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An Innovative Approach to Design a Sensor for Environmental Hazardous Waste Management Using L-Alanine reinforced with Diglycine Picrate (LADGP) Crystal

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Abstract

L-Alanine Diglycine Picrate (LADGP) single crystals were successfully grown at room temperature using the slow evaporation solution growth technique. The optical properties of the grown crystals were studied using UV–Vis–NIR spectroscopy, revealing good optical transparency in the visible region. The electrical properties were examined through dielectric and conductivity measurements, indicating favorable dielectric behavior. The laser damage threshold (LDT) study demonstrated that the LADGP crystal possesses a high resistance to laser-induced damage, suggesting its suitability for laser-related and optoelectronic applications. In addition, picrate ions are known for their strong affinity toward binding organic compounds and heavy metal ions, and the crystalline structure of diglycine picrate provides a stable matrix with a relatively high surface area advantageous for adsorption processes. By incorporating L-alanine into the diglycine picrate lattice and optimizing the growth conditions at different pH values, the material's adsorption capacity, stability, and selectivity can be enhanced. These characteristics indicate that LADGP crystals have potential not only in optical applications but also as promising candidates for hazardous waste treatment and environmental remediation.

1. INTRODUCTION

Third-order NLO properties involve interactions where the induced polarization is proportional to the cube of the electric field. These properties are utilized in a variety of advanced optical and photonic applications. The balance between third-order nonlinear susceptibility and laser damage threshold is crucial for the practical application of NLO materials. By addressing the inherent drawbacks through advanced materials engineering and innovative design strategies, it is possible to harness the full potential of third-order NLO properties in a variety of high-performance optical and photonic devices. These applications span from telecommunications and data processing to

biomedical imaging and safety systems, highlighting the significant impact of these advanced materials. By leveraging the multiple functional groups present in L-alanine and diglycine picrate, electrochemical sensors can achieve enhanced sensitivity towards detecting low concentrations of heavy metals. These functional groups, including amino, carboxyl, and picrate ions, provide multiple binding sites that facilitate strong interactions with heavy metal ions. Through careful tuning of the composition and structure of the sensor material, selectivity can be tailored to distinguish between different types of heavy metal ions based on their unique coordination chemistry with the sensor surface. This approach not only enhances the sensor's performance in detecting specific contaminants but also broadens its applicability in environmental monitoring, biomedical diagnostics, and industrial process control. Extinction coefficients, denoted as ε, are crucial in spectroscopic analysis for their sensitivity to molecular environments, including pH variations[1].Changes in pH can profoundly influence the extinction coefficient by altering the electronic structure or the protonation states of functional groups within a molecule. For instance, acidic or basic conditions can shift the equilibrium between different ionization states of functional groups, thereby modifying the molecule's absorption spectrum. This sensitivity forms the basis for pH-dependent spectroscopic techniques used in detecting hazardous substances. By monitoring how the extinction coefficient varies with pH, analysts can infer the presence or concentration of substances that alter the solution's pH or directly interact with the analyte. This approach not only aids in identifying hazardous materials but also enhances sensitivity in environmental monitoring and chemical analysis applications where pH variations are significant factors influencing molecular interactions and absorption characteristics[2].

Experimental section
Growth and synthesis procedure
The LADGP single crystals were synthesized using the slow evaporation solution method. Specific amounts of L-Alanine and Diglycine Picrate were dissolved separately in distilled water, each in its own beaker. Once dissolved, the solutions were gradually combined and stirred thoroughly for 8 hours at room temperature to ensure complete reaction. The resulting solution exhibited a yellow hue, indicating successful chemical transformation. Subsequently, the solution was set to have different PH values with addition of L-alanine solution. It is then evaporate naturally at ambient conditions, resulting in the formation of yellow crystalline DGP crystals. The well-developed LADGP single crystal reaching optimal condition with PH=6 is grown with dimensions of 9 mm × 8 mm × 5 mm and it was cultivated over a growth duration of 14 days. Figure.1a illustrates the resulting LADGP single crystal reached optimal condition.
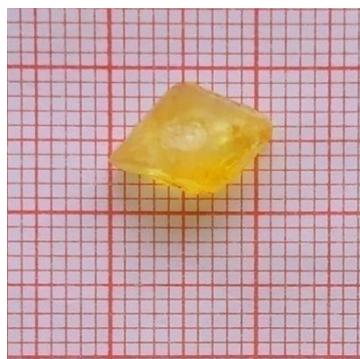

Fig1a.Picture of LADGP single crystal

Results and Discussion
Microhardness Analysis
 Microhardness is the assessment of material hardness at very small scales, usually measured in micrometers. It involves applying a precise force to create an indentation on the material's surface, which is then measured. This method is essential for analyzing specific mechanical properties of

materials in localized areas. Figure 2a illustrates the plot showing the relationship between the logarithm of P and the logarithm of 'd'. The measured value of n=0.4091 on the graph confirms that optimized LADGP crystal is classified as hard[3][4][5][6]. In Figure 2a,b graph demonstrates the relation between the hardness number 'H_v' and the applied load 'P'. The hardness value obtained from the grown LADGP crystal indicates that higher stress is required to induce micro-damages, affirming its superior crystalline perfection. This quality makes the crystal highly suitable for device fabrication purposes.
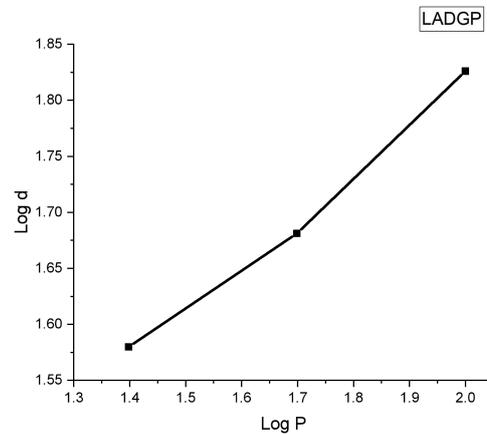

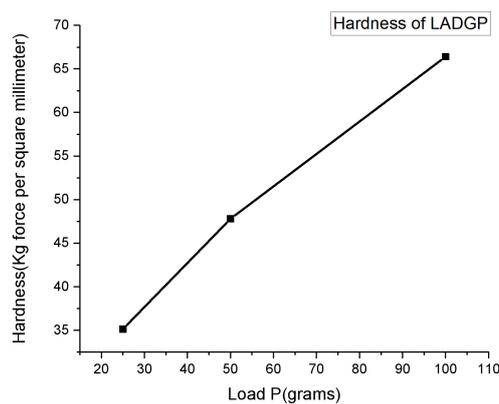**Fig2a.variation of log P with log d**

Fig2b.variation of H_v with load P

UV-VIS NIR analysis

pH can alter the refractive index of a solvent due to changes in its ionization state or interactions with solvent molecules. For example, acidic or basic conditions can affect the ionization of water molecules, leading to variations in its refractive index. This change is particularly relevant in aqueous solutions where pH fluctuations can modify the density and polarizability of the solvent molecules, thereby influencing their refractive index.The absorption spectrum of LADGP at different pH values is plotted and it is shown in figure 3a. The extinction co-efficient graph of LADGP at different PH values is plotted and it is shown in figure 3b. Less absorbance and less extinction Co-efficient in LADGP at ph=6 is shown in figures 3c, 3d. Understanding these mechanisms is crucial in various fields such as chemistry, biology, and materials science where pH-sensitive optical properties play a significant role in analytical techniques and sensor development.The concentration of the added amino acid and its molar ratio relative to diglycine picrate will determine the magnitude of the pH change. If the molar extinction coefficient changes with pH, the absorbance measured at a given wavelength will also change according to Lambert's Law, even if the concentration and path length remain constant[7][8]. Figure 3e shows at ph=6,there is a maximum extinction co-efficient.
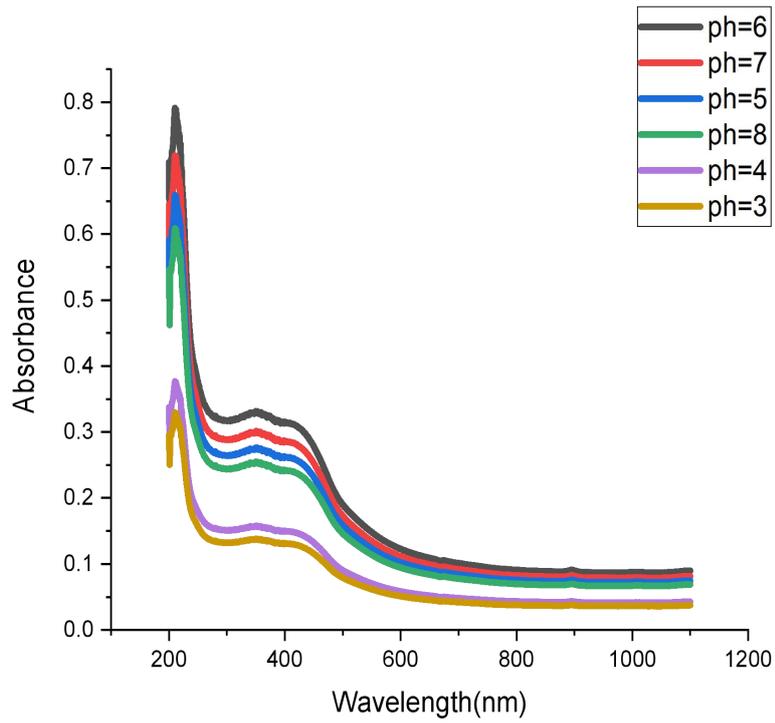
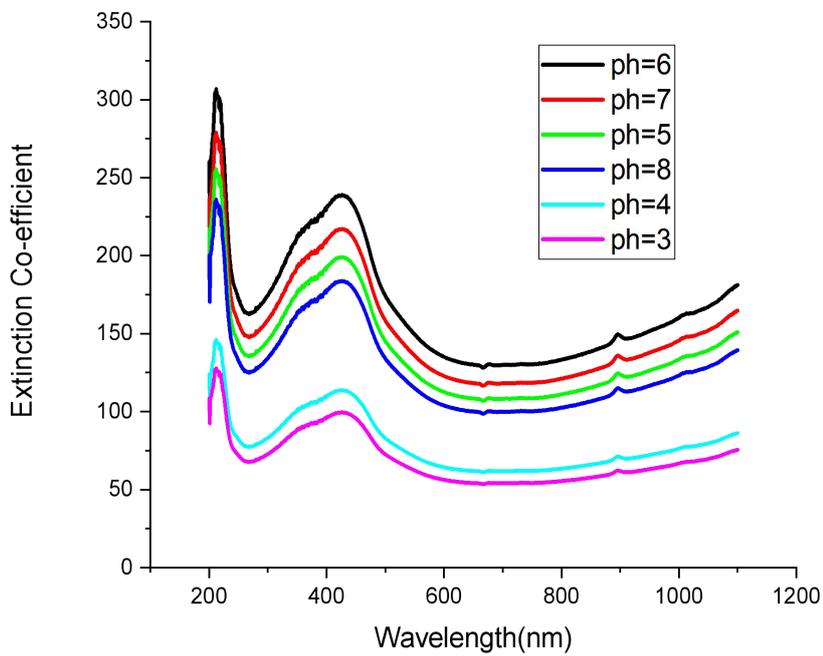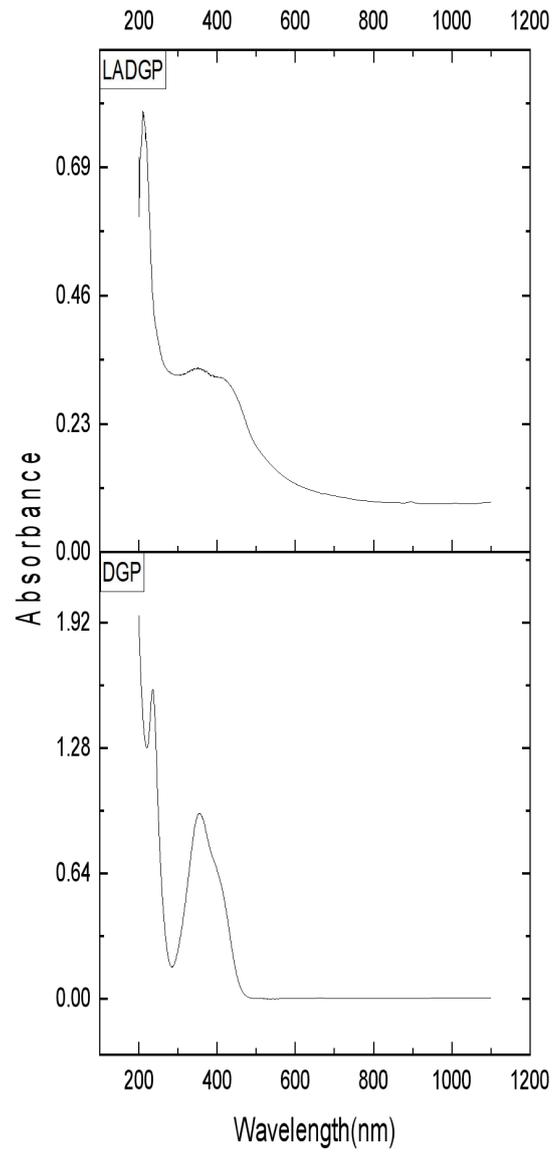**Fig 3a.Absorption spectrum of LADGP at different pH Values**

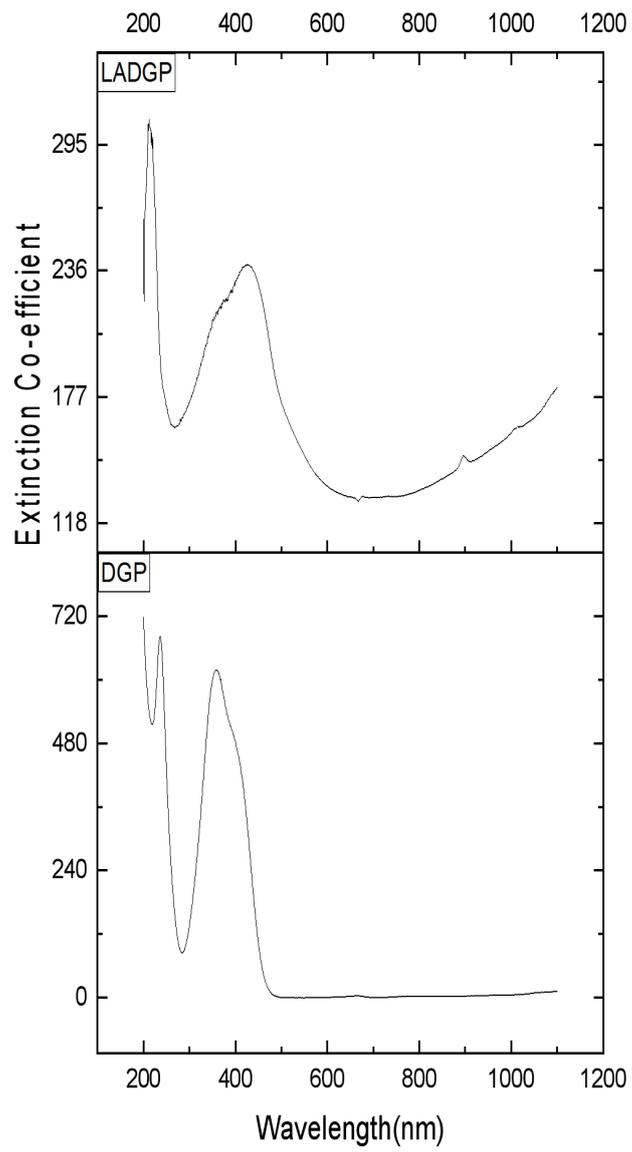**Fig 3b.Extinction co-efficient of LADGP at different pH levels**

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Fig 3c. variation of absorbance   Fig.3d.variation of extinction coefficient

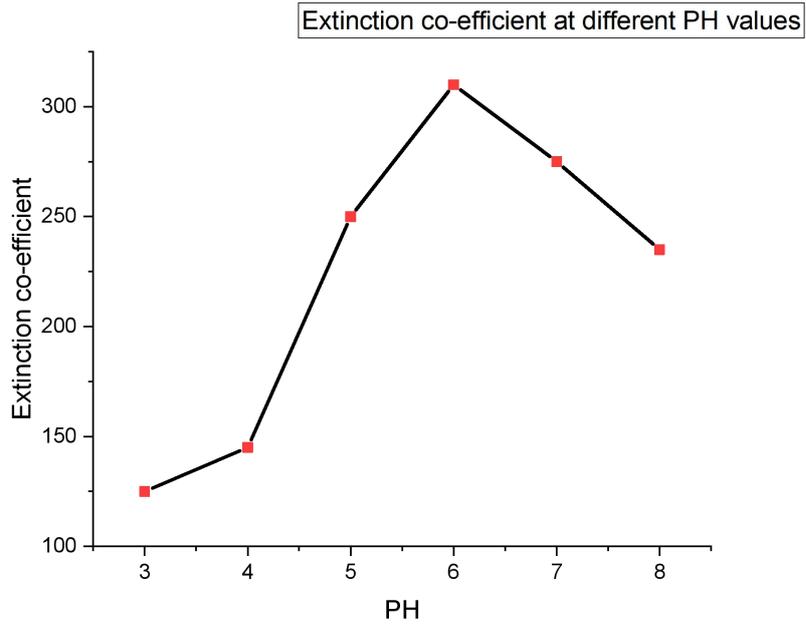Extinction co-efficient at different PH values

Fig 3e. Extinction co-efficient versus pH

Materials with a reduced bandgap require lower energy photons to excite electrons from the valence band to the conduction band. This allows the sensor to operate effectively under lower light conditions, enhancing its sensitivity to weak signals[9]. The bandgap energy diagram shown in figure 3f.
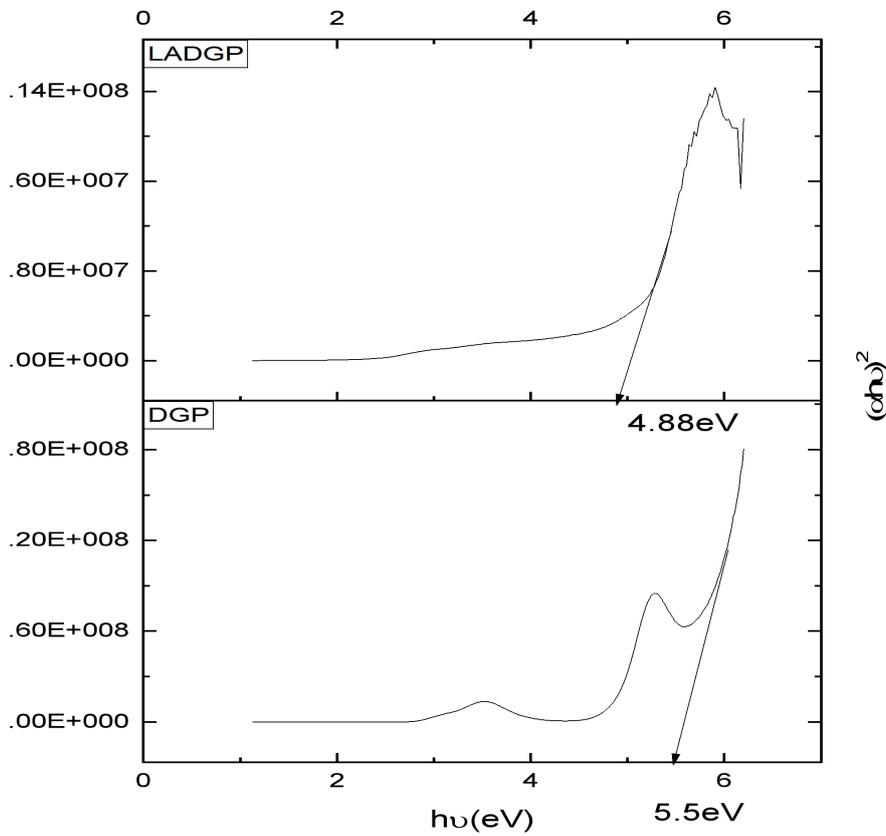
Fig 3f . Tauc plot

Dielectric study

The dielectric constant and dielectric loss for LADGP for three different temperatures are shown in figures 4a and 4b. AC Conductivity of LADGP is shown in figure 4c Activation energy of LADGP is shown in table 1.The properties of high AC conductivity and low activation energy make the material suitable for different operational environments, including those with varying temperatures and electrical conditions. Choosing materials with intrinsic low activation energy characteristics that exhibit favorable electronic or catalytic properties is crucial for effective sensor design. Low activation energy plays a critical role in sensor technology by enhancing sensitivity, selectivity, and energy efficiency. Sensors utilizing materials with low activation energy can operate effectively at lower temperatures, respond quickly to changes in analyte concentration, and maintain stability under various environmental conditions. These attributes make them suitable for a wide range of applications, from environmental monitoring to biomedical diagnostics, ultimately leading to improved sensor performance and reliability[10][11][12][13].
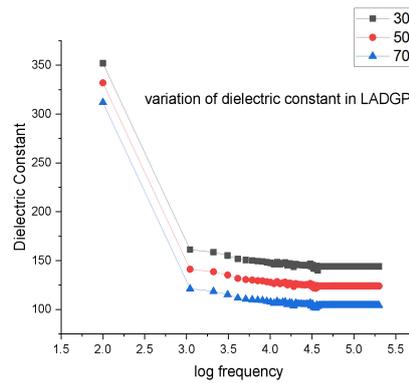
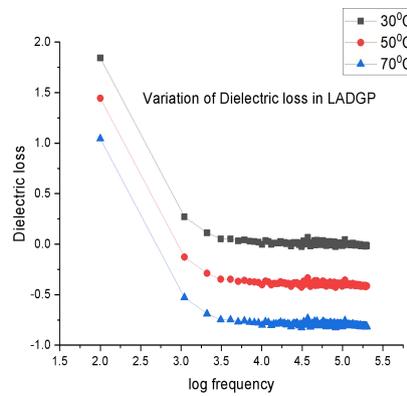

Fig 4a. **dielectric constant in LADGP**
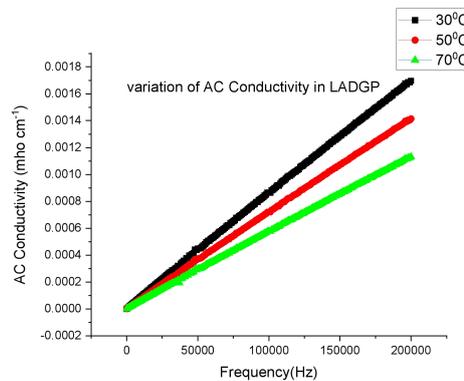

Fig 4b.**dielectric loss in LADGP**

Fig 4cAC conductivity in LADGP

Table 1.Activation energy in LADGP

Frequency	Ea/K	in eV
100	31.8256	0.002742412
1099	12.2159	0.001052644
10095	3.956	0.000340889
50075	3.556	0.000306421
100050	2.75	0.000236968
200000	2.55	0.000219734

Laser Damaged Threshold (LDT) study

A laser damage threshold study on crystals involves examining the point at which a crystal material begins to deteriorate or sustain irreversible damage when exposed to intense laser radiation. This research aims to determine the limits of a crystal's resilience to high-energy photon interactions, which is crucial for various applications in laser technology, optics, and materials science. The investigation into the Laser Damage Threshold involved subjecting the LADGP crystal to a high-energy Nd: YAG laser operating at a wavelength of 1064 nm in a Q-switched configuration. The incident laser beam was focused using a lens with a 10 cm focal length. The laser light's pulse energy was measured with a power meter, and the power density was calculated using the following expression:

$$\text{Power density, } (P_d) = E/\tau\pi r^2$$

In this equation, 'E' stands for the input energy density measured in millijoules (mJ), 'τ' represents the pulse width in nanoseconds (ns), and 'r' is the radius of the circular spot in millimeters (mm). Notably,LADGP crystal exhibits an impressive laser damage threshold 2.6 GW/cm², which surpasses that of KDP (0.20 GW/cm²) and urea (1.50 GW/cm²). This characteristic underscoresLADGP crystal's exceptional optical damage tolerance[14], making it a promising candidate for integration into high-energy laser devices. At extreme pH levels, materials may undergo chemical degradation, altering their physical and optical properties. This degradation can lower the material's resistance to laser-induced damage. In highly acidic or basic environments, certain materials, especially organic compounds, can undergo hydrolysis, leading to structural breakdown and reduced LDT.

Z-Scan Analysis

The Z-scan method measures the nonlinear refractive index by moving the sample through the focus of a tightly focused laser beam and monitoring the transmitted intensity as a function of the sample position (z).In open aperture both the linear and nonlinear absorption effects are measured. In closed aperture Z-scan, a small aperture is placed before the detector to measure changes in the beam's phase due to the nonlinear refractive index. The nonlinear absorption coefficient is measured using the z-scan open aperture configuration, where the entire transmitted beam is collected without any aperture, similar to the closed aperture Z-scan, but without the aperture before the detector. The sample is scanned along the z-axis, and the transmitted intensity is also to be measured.In closed-aperture configuration, the nonlinear third order refractive index 'n_2' value was measured at 2.6550×10^{-12} m²/W for LADGP single crystal. Under the open aperture configuration, the nonlinear absorption coefficient 'β' evaluated as 9.2217×10^{-5} m/W for LADGP single crystal. The magnitude of the nonlinear third order susceptibility '$\chi^{(3)}$' recorded at 3.8189×10^{-8} esu for LADGP. The presence of a positive nonlinear refractive index (n_2) signifies that the material exhibits self-focusing characteristics. Figure 5a and5b shows Normalized transmittance graph of LADGP when observed through open aperture method and Closed aperture method. By systematically studying the changes in nonlinear magnetic susceptibility with pH, we can gain insights into the underlying mechanisms and potentially use this relationship for applications such as pH sensors or in materials science research. Changes in nonlinear magnetic susceptibility (χ3) can significantly influence the refractive index of adjacent materials. In our study, we observed that the enhanced magnetic interactions due to increased(χ3) lead to a measurable change in the refractive index of nearby optical materials. This

effect underscores the potential for designing advanced optical devices that leverage nonlinear magnetic properties to dynamically control refractive index[15][16][17][18]
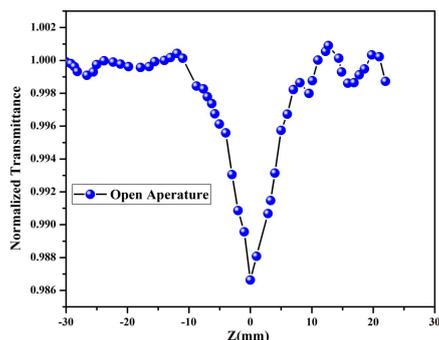

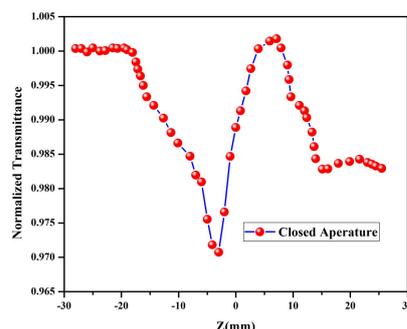**Fig.5a.Normalized transmittance of LADGP in open aperture**

Fig.5b.Normalized transmittance of LADGP in closed aperture

The relationship between transmittance and impedance in sensor technology provides valuable insights into the interaction of electromagnetic waves with sensor materials. Understanding this relationship helps optimize sensor design for enhanced sensitivity, selectivity, and performance. By combining measurements of transmittance and impedance, sensors can achieve more accurate and comprehensive detection capabilities, making them suitable for a wide range of applications, from environmental monitoring to biomedical diagnostics[19][20][21].

CONCLUSION

High-quality L-Alanine Diglycine Picrate (LADGP) single crystals were grown under optimized conditions using the slow evaporation solution growth method, yielding transparent yellow crystals with dimensions of $9 \times 8 \times 5$ mm³. Sensor calibration can be performed using known concentrations of analytes to establish baseline responses based on variations in the extinction coefficient and dielectric properties. Optical parameters, particularly the extinction coefficient and third-order nonlinear magnetic susceptibility (χ^3), play a crucial role in enhancing sensor performance. The extinction coefficient, which quantifies light absorption, is highly sensitive to changes in the chemical environment, enabling precise detection of analytes through measurable absorption variations. Furthermore, the third-order nonlinear magnetic susceptibility contributes to enhanced sensor sensitivity by amplifying nonlinear optical responses under applied magnetic fields, allowing detection of subtle changes in the magnetic environment. By integrating extinction coefficient analysis with nonlinear magnetic and dielectric properties, LADGP-based sensor technology can achieve high sensitivity, selectivity, and multifunctionality, making it suitable for applications ranging from environmental monitoring to biomedical diagnostics. Future research will focus on investigating refractive index variations in the presence of different metal ions and exploring the feasibility of LADGP crystals as electrochemical sensors.

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