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Research Article

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Posted Date: October 15th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-11076849/v1>

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Additional Declarations: No competing interests reported.

**Multi-Parametric Characterization and DFT Analysis of L-Proline-Doped Strontium Nitrate
(LPSN) Single Crystal**

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Abstract

The Mounting demand for advanced optoelectronic devices has generated curiosity over the optical and functional nature of crystalline structures. The present work focuses on synthesizing and evaluating the structural, thermal, optical, electrical, and quantum chemical properties of semi-organic L-proline-doped strontium nitrate (LPSN) single crystals. Single crystal X-ray diffraction (SCXRD) analysis revealed that LPSN crystallizes in the cubic centrosymmetric $Fm\bar{3}m$ space group, while powder X-ray diffraction (PXRD) verified phase purity. Fourier-Transform Infrared spectroscopy identified key functional groups and conformed structural interaction between the L-proline component and nitrate-bearing host lattice. Thermogravimetric and Differential Thermal Analysis (TG-DTA) revealed exceptional thermal stability up to 550°C before decomposition. Kinetic parameters of major decomposition process studied using Coats-Redfern Method yielded activation energy of 304.01 kJ mol⁻¹. UV-Vis-NIR analysis showed significant transparency within the region of wavelength investigated. Results of scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy analysis verified a smooth surface morphology, besides confirming the presence of strontium, nitrogen, carbon and oxygen. Complex impedance analysis confirmed a bulk relaxation mechanism, characterized by an ohmic resistance of 50

Ω , a charge-transfer resistance of $970\ \Omega$ and a low AC conductivity of $(1.25 \times 10^{-2}\ \Omega\cdot\text{m})^{-1}$. Density Functional Theory (DFT) and molecular electrostatic potential (MEP) analyses were employed at the B3LYP/LANL2DZ level to investigate electronic properties of the LPSN crystal. High global electrophilicity and extremes of electrostatic potential indicated strong regional reactivity and intermolecular hydrogen-bonding capability. These combined findings highlighted the suitability of LPSN crystals for next generation optoelectronic devices like, optical modulators, photodetectors, optical sensors, organic LEDs, signal detectors and generators.

Keywords: $Fm\bar{3}m$ space group; Eyring transition-state approach; Gibbs free energy; Warburg-type diffusion; Charge-acceptance capacity.

1. Introduction

Ever growing demand for high quality optical and electronic devices has prompted researchers to study crystalline materials with customised structural, mechanical, thermal, and optical characteristics. In particular, amino acid-derived organic and semi organic crystals have garnered attention, as their molecular structures enable varied intermolecular interactions, involving hydrogen bonding and ionic interactions, having effect on their physicochemical and optical behaviour [1-4]. When combined with inorganic constituents, their structural stability, optical transparency, dielectric response, etc. get modified. Some recent researches have reported certain functional properties in amino acid derived semi organic crystals which illustrate their utility in optical, optoelectronic and photonic technologies [5-8]. A network of intermolecular hydrogen bonds and ionic interactions stabilize the amino acid molecules in crystalline form, thus playing an important role for maintaining lattice integrity. Certain functional groups, viz. carboxylate and protonated amino groups provide several sites for interaction which tend to influence the structure and physicochemical characteristics of the grown crystals [7-9]. Thus, by incorporating amino acids into inorganic or semi organic crystal matrices their structural, optical, dielectric and thermal properties can be tailored effectively.

In one study, for example, L-proline-modified imidazolinium L-tartrate crystals reportedly exhibited variations in crystal structure, diffraction features, optical transmission and dielectric response, which demonstrate the impact of the incorporated amino acids on the physicochemical properties of crystals [10]. The structural uniqueness of the cyclic amino acid L-proline results from a pyrrolidine ring in which the amino nitrogen forms a distinct secondary amine core. Such a molecular configuration supplies conformational stability apart from facilitating within the crystal lattice diverse intermolecular

interactions. L-proline based semi organic crystals have therefore, been examined in view of their distinct structural and optical traits. Further L-proline potassium bromide crystals have reportedly exhibited fair optical transparency over the spectral range studied [11]. The present study has focussed keenly on the controlled synthesis and systematic characterization of semi-organic L-proline-doped strontium nitrate (LPSN) single crystals using slow evaporation solution growth process.

The LPSN crystals underwent comprehensive structural, vibrational and optical characterization using SCXRD, PXRD, FTIR spectroscopy and UV–Vis–NIR spectrophotometry, Thermogravimetric–differential thermal analysis (TG-DTA) and complex impedance measurements to study its structural architecture, chemical bonding environments, optical transmission behaviour, thermal kinetics and dielectric characteristics. SEM-EDX studies confirmed smooth crystalline surface and uniform elemental distribution. The significant HOMO-LUMO energy gap and molecular electrostatic potential (MEP) surfaces were identified by DFT calculations at the B3LYP/LANL2DZ level. The combined experimental and theoretical results confirm the strong structure-property relationship of the LPSN single crystal, demonstrating its potential for deployment in next-generation optical, photonic and optoelectronic systems.

2. Material Synthesis

Analytical reagent (AR)-grade L-proline and strontium nitrate were used as starting materials to synthesize L-proline doped strontium nitrate (LPSN). Equimolar quantities of the reagents were dissolved in double-distilled water and stirred continuously for three hours. The homogeneous solution was then passed through Whatman filter paper to remove particulate impurities. It was next transferred to a clean petri dish and covered with a thin perforated aluminum foil to control the rate of solvent evaporation and prevent contamination. Thereafter, the solution was maintained undisturbed at room temperature, to facilitate supersaturation, nucleation and crystal growth [12]. Upon controlled evaporation of the solvent, well developed, optically transparent LPSN crystals exhibiting distinct morphology were successfully formed. The as-grown LPSN single crystal thus obtained through slow-evaporation solution-growth technique is shown in **Fig.1**.



Fig1. As-grown (LPSN) single crystal

3. Single-crystal and powder X-ray diffraction analysis

The PXRD pattern of the grown LPSN crystal displays sharp and well-defined reflections which evidences its high degree of crystallinity, as shown in **Fig. 2**.

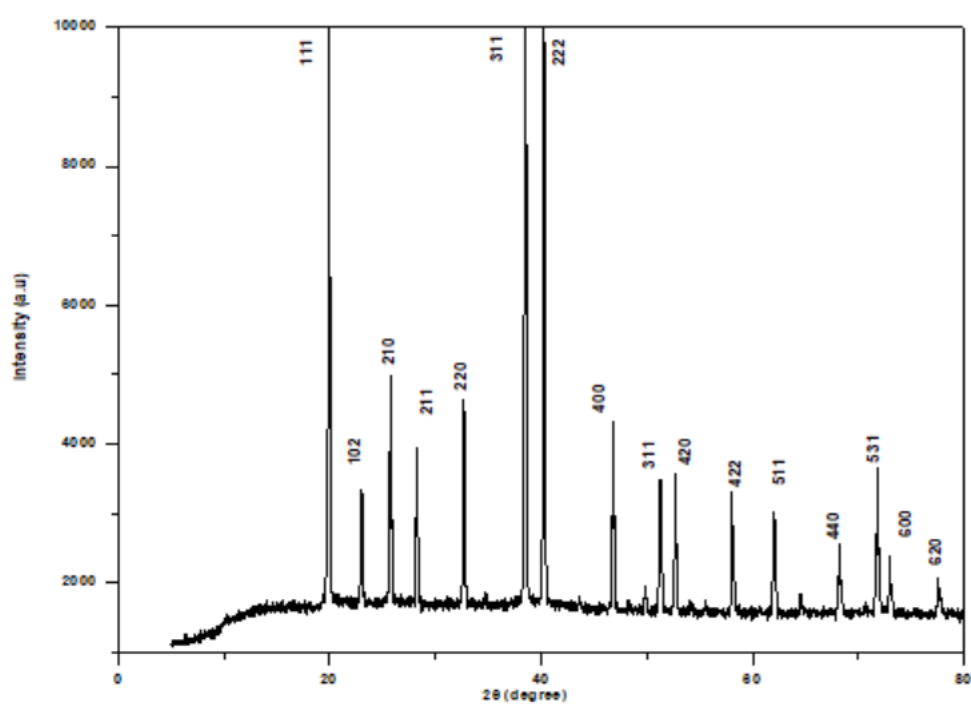


Fig2. The powder X-ray diffraction pattern of LPSN Crystal

The diffraction profile observed matches with the standard diffraction data of strontium nitrate (JCPDS No.00-025-0746), indicating that the crystalline phase is dominantly associated with $\text{Sr}(\text{NO}_3)_2$ [13]. Furthermore, the SCXRD investigation established the as-grown crystal having crystallized in the cubic system, described by the $\text{Fm}\bar{3}\text{m}$ space group (No.225), having density of 2.416 g cm^{-3} . Though pure L-proline is orthorhombic, its integration into the host matrix maintains the core cubic frame even as it induces a lattice contraction from $7.8220 \text{ \AA}$ to $7.7860 \text{ \AA}$ and a volume reduction from $478 \text{ \AA}^3$ to $472 \text{ \AA}^3$, asserting the integration of L-proline into the lattice structure. Comparative crystallographic parameters and cell volumes of pure L-proline, strontium nitrate and LPSN crystals is given in **Table 1**.

Table:1 Crystallographic parameters and cell volumes of pure L-proline, strontium nitrate and LPSN

Sample	Lattice Parameters ($\text{\AA}$)			Unit cell volume ($\text{\AA}^3$)	Crystal structure	Reference
	a	b	c			
L-proline	5.2794	8.8686	11.5321	539.94	Orthorhombic	[14]
Strontium nitrate	7.8220	7.8220	7.8220	478	Cubic	[13]
L-proline doped Strontium nitrate	7.786	7.786	7.786	472	Cubic	Current work

3.1. Fourier-transform infrared (FTIR) spectral evaluation

The FT-IR spectrum recorded for the synthesized LPSN crystal provides evidence of the characteristic vibrational modes arising from the L-proline and strontium nitrate components. The corresponding spectrum is shown in **Fig. 3**.

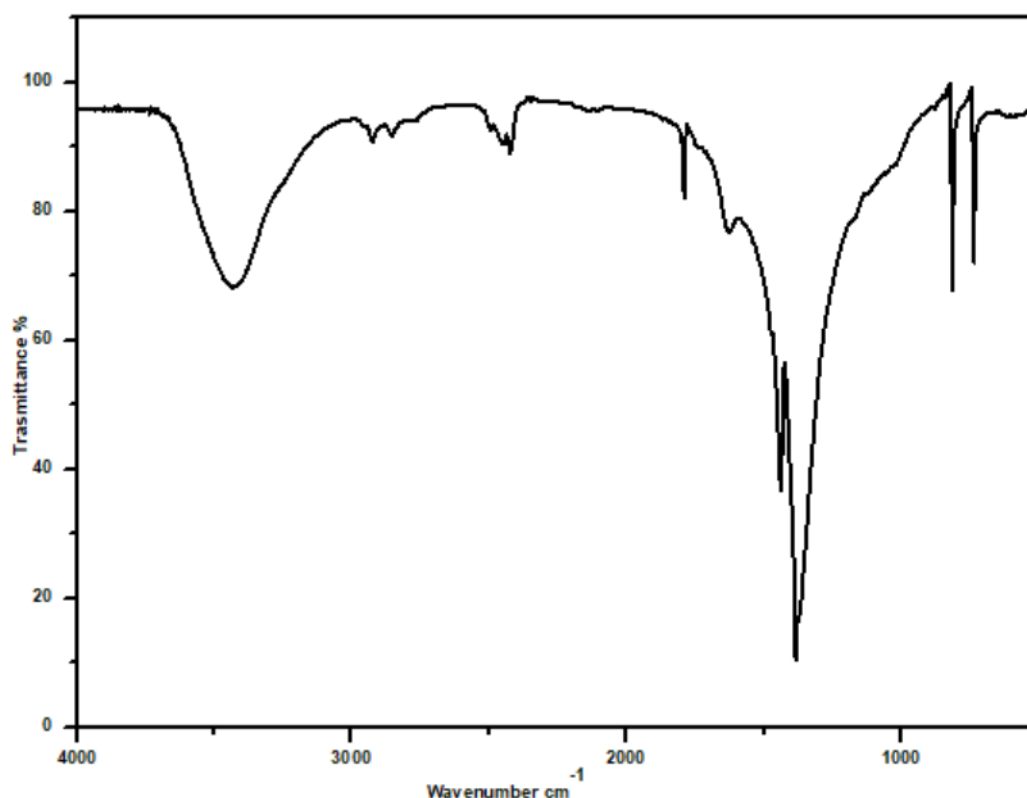


Fig3. FTIR spectrum of LPSN crystal.

The broad band in the 3200–3600 cm^{-1} region is attributed to the overlapping stretching vibrations of N–H/O–H induced by hydrogen bonding [15]. The bands at 2941 and 2855 cm^{-1} correspond respectively to CH_2 asymmetric and symmetric stretching vibrations [16]. In addition, the existence of zwitterionic L-proline inside the LPSN framework is confirmed by the distinctive vibrational bands at 1626 cm^{-1} (COO^- asymmetric stretching) and 1441 cm^{-1} (CH_2 scissoring) [17]. The intense peak that appears at 1384 cm^{-1} arises mainly from the ν_3 asymmetric stretching mode of the (NO_3^-) anions, while bands at 812 and 741 cm^{-1} are attributed to nitrate deformation vibrations [18]. The observed shifts in the characteristic L-proline bands indicate changes in the local molecular environment and intermolecular interactions following incorporation of the strontium nitrate component, supporting the formation of the LPSN crystal

3.2 Thermal properties

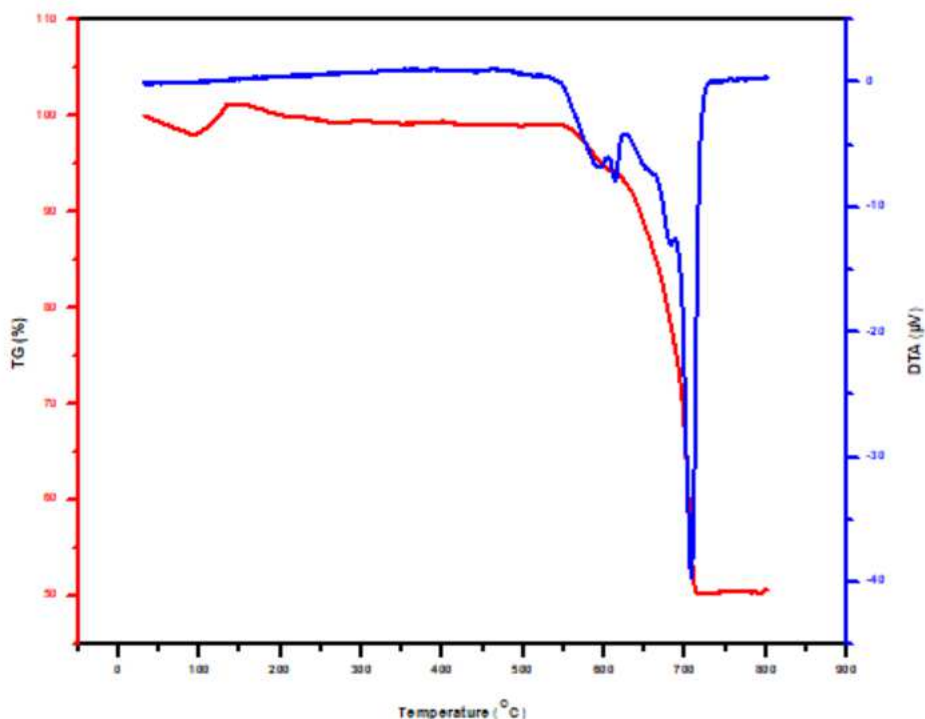


Fig4. TGDTA plot of LPSN crystal

Fig. 4 shows the TG-DTA profile for the LPSN crystal. The TG–DTA profile of the LPSN single crystal indicates good thermal stability up to approximately 550 °C, with only a minor mass variation at lower temperatures. A pronounced mass loss occurs between ~550 and 720 °C, accompanied by a strong DTA response, indicating the major decomposition of the crystal. This behaviour can be associated with the thermal degradation of the organic and nitrate-containing constituents. Above ~720 °C, the TG curve becomes nearly constant, leaving approximately 50% residual mass, suggesting the formation of a stable inorganic residue [19,9]. The temperature-dependent decomposition stages identified from the TG–DTA profile of LPSN are presented in **Table 2**.

Table 2: Decomposition stages of LPSN

Phase	Temperature range (°C)	Thermal behaviour
I	50-150	Minor mass loss; removal of weakly bound moisture, volatile species
II	150-550	Relatively stable region with negligible mass loss
III	550-720	Major decomposition of the crystal constituents
Residual region	Above 720	Nearly constant mass; formation of thermally stable residue

3.2.1 Coats–Redfern kinetic analysis

The thermal decomposition kinetics of LPSN were investigated using the integral Coats–Redfern method, with particular attention on the dominant weight loss stage observed from the TG-DTA profiles [20]. Above TG results indicate that the principal decomposition event takes place approximately within the temperature range of 550–720 °C. Among the investigated temperature intervals, the 630–680 °C region produced the most reliable linear relationship, with a correlation coefficient of $R^2 = 0.95928$. The extent of conversion at each temperature was determined from the following expression:

$$\alpha = \frac{W_0 - W_t}{W_0 - W_f}$$

where W_0 denotes the sample mass at the onset of the selected decomposition stage, W_t corresponds to the mass measured at a particular temperature, and W_f represents the residual mass at the completion of that decomposition stage.

For the assumed first-order degradation mechanism, the Coats–Redfern equation was employed in the following form:

$$\ln \left[\frac{-\ln(1-\alpha)}{T^2} \right] = \ln \left(\frac{AR}{\beta E_a} \right) - \frac{E_a}{RT}$$

In this kinetic equation, E_a represents the activation energy, T denotes the absolute temperature, A stands for the pre-exponential factor, β for the constant heating rate and R to the universal gas constant, which is $8.314 \text{ J mol}^{-1} \text{ K}^{-1}$. A plot of $\ln[-\ln(1-\alpha)/T^2]$ as a function of $1000/T$ as constructed to evaluate the kinetic parameters are illustrated in **Fig. 5** [21]. The slope of the obtained linear plot was employed to evaluate the kinetic activation energy $E_a = -mR$, where R represents the universal gas constant.

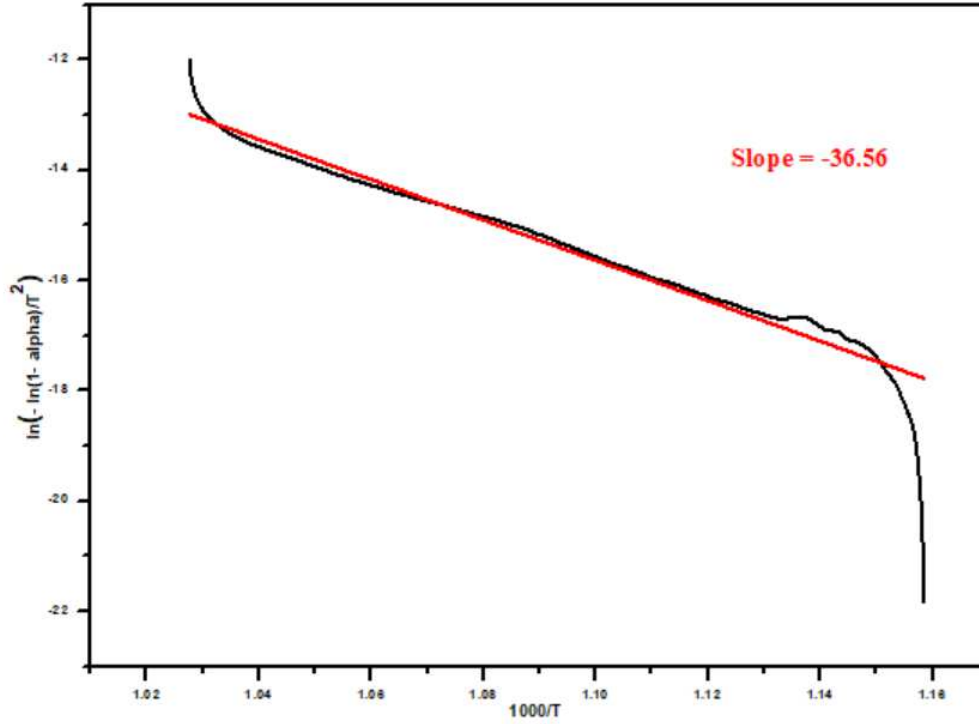


Fig 5. Activation energy plot for the LPSN crystal

For LPSN, the calculated activation energy was 304.01 kJ mol⁻¹. The intercept (*b*) obtained from the linear kinetic plot was subsequently used to estimate the pre-exponential factor using

$$A = \frac{\beta E_a}{R} \exp(b)$$

The thermodynamic characteristics of the decomposition process were further determined using the Eyring transition-state approach. The activation entropy was evaluated from

$$\Delta S = R \left(\ln \left[\frac{A h}{K_B T_p} \right] - 1 \right)$$

where *h* and *k_B* are Planck's constant and Boltzmann's constant, respectively. The activation enthalpy was calculated from

$$\Delta H = E_a - RT_p$$

obtaining the associated Gibbs free energy of activation using

$$\Delta G = \Delta H - T_p \Delta S$$

Progressive increase in the decomposition rate with increasing temperature, together with the associated reduction in the half-life, demonstrates that the degradation of LPSN is a thermally activated process.

The evaluated kinetic and thermodynamic parameters obtained from the analysis are presented in **Table 3**.

Table 3. LPSN kinetic and thermodynamic parameters

Stage	Temp. range (°C)	1000/T range	Slope	Ea	ΔS	ΔH	ΔG	R ₂
Major Decomposition	550–720	1.158–1.028	-36.56	304.01	22.09	295.89	274.30	0.95928

3.2.2 TG-DTA confirmation of Thermal Stability of L-proline based single crystals

The TG-DTA results presented in the **Table 4** confirm that LPSN offers a much wider working temperature range, i.e. s thermally stable up to ~550 °C, which is two to three times higher than other L-proline crystals. Such broad operational temperature window confirms the thermal stability of the grown LPSN crystal as a highly reliable for high-power laser and optoelectronic applications.

Table 4: Comparative thermal stability of L-proline-based single crystals

No.	Sample Name	Thermal Stability (°C)	Reference
1	L-Proline Strontium Nitrate (LPSN)	~550 °C	<i>Present study</i>
2	Dichlorobis (L-proline) zinc (II) (DBLPZ)	~242.3 °C	[21]
3	Bis L-proline hydrogen nitrate (BLPHN)	~235 °C	[22]
4	L-proline cadmium chloride monohydrate + ZnCl ₂	~208.9–211.9 °C	[23]
5	L-Proline doped Potassium Dihydrogen Phosphate (LP-KDP)	~190	[24]
6	L-proline strontium chloride monohydrate	~126 °C	[25]

3.3. UV-Visible spectral behaviour and optical constants

The light transmittance properties related to the grown LPSN single crystal were evaluated across wavelength spectrum of 250 nm to 800 nm. The crystal exhibited transmittance above 70% in the region that is visible with an absorption edge centered at about 305 nm. The higher transmission and clear absorption edge are relatable to low optical losses and higher optical quality, emphasizing its potential for photonic and optoelectronic applications [26]. Further, the estimation of the LPSN crystal's absorption coefficient (α) derived out of the measured transmittance, from the relation

$$\alpha = \frac{2.303 \log(1/T)}{t}$$

where T denotes the measured transmittance and t represents the crystal thickness. The corresponding variations in absorbance, transmittance and absorption coefficient as a function of wavelength and photon energy are illustrated in **Fig. 6-8** respectively.

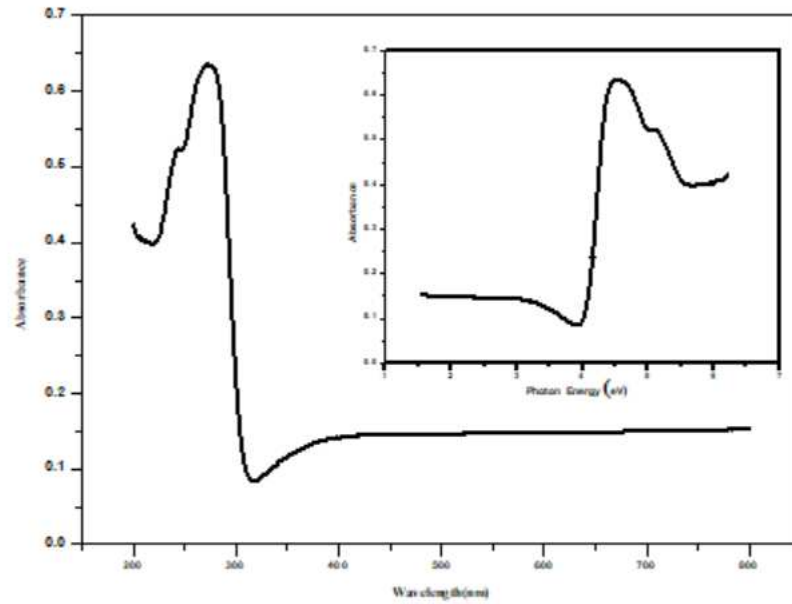


Fig6. Absorbance versus wavelength with photon energy shown in the inset.

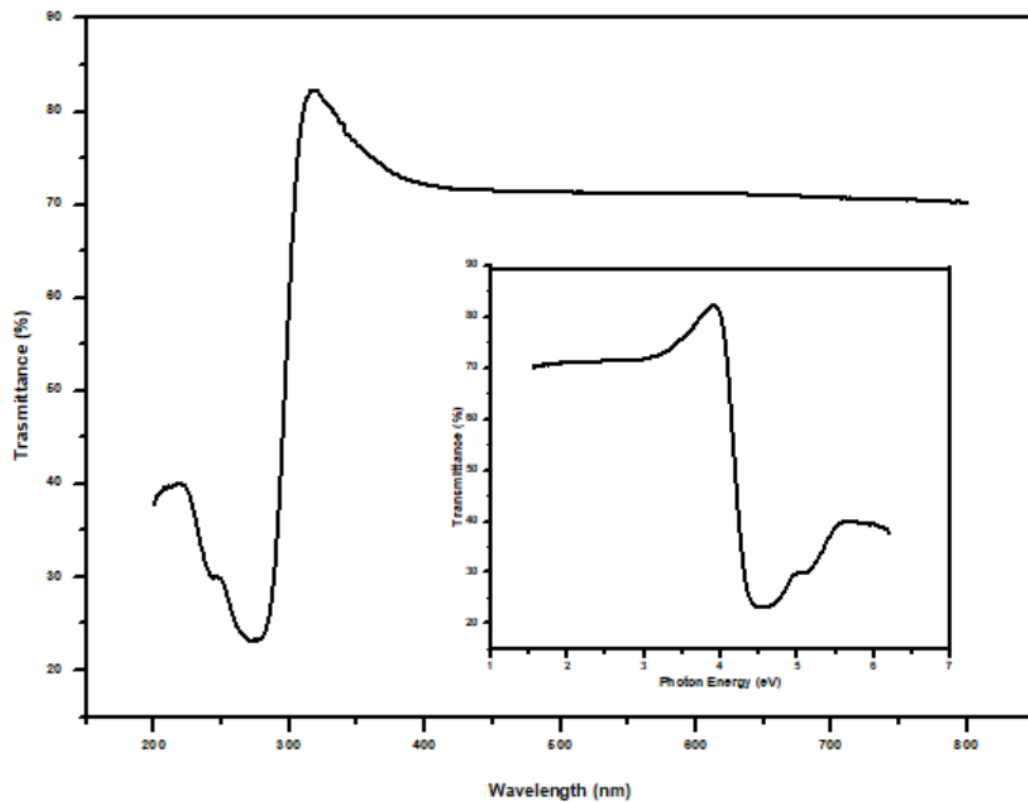


Fig7. Transmittance verses wavelength and with photon energy as inset

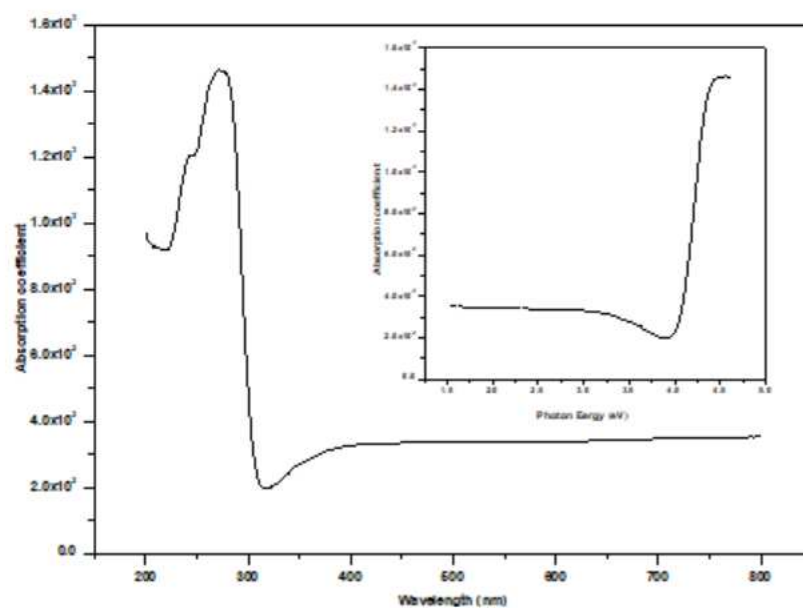


Fig 8. Absorption coefficient verses wavelength and with photon energy as inset

3.3.1. Determination of optical constants

The LPSN single crystal's extinction coefficient (K) had been determined using the absorption coefficient (α) as specified via [27]:

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

where (λ) is the incident radiation's wavelength. The extinction coefficient's dependence on wavelength along with corresponding photon energy is evident in **Fig. 9**.

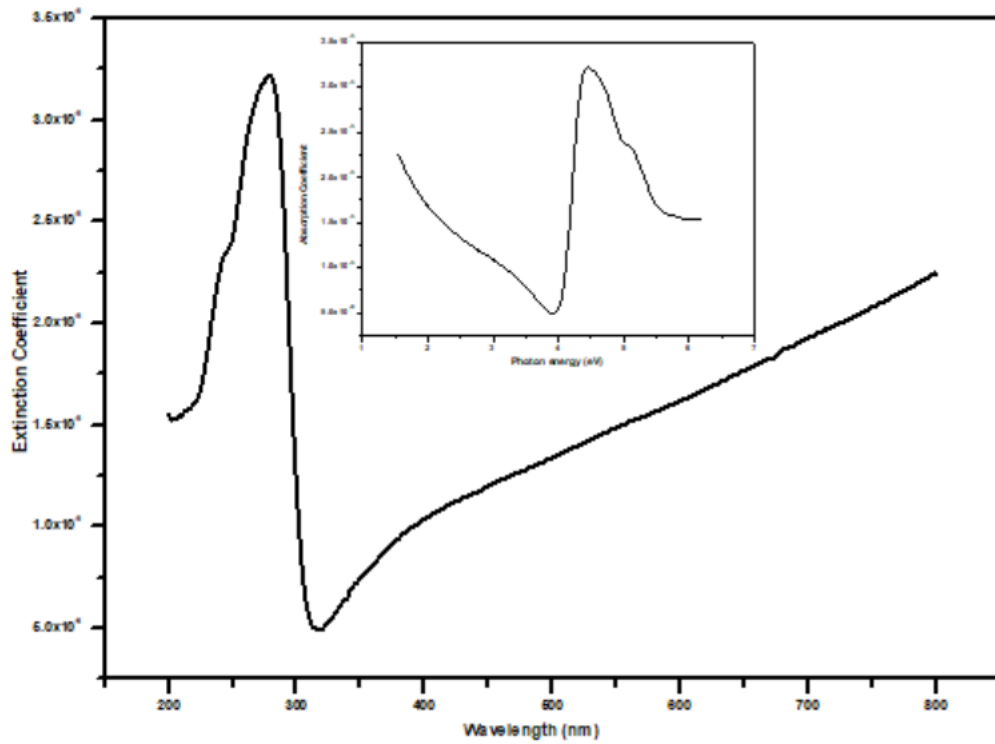


Fig9. Extinction coefficient verses wavelength and with photon energy as inset

The observed frequency spectrum variation of (K) reveals more insight pertaining to the optical response of the crystal and is consistent with its wavelength-dependant absorption properties. The reflectance (R) was calculated from the absorption coefficient (α) and crystal thickness (t) using [12]:

$$R = \frac{\sqrt{1 - \exp(-\alpha t) + \exp(\alpha t)}}{1 + \exp(\alpha t)}$$

The value of the refractive index (n) for the LPSN single crystal was derived from the reflectance (R) through standard optical relation [28]

$$n = \frac{1 + \sqrt{R}}{1 - \sqrt{R}}$$

The variation of n with wavelength and photon energy is presented in **Fig. 10**, providing insight into the wavelength-dependent optical response of the crystal.

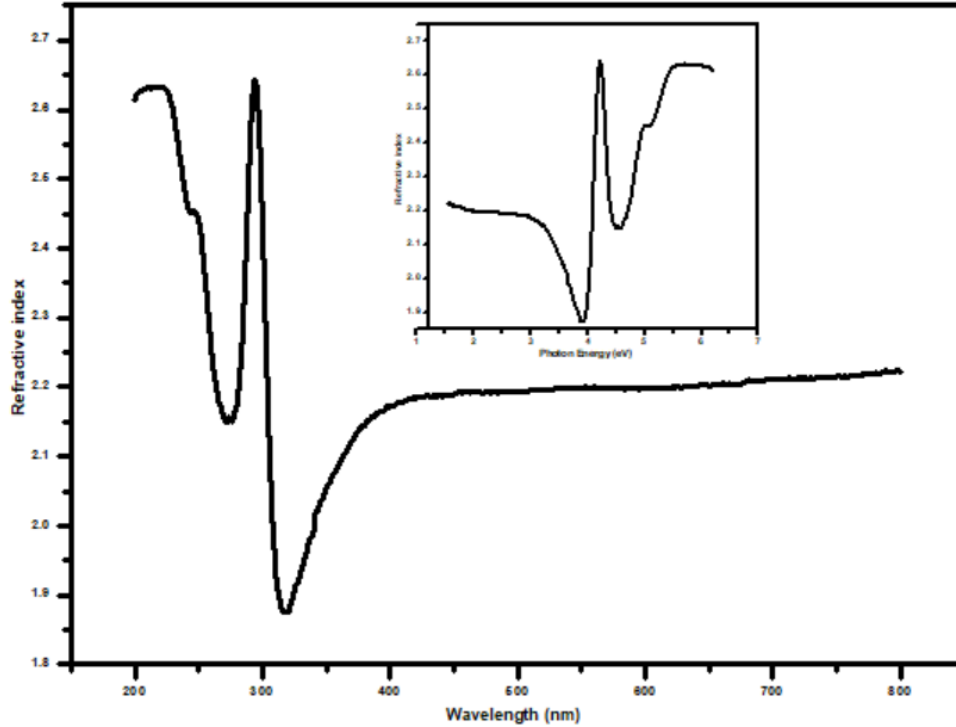


Fig10. The variation of the refractive index with wavelength and photon energy as inset

The optical conductivity (σ_{op}) was calculated from the absorption coefficient and refractive index using

$$\sigma_{op} = \frac{Knc}{\lambda} = \frac{\alpha nc}{4\pi}$$

The optical conductivity (σ_{op}) was computed from the refractive index and absorption coefficient

$\sigma_{op} = \frac{knc}{\lambda} = \frac{\alpha nc}{4\pi}$. In which (α) corresponds to the optical absorption coefficient, (n) symbolizes the refractive index and (c) for the speed of light in free space.

The variation of (σ_{op}) with wavelength photon energy is shown in **Fig. 11**. The increase in optical conductivity with photon energy indicates enhanced optical excitation and photo-response in the investigated spectral region.

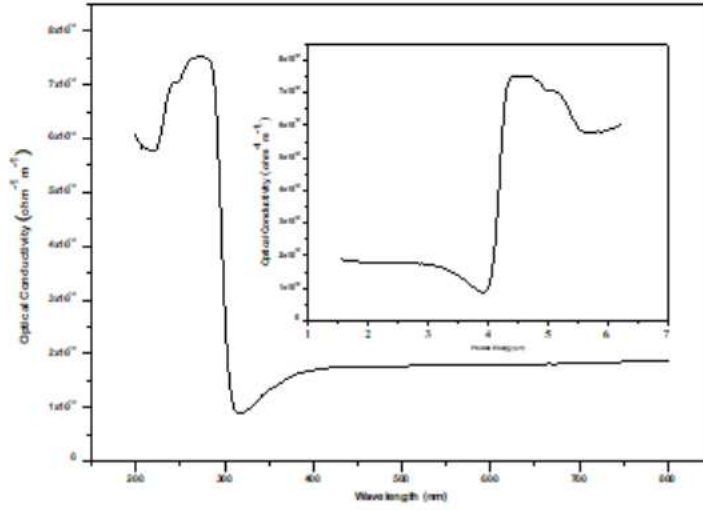


Fig 11. Optical Conductivity verses wavelength and with photon energy as inset

The electrical conductivity (σ_{el}) was evaluated using $\sigma_{el} = \frac{2Knc}{\alpha} = \frac{2\lambda\sigma_{op}}{\alpha}$ [29] where (K) is the extinction coefficient and (λ) is the wavelength of incident radiation. The variation of (σ_{el}) with wavelength and photon energy shown in **Fig. 12** provides information on the energy-dependent charge-transport characteristics of the LPSN crystal.

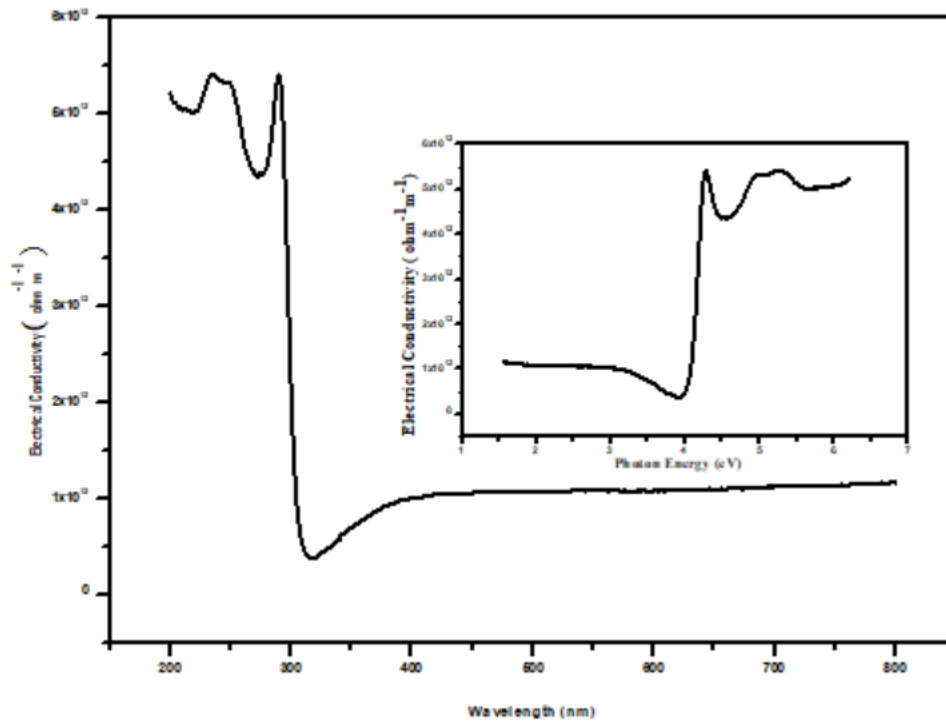


Fig 12. Electrical conductivity verses wavelength and with photon energy as inset

The electrical susceptibility and optical polarizability were subsequently estimated from the refractive index and extinction coefficient using the corresponding relations [12].

$$\chi_{el} = \frac{n^2 - k^2 - \epsilon_0}{4\pi} \quad \text{and} \quad P = \frac{h \epsilon_0 c \chi_{el}}{\lambda}$$

The variations of (χ_{el}) and (P) with wavelength and photon energy are shown in **Figs. 13 and 14**,

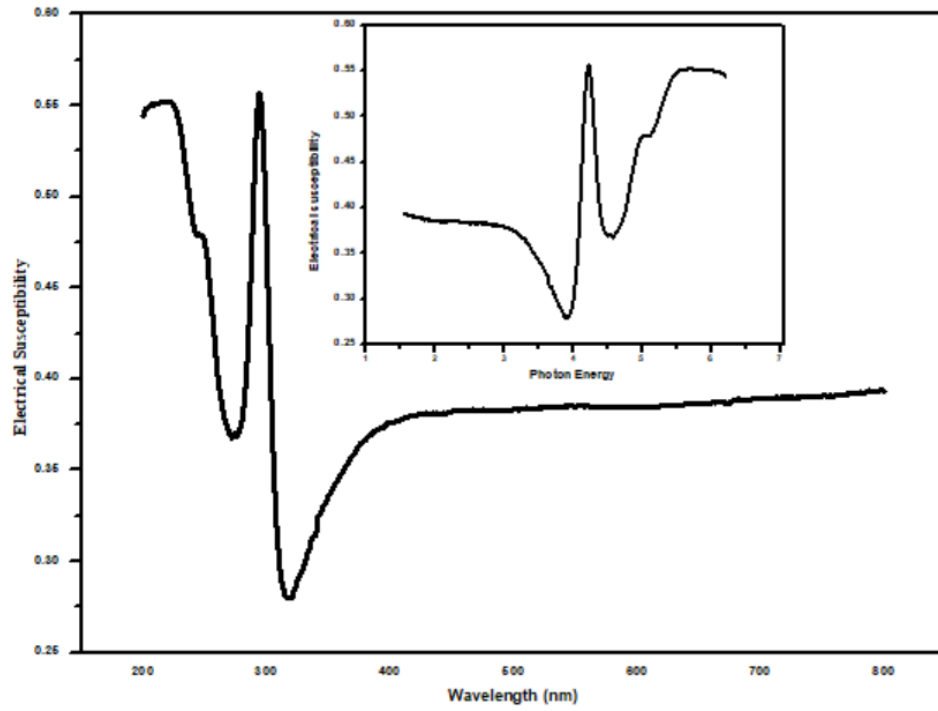


Fig13. Electrical Susceptibility verses wavelength and with photon energy as inset

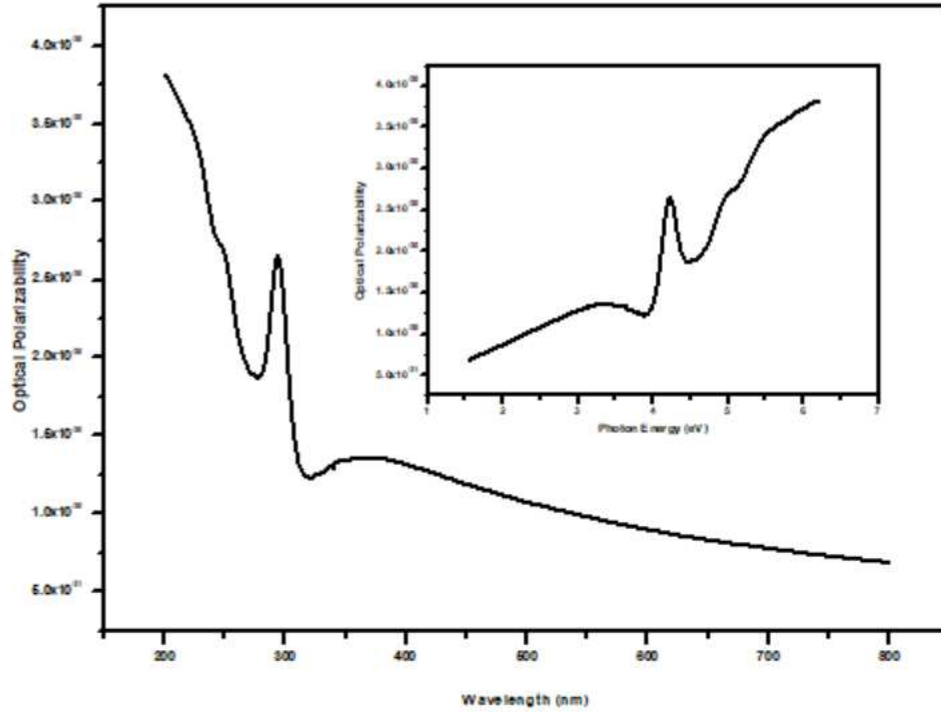


Fig14. Optical Polarizability verses wavelength and with photon energy as inset

respectively. The dielectric behaviour of the LPSN grown crystal was evaluated in terms of its real (ϵ') and imaginary (ϵ'') components. The corresponding optical parameters were determined from the refractive index (n) and extinction coefficient (K) according to the following equations:

$$\epsilon' = n^2 - k^2 \text{ and } \epsilon'' = 2nk$$

The dielectric response of the LPSN crystal can be described through its real and imaginary components, which are associated with energy storage and dielectric loss, respectively. The skin depth (δ) was determined from the absorption coefficient using $\delta = 1/\alpha$, where the absorption coefficient is represented by (α). Figure 15 illustrates the dependence of (δ) on photon energy and the variation of electromagnetic-wave penetration with incident photon energy. The acquired optical parameters are compiled in Table 5.

Table 5: Optical parameters of LPSN

S.No.	Parameter	LPSN
1	Optical cut-off wavelength	305 nm
2	Absorption coefficient, α at 800 nm	352 m ⁻¹

3	Extinction coefficient, k at 800 nm	2.24496×10^{-5}
4	Refractive index, n at 800 nm	2.2
5	Optical conductivity, σ_{op} at 800 nm	$1.8 \times 10^{10} \text{ ohm}^{-1}\text{m}^{-1}$
6	Electrical conductivity, σ_{el} at 800 nm	$1.16 \times 10^{12} \text{ ohm}^{-1}\text{m}^{-1}$
7	Electric susceptibility, χ at 800 nm	0.393363
8	Optical polarizability, P at 800 nm	6.89602×10^{-37}
9	Real dielectric constant, ϵ' at 800 nm	9.98×10^{-05}
10	Imaginary dielectric constant, ϵ'' at 800 nm	- 4.940643
11	Skin depth, d at 800 nm	0.0028 m

3.4. SEM image with EDAX

SEM analysis of the sample surface at 500X magnification revealed a heterogeneous, crystalline morphology characterized by defined cleavage planes and irregular grains as shown in **Fig. 15**. Step-like facets, lustrous fracture surfaces and wide range of particle sizes from minute micro fragments to giant agglomerated grains ($< 10 \mu\text{m}$ to $100 \mu\text{m}$) highlighted the sample's brittleness and crystalline integrity. Surface charge accumulation was correlated with localized light patches on sharp boundary edges under the applied functional voltage of 20 kV. These irregular micro-grain architectures and high-surface-area particulate morphologies with defined facets and sharp fracture sites are advantageous for optoelectronic and photonic applications because they perform the role as active host matrices for optical sensors, luminescent phosphor systems and precursors for compacted dielectric ceramics [30].

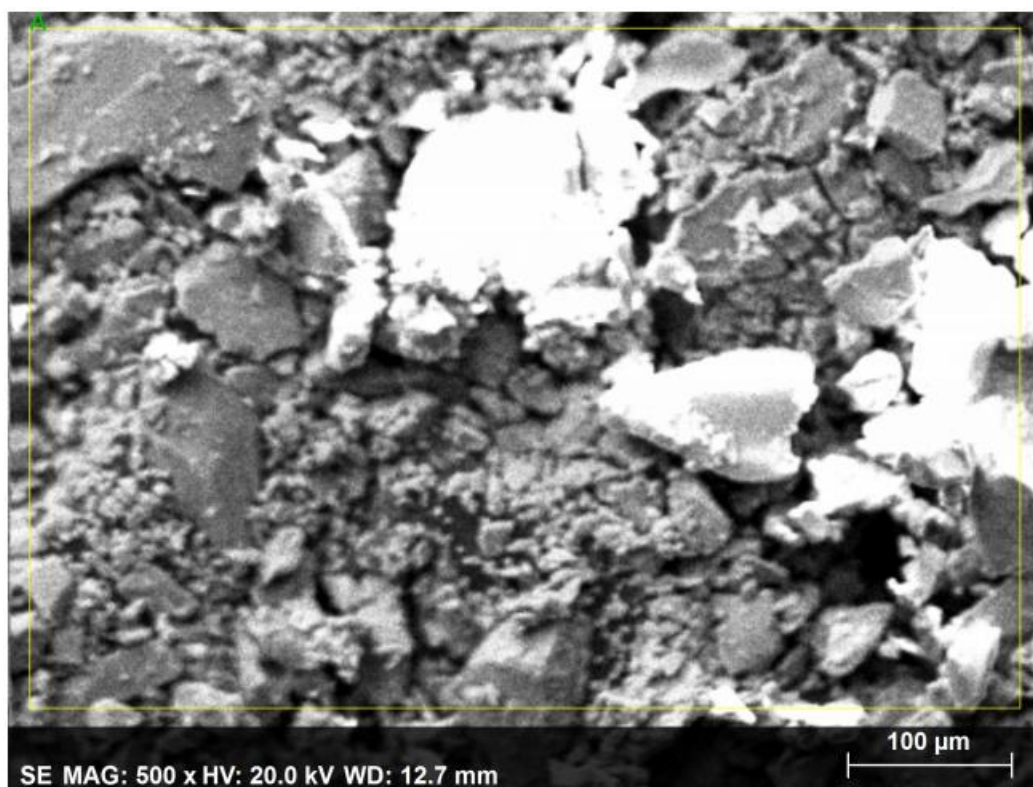


Fig15. SEM image of LPSN crystal.

EDX was adopted to check the grown material's elemental composition, chemical purity and relative atomic distribution. The EDX spectrum in **Fig. 16**, which highlights well-defined characteristic emission modes linked to carbon (C), nitrogen (N) and strontium (Sr) with no notable peaks from extraneous elements, supports the sample's notable chemical purity.

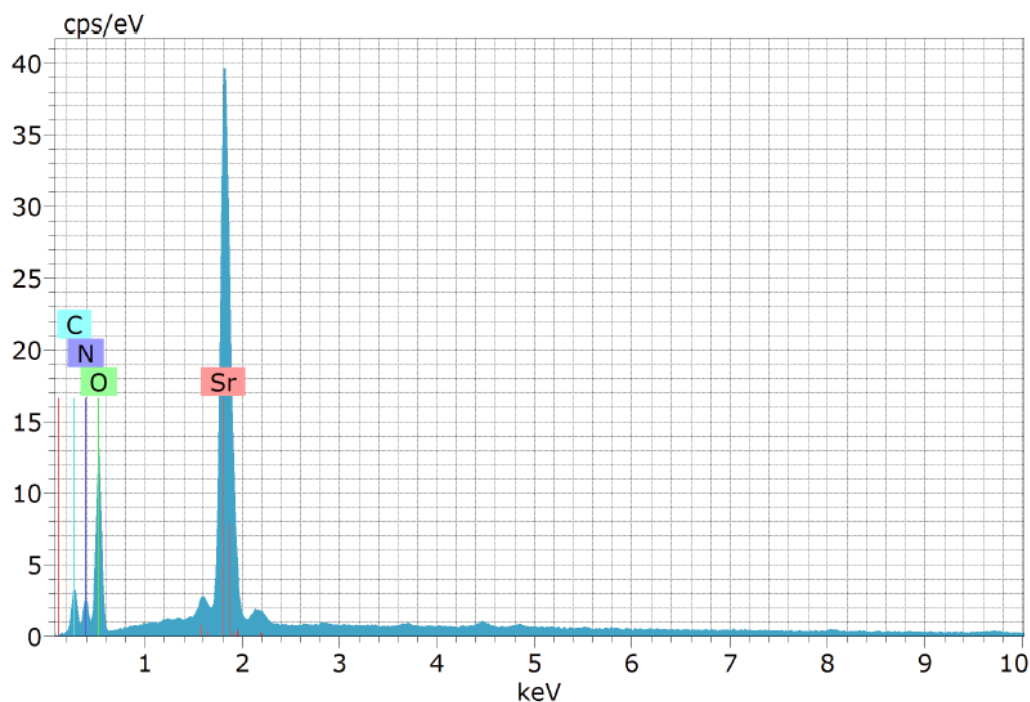


Fig16. EDAX spectrum of crystal.

Characteristic K- series emission peaks for C, N and O appear at ~0.28 keV, ~0.39 keV and ~0.52 keV respectively, accompanied by a prominent Sr L- series peak at ~1.80 keV. Quantitative elemental analysis provided normalized weight percentages of Sr, O, N and C as 33.15%, 36.80%, 14.72% and 15.16% respectively. Sample's atomic composition of 7.56 at.% Sr, 46.21 at.% O, 21.01 at.% N and 25.23 at.% C confirms the incorporation of all constituent element in the final structure. The quantitative material composition, weight and percentages corresponding to the synthesized sample, assessed by EDX analysis, are presented in **Table 6**.

Table 6: Quantitative elemental composition (weight and percentages) of LPSN

Element	Line Type	Wt%	Atomic %
Strontium	L-series	33.15	7.56
Oxygen	K-series	36.98	46.21
Nitrogen	K-series	14.72	21.01
Carbon	K-series	15.16	21.01
Total:	-	100	100

3.5. Impedance studies

Complex impedance spectrum analysis, which thoroughly analyzed a systems AC response to a sinusoidal stimulus and quantified its impedance and related parameters as a measure of frequency, was executed to examine the electrical parameters of the material. $Z^* = Z' - jZ''$ is the formula for the complex impedance Z^* , Where Z' denotes the real impedance component and Z'' stands for real impedance component, respectively [30]. Plotting the imaginary and real components of impedance against each other reveals an inverse connection, as seen in **Fig. 17**.

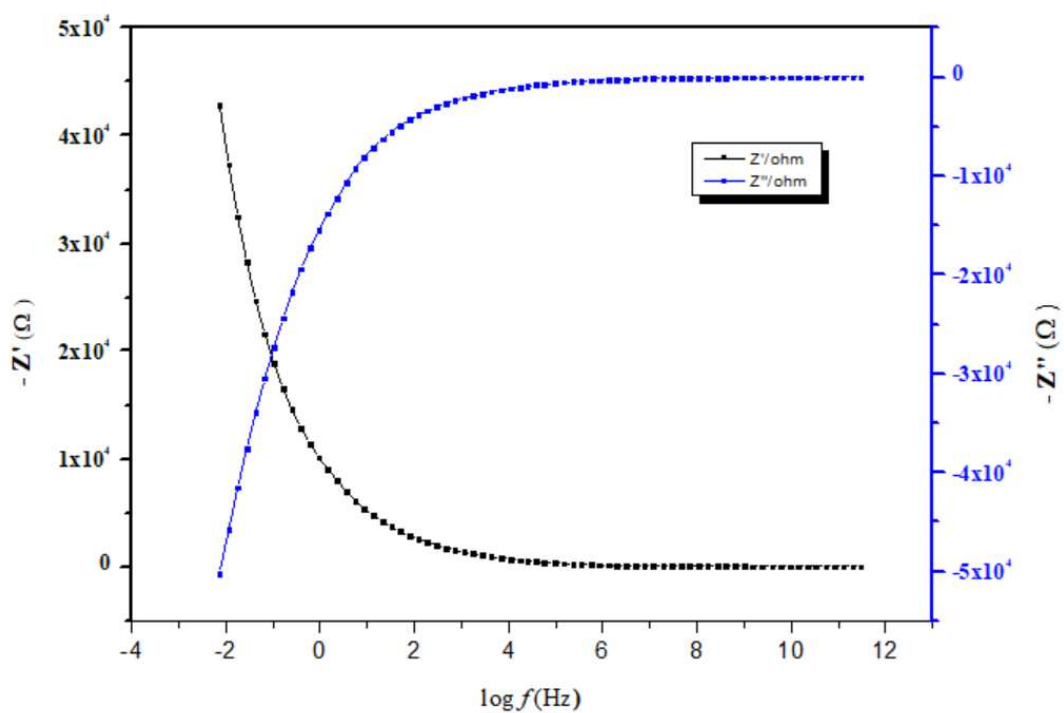


Fig17. Real (Z') and imaginary ($-Z''$) components of impedance with frequency

This behaviour provides a grain boundary resistance of $970 \, \Omega$ for the LPSN single crystal, providing basic insights into the dielectric response of the lattice.

The Cole-Cole (Nyquist) impedance profile for the LPSN crystal is shown in **Fig.18** along with a complex non-linear least-squares (CNLS) numerical fit that was obtained using a suitable equivalent electrical circuit model [31]. A bulk relaxation mechanism controlled by the combined resistive and capacitive characteristics of the crystalline matrix is indicated by the single, dominant semi-circular arc. Notably, the absence of a low-frequency linear Warburg diffusion tail confirms that ion-diffusion

processes do not influence the conduction dynamics across the measured frequency range. Importantly, the absence of a low-frequency linear tail – a characteristic of Warburg diffusion impedance – shows that ion-diffusion processes have no effect on the conduction dynamics throughout the studied frequency range. The lack of a characteristic Warburg-type diffusion response at low frequencies rules out any significant ion-diffusion contribution to the overall conduction mechanism within the investigated frequency regime [31,32].

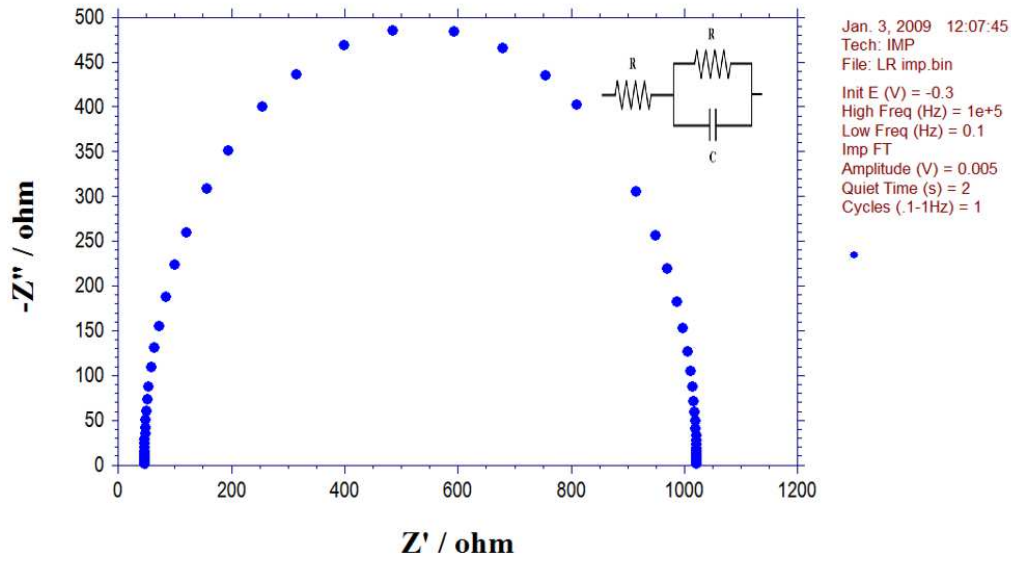


Fig 18. Nyquist plot of the LPSN single crystal along with the corresponding non-linear least-squares (CNLS) fit

3.5.1. High- and Low-Frequency Impedance Intercepts (R_s and R_{ct})

Within the framework of the Randles equivalent-circuit model [33], the complex impedance response of the crystal can be described in terms of its real component (Z') and imaginary component ($-Z''$) as functions of angular frequency, where ($\omega = 2\pi f$). The impedance response is expressed by the corresponding theoretical relations:

$$Z' = R_s + \frac{R_{ct}}{1 + (\omega R_{ct} C_{dl})^2}$$

$$-Z'' = \frac{\omega R_{ct}^2 C_{dl}}{1 + (\omega R_{ct} C_{dl})^2}$$

In the high-frequency regime ($\omega \rightarrow \infty$), the capacitive reactance approaches zero ($1/\omega C_{dl} \rightarrow 0$) short-circuiting the capacitive branch. The uncompensated electrolyte solution resistance $R \approx 50 \, \Omega$ is thus

obtained from the real impedance intercept along the horizontal axis. In line with high-frequency Bode magnitude plateaus ($\log |Z|$), this shows low ohmic potential dips across the bulk electrolyte ($G = 1/R = 20\text{ms}$) [33].

On the other hand, the electrical double-layer capacitor functions as an open circuit at the low-frequency limit ($\omega \rightarrow 0$). The ohmic solution and interfacial charge-transfer resistances add up to the total real impedance ($R_{\text{total}} = R_s + R_{\text{ct}} = 1020 \Omega$). The extracted charge-transfer resistance is as follows after deducting the ohmic electrolyte contribution: $R_{\text{ct}} = R_{\text{total}} - R_s = 1020 \Omega - 50 \Omega = 970 \Omega$. The activation energy barrier for electron transport across the modified crystal-electrolyte border is measured by the magnitude of (R) [34]. For an electrode radius of 5 mm, the cross-sectional area was determined to be $78.5 \times 10^{-6} \text{ m}^2$ via $A = \pi r^2$. The electrical conductivity of the developed crystal was calculated using $\sigma = t/(RC)$ based on its thickness of $1 \times 10^{-3} \text{ m}$ and resistance as determined by impedance analysis of 1020Ω . The electrical conductivity of the prepared sample was determined to be $1.25 \times 10^{-2} (\Omega \cdot \text{m})^{-1}$. This relatively low conductivity reflects features of the LPSN crystal and further indicates a limited charge-carrier transport under the laboratory conditions. A weak conducting or semiconducting type of material is recognised by the crystal's electrical response and notable resistance. In crystal-based dielectric and optoelectronic components, where electrical stability and current leakage suppression are crucial, this specific type of resistive response seems to be beneficial [35].

3.5.2. Relaxational Kinetics and Double-Layer Capacitance (C_{dl})

The optimum rate of charge transportation across the double layer can be estimated by the interfacial relaxation time constant ($\tau = R_{\text{ct}}C_{\text{dl}}$) [36]. At the apex of the semi-circular arc, the imaginary impedance achieves its maximum value: $-Z''_{\text{max}} = \frac{R_{\text{ct}}}{2} = 485 \Omega$. The characteristic relaxation frequency at this maximum was determined experimentally at $f_c = 215 \text{ Hz}$, corresponding to a characteristic angular frequency of $\omega_c = 2\pi f_c = 1350.88 \text{ rad s}^{-1}$. Applying the resonance criterion ($\omega_c C_{\text{dl}} R_{\text{ct}} = 1$) determination of the interfacial double-layer capacitance (C_{dl}) [37]:

$$C_{\text{dl}} = \frac{1}{2\pi f_c R_{\text{ct}}} = 0.763 \mu\text{F} .$$

3.5.3. Mass-Transport Mass Kinetics (Warburg Diffusion).

At frequencies below $f_c = 215 \text{ Hz}$, the impedance response transitions from charge-transfer control to semi-infinite linear diffusion control [29]. This behaviour is represented by the complex Warburg impedance (Z_w) [38]:

$$Z_w = \sigma \omega^{-1/2} (1-j)$$

where σ denotes the Warburg diffusion coefficient. The characteristic 45° slope relative to the real axis demonstrates that mass transport of electroactive species becomes the rate-determining step at lower perturbation frequencies. **Table 7** presents the principal impedance parameters obtained from the EIS measurements of the LPSN crystal.

Table 7: The electrochemical impedance parameters of LPSN

Parameter	Description Symbol	Value
Electrical conductivity	σ	$0.25 \times 10^{-2} (\Omega \cdot m)^{-1}$
Total Interfacial Resistance	R_{total}	1020 Ω
Charge Transfer Resistance	R_{ct}	970 Ω
Apex Characteristic Frequency	f_c	215 Hz
Characteristic Angular Frequency	ω_c	1350.88 rad s ⁻¹
Double-Layer Capacitance	C_{dl}	0.763 μF .

3.6 Theoretical Studies

The theoretical parameters were measured with Gaussian 09W software package [39]. The geometry of L-proline doped strontium nitrate (LSPN) and zwitterion L-proline-strontium nitrate (ZLSPN) were built using Spartan 08 and also optimized by means of density functional theory B3LYP/LANL2DZ method. Theoretical parameters, frontier molecular orbitals and electrostatic potential map were calculated for LSPN in the gas phase. The reactivity indicators of the DFT were evaluated from the frontier molecular orbital E_{HOMO} and E_{LUMO} energies by the use of standard mathematical formulations, according to Koopmans' Theorem, which is given in expressions 1 to 15 below [40, 41].

Vertical ionization potential ($I = -E_{HOMO}$) and electron and electron affinity ($A = -E_{LUMO}$) were calculated with the use respectively of Equations (1) and (2).

$$\text{ionization potential } (I = -E_{HOMO}) \quad (1)$$

$$\text{electron affinity } (A = -E_{LUMO}) \quad (2)$$

Relying on these energetic parameters, the absolute electronegativity (χ) and chemical potential (μ) were studied respectively applying Equations (3) and (4).

$$\text{Electronegativity} \quad \chi = I + A/2 \quad (3)$$

$$\text{Chemical Potential } \mu = -\chi \quad (4)$$

Resistance of the electronic cloud towards deformation was valued through the chemical hardness and, reciprocally, its relationship defined the global chemical softness, applying respectively Equations (5) and (6).

$$\text{Chemical Hardness } \eta = I - A/2 \quad (5)$$

$$\text{Chemical Softness } S = 1/\eta \quad (6)$$

In order to estimate the net stabilization energy upon charge transfer, the electrophilicity index was deduced by use of Equation (7).

$$\text{Electrophilicity Index } \omega = \mu^2/2\eta \quad (7)$$

The charge-acceptance capacity (ω^+) and charge-donation index (ω^-) were calculated respectively as per Equations (8) and (9).

$$\text{Electron accepting capability } \omega^+ = \frac{(I+3A)^2}{16(I-A)} \quad (8)$$

$$\text{Electron donating capability } \omega^- = \frac{(3I+A)^2}{16(I-A)} \quad (9)$$

Here, I represents the vertical ionization energy, whereas A denotes the electron affinity.

$$\text{Differential electrophilicity is given as } \Delta\omega^2 = (\omega^+ - \omega^-) \quad (10)$$

$$\text{Chemical Potential } \mu = -\chi$$

Global molecular softness (S) and back-donation stabilization energy (ΔE_{back}) were calculated respectively using Equations (11) and (12)

$$\text{Global Softness } S = 1/2\eta \quad (11)$$

$$\Delta E_{\text{back donation}} = -\eta/4 \quad (12)$$

$$\text{Electron donating capability} = \omega^- = \frac{(3I+A)^2}{16(I-A)}$$

The nucleophilic reactivity index (N) and the maximum charge-transfer capacity (ΔN_{msx}) were also determined using Equations (13) and (14).

$$\text{Nucleophilicity index } N = 1/\omega \quad (13)$$

$$\text{Additional electronic charge } \Delta N_{\text{msx}} = -\mu/\eta \quad (14)$$

Finally, the optoelectronic softness threshold (σ_0) is defined by Equation (15).

$$\text{Optoelectronic softness } \sigma_0 = -1/\Delta E \quad (15)$$

3.6.1. Optimized Geometry

The optimized geometry of the title compound is made up of one organic substance L-proline (amino acid) and one inorganic $\text{Sr}(\text{NO}_3)_2$. The optimized geometry is shown in **Fig. 19**. In L-proline, the carboxyl group ($-\text{COOH}$) and amino group ($-\text{NH}_3$) exist as zwitter ionic in nature. Various structural parameters such as energy ($E=-622128.27$ KJ/mol), E_{HOMO} (-6.65 eV), E_{LUMO} (-5.77 eV), energy gap (-0.87 eV), ionization potential (6.65), electron affinity (5.77), electronegativity (6.21), chemical potential (-6.21), chemical hardness (0.43), chemical softness (2.28), dipole (8.58), electrophilicity index ($\omega=44.04$), electron accepting capability ($\omega^+=41.05$), electron donating capability ($\omega^-=47.27$), net electrophilicity ($\Delta\omega_{\pm}=38.65$), global softness ($s=1.14$), $\Delta E_{\text{Back donation}}$ (-0.10), nucleophilicity index ($N=0.022$), additional electronic charge ($\Delta N_{\text{max}}=14.19$), optical softness ($\sigma_0=-9.13$) were measured for the LPSN using theoretical method.

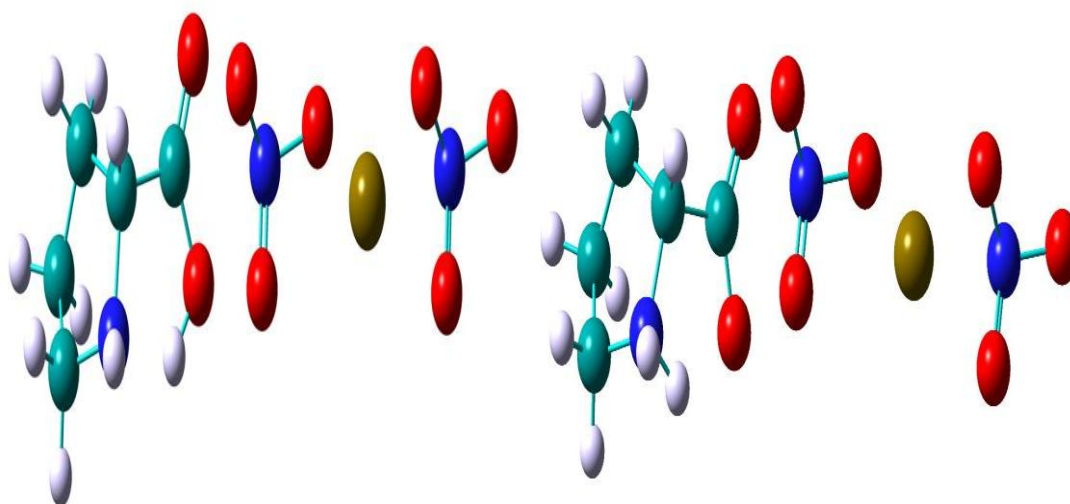


Fig.19 The optimized structure of LPSN and zwitterion LPSN

3.7.2. Frontier Molecular Orbitals

The HOMO and LUMO energy diagram for LPSN and ZLPSN are shown in **Figures 21 and 22**.

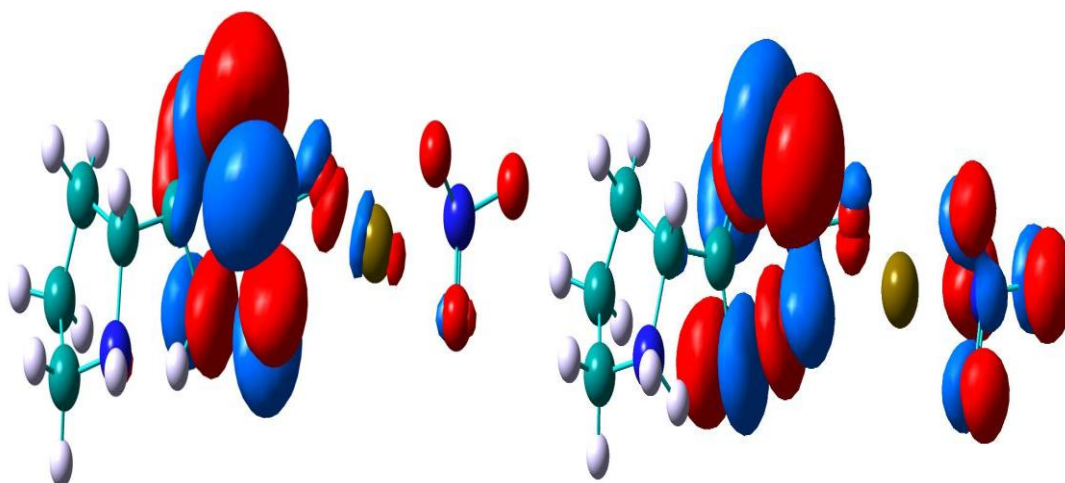


Fig 20. The HOMO energy structure of LPSN and zwitterion LPSN

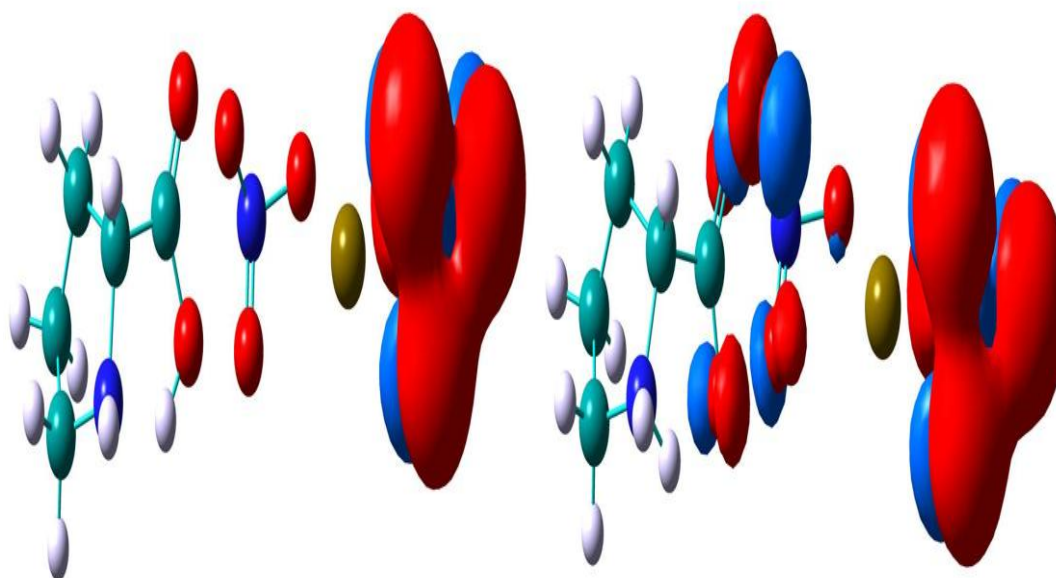


Fig21. The LUMO energy structure of LPSN and ZLPSN nitrate.

The calculated HOMO and LUMO energies were determined to be -6.65 and -5.77 eV, respectively, with an energy separation of 0.87 eV. This narrow energy gap reveals the high chemical reactivity and chemical softness of the material which directly accounts for its enhanced molecular polarizability [31]. Calculated quantum chemical parameters and electronic properties of LPSN and its zwitterionic form was presented in the **Table 7**, which directly accounts for its enhanced molecular polarizability.

Table 7. Quantum chemical parameters and electronic properties of LPSN and its Zwitterion **LPSN** form (DFT B3LYP/ LANL2DZ).

S.No.	Parameter	LPSN	Zwitterion LPSN
1	E _{HOMO}	-6.65	-4.80
2	E _{LUMO}	-5.77	-4.32
3	Energy gap (ΔE)	-0.87	-0.48
4	Ionisation potential (I)	6.65	4.80
5	Electron affinity (A)	5.77	4.32
6	Electronegativity (χ)	6.21	4.56
7	Chemical potential (μ)	-6.21	-4.56
8	Chemical hardness (η)	0.43	0.24
9	Chemical softness (S)	2.28	4.16
10	Dipole	8.58	19.57
11	Energy (KJ/mol)	- 622128.27	- 622049.86
12	Electrophilicity index (ω)	44.04	43.31
13	Electron accepting capability (ω^+)	41.05	41.06
14	Electron donating capability (ω^-)	47.27	45.62
15	Net electrophilicity ($\Delta\omega_{\pm}$)	38.65	20.81
16	Global softness (s)	1.14	2.08
17	ΔE Back donation	-0.10	-0.05
18	Nucleophilicity index (N)	0.022	0.023
19	Additional electronic charge (ΔN_{max})	14.19	18.98
20	Optical softness (σ_0)	-9.13	-19.02

Fig21. The LUMO energy structure of LPSN and ZLPSN nitrate.

3.6.3. Molecular Electrostatic Potential Map Mapping

Fig. 22 portrays the MEP surface computed at the DFT/B3LYP/LANL2DZ level. The electron-density distribution is highlighted by multiple colours, with red and yellow domains symbolizing electron-rich spots nearby the nitrate and carboxyl group of oxygen atoms. The blue electron electron-deficient zones can reinforce electrophilic interactions, even though they are primarily found adjacent to the strontium core and -NH group.

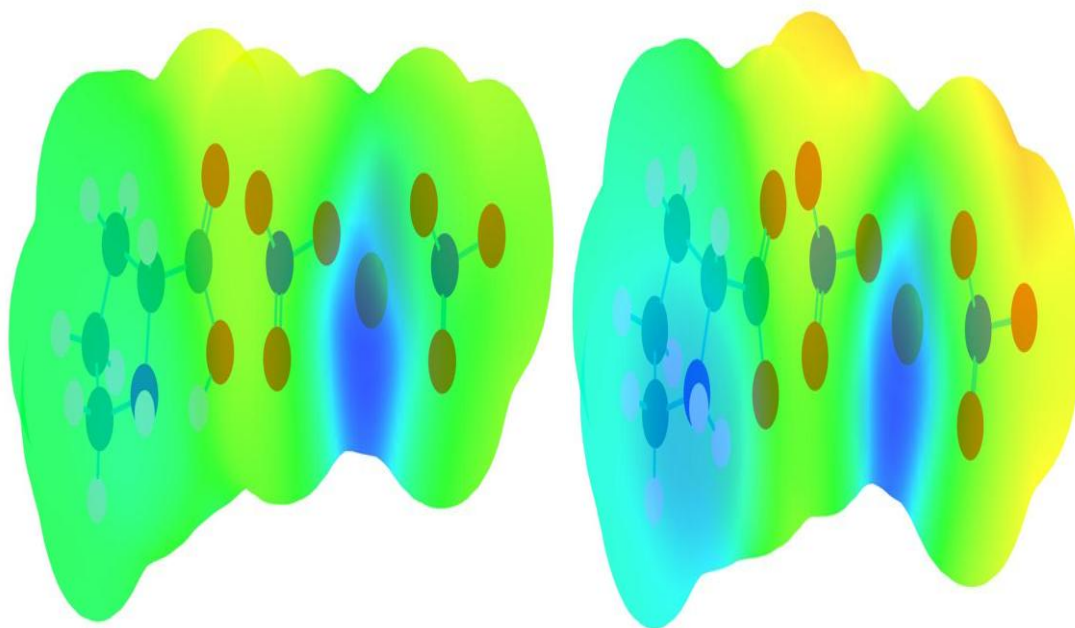


Fig22. The electrostatic potential map of LPSN and ZLPSN

Conclusion

Single crystals of L-proline-doped strontium nitrate (LPSN) were grown using the slow-evaporation solution technique. SCXRD confirmed that the crystal retains the cubic centrosymmetric lattice. Successful incorporation of L-proline into the host matrix was verified by PXRD. The observed shifts in the characteristic COO^- and NO_3^- absorption bands in the FTIR spectrum indicate changes in their chemical environments, supporting the coordination of L-proline and nitrate groups with Sr^{2+} in the LPSN crystal structure. TG-DTA analysis indicated thermal stability up to $\sim 550^\circ\text{C}$, with a Coats-Redfern kinetic activation energy (E_a) of $304.01\text{ kJ mol}^{-1}$. Optical characterization revealed an absorption edge near 305 nm with transparency above 70% in the visible region. Optical constant dispersion profiling further indicated low optical loss, while dielectric and photo-response measurements demonstrated good electrical stability. EDX elemental distribution maps confirmed a homogeneous, phase-pure material composed of Sr, O, N and C. Coupled with these compositional findings, the observed cleavage facets and large grain size variation showed the mechanical fracture behaviour and structural coherence of the synthesized LPSN crystals under applied strain. Impedance spectroscopy confirmed a single bulk relaxation mechanism in LPSN, where high charge-transfer resistance ($970\ \Omega$) and low conductivity ($1.25 \times 10^{-2}\ \Omega\cdot\text{m})^{-1}$) effectively suppress leakage currents for stable optoelectronic applications. Theoretical calculations using DFT/B3LYP/LANL2DZ demonstrated high polarizability

and electronic reactivity in LPSN, as evidenced by a small 0.87 eV orbital gap, substantial electrophilicity ($\omega = 44.04$ eV), and clear spatial potential gradients identified through MEP mapping. These combined experimental and theoretical results confirm the strong structure-property relationship of the LPSN single crystal, demonstrating its potential for deployment in next-generation optical, photonic and optoelectronic systems.

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Statement &Declarations

The authors declare that they did not receive any funding, grants, or other forms of assistance while working on this manuscript.

Competing Interests

The authors have no relevant financial or non-financial interests to report.

Author Contributions

A All authors developed the study, did the experiments, examined the data, and composed the report.

The final text was reviewed and approved by all authors. [L.R.L], [P.S], [A.A] and [J.U].