation depression in diameter. The relation between hardness number (Hᵥ) and load (P) for LACaCl₂ is shown in fig 5. The plot of log p vs log d is a straight line and is shown in fig 6, which is in good agreement with Meyer’s law. The slope of the graph gives the n value as 2.933. According to Onitsch and Hanneman, for hard materials, value of n should be less than 1.6 and for the soft one, n should be greater than 1.6. Hence the grown crystal is a relatively softer material. The elastic stiffness constant is calculated for different loads using the relation C₁₁=(Hᵥ)⁷/³ [20] and the table 2 lists the computed values of C₁₁ for LACaCl₂.

Table 2: Elastic stiffness constant for different Loads

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Hᵥ kg/mm²</th>
<th>C₁₁ x 10⁻¹¹ Pa</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>30.45</td>
<td>3.9</td>
</tr>
<tr>
<td>2.</td>
<td>38.35</td>
<td>5.9</td>
</tr>
<tr>
<td>3.</td>
<td>45.8</td>
<td>8.06</td>
</tr>
<tr>
<td>4.</td>
<td>51.0</td>
<td>9.7</td>
</tr>
</tbody>
</table>

![Fig.5.Variation of Hᵥ with applied load P](image)
IV. CONCLUSION

LACaCl₂ crystal has been grown from aqueous solution by slow evaporation technique at room temperature. The sharp and well defined Bragg’s peaks of powder XRD pattern at specified 2θ angles shows the crystalline nature and purity of the crystal. The lattice parameters of LACaCl₂ are determined by single crystal XRD. It belongs to orthorhombic crystal system with the space group P2₁2₁2₁. The FTIR analyses confirm the presence of various functional groups. The lower cutoff wavelength at 210nm and the wide transparency range (200nm–800nm) observed from the UV–Vis spectrum confirms suitability of the material for optoelectronic applications. SHG studies validate the use of LACaCl₂ crystal as a promising material for NLO applications. Vickers Microhardness value was calculated in order to understand the mechanical stability of the grown crystal and the calculated value of n being 2.933 proves that the grown crystal belongs to the category of soft materials.

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