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Z-scan, antibacterial activity and photocatalytic studies of sodium bromide-doped L-alanine single crystals

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The slow evaporation method was used to produce sodium bromide-doped L-alanine (SBLA) single crystals at room temperature. Advanced techniques including single crystal XRD, FTIR, Energy-dispersive X-ray spectroscopy (EDS or EDX), SEM, Impedance analysis, Photocatalytic activity test, Z-scan and antibacterial activity studies were used to investigate the grown SBLA crystal. Through single crystal XRD analysis, the SBLA single crystal exhibits the orthorhombic structure. To identify the functional groups, FTIR examines the unique fingerprint of SBLA single crystal. To determine the percentage amount of the elements in the SBLA sample, an EDS analysis was conducted. To determine the surface morphology in the SBLA sample, a SEM analysis was conducted. The bulk resistance, grain boundary, AC and DC conductivity values were determined for SBLA sample through an impedance analysis. The photocatalytic activity SBLA sample was tested to check the dye removal in congo red and methylene blue dyes. By examining Z-scan, the nonlinear refractive index (n_2) (or Kerr index), nonlinear optical absorption coefficient (β), and absolute third order susceptibility values of the SBLA crystal were ascertained. The antibacterial activity was also carried out for sodium bromide-doped L-alanine (SBLA) crystal and the results are analyzed.

Keywords: Single crystal; FTIR; EDS; SEM; photocatalytic activity; Z-scan study; antibacterial activity.

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Introduction

Nonlinear optical (NLO) crystals are the intriguing materials since they are widely used in so many different sectors, including photonics, optoelectronics, fiber optic computers, and many more [1]. One of the most notable characteristics of amino acids is their molecular chirality, which also helps to maintain their non-centrosymmetric crystallographic structure. Moreover, the zwitter ionic nature of amino acids promotes crystal hardness, which is advantageous for their use in devices, as strong conjugated bonding is absent and allows for wide transparency ranges in the visible and ultra-violet spectral regions [2, 3]. The study on doped potassium dihydrogen orthophosphate single crystals was completed by Fernando Loretta *et al.*,

(2014). The existence of the elements corresponding to the integrated semiorganic dopants in the KDP crystal is confirmed by energy dispersive spectrum analysis, which also discloses the chemical makeup of the pure and semiorganic impurity doped KDP crystals [4]. Retnakumar *et al.*, (2015) have grown pure and strontium chloride-doped L-alanine cadmium chloride by slow evaporation technique. An EDS analysis verified the presence of strontium ions in the crystal lattice of the LACC crystals [5]. Merline Priya *et al.*, (2018) have grown crystals of antimony potassium tartrate l-alanine using the long evaporation solution growth technique. To determine the elemental makeup of the title substance, an energy dispersive spectrum analysis was conducted [6]. Shi Ping Gai *et al.*, (2024) have grown a new N, N'-bis (L-alanine)

naphthalene diamide by solvothermal conditions and it has strong photo-catalytic degradation activity against a range of dyes, particularly the cationic dyes Janus green B, methyl violet (MV), and crystal violet (CV) [7]. L-alanine has high antibacterial effect against gram-negative bacteria of *E. Coli*. The L-alanine single crystal under investigation is hence very suitable for wastewater treatment. Amino acid of L-alanine material suitable for biomedical applications by antibacterial activity studies [8]. Solvent evaporation was used to generate optically excellent translucent L-alanine crystals doped with cadmium chloride from aqueous solution. The crystal's good crystalline quality and orthorhombic crystal system are confirmed by X-ray diffraction examination. Z-scan analyses reveal that the material's nonlinear optical refractive index and nonlinear absorption coefficient are both high [9]. Based on the literature survey, it is decided to grow sodium bromide-doped L-alanine (SBLA) single crystals by solution method and then to characterize the sample by a variety of methods, including FTIR and EDS analysis, SEM, Impedance analysis, photo-catalytic activity, Z-scan measurement and antibacterial activity studies.

I. Growth of SBLA crystal

In double-distilled water, 99% pure sodium bromide and L-alanine were dissolved at a stoichiometric ratio of 1:0.02 molar ratio. After making the saturated solution, After being continuously stirred, it was let to stand at room temperature for five hours. In a jar, the mixture was filtered via Whatman filter papers before being stored in an undisturbed environment. After 55 days, the slow evaporation approach was used to recover the optically excellent crystals of SBLA (sodium bromide-doped L-alanine) from the supersaturated solution. In the growing vessel, a few crystals of the highest caliber were submerged in the supersaturated solution and the size of the sample is $1.5 \times 1 \times 0.5 \text{ cm}^3$. The sample is found to be colourless and transparent as shown in figure 1.

Sodium bromide-doped L-alanine crystal

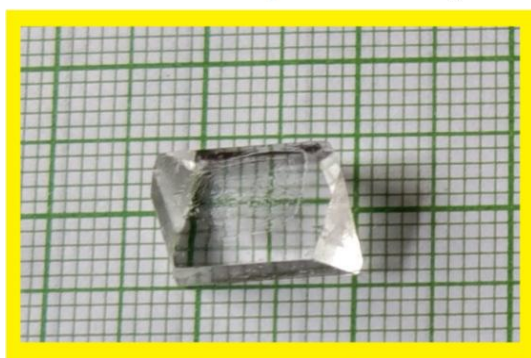


Fig. 1. Photograph of sodium bromide-doped L-alanine (SBLA) single crystal.

II. Result and discussions

2.1. XRD study

When evaluating single crystal X-ray diffraction (XRD), a Bruker Kappa Apex II single crystal X-ray

diffractometer was used $\text{MoK}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) to find crystal structure. The findings demonstrated that the SBLA crystal crystallizes in an orthorhombic shape with values for unit cell dimensions values of $a = 5.778(2) \text{ \AA}$, $b = 6.026(3) \text{ \AA}$ and $c = 12.326(6) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, and $\gamma = 90^\circ$ and volume of the unit cell is $429.2(2) \text{ \AA}^3$ [10].

2.2. Fourier transform infrared (FTIR) spectroscopy

A Scientific Nicolet iS5 FT-IR spectrometer was used to record the FTIR spectra of a generated sodium bromide-doped L-alanine (SBLA) single crystal at room temperature in the frequency range of $500\text{--}4000 \text{ cm}^{-1}$. Figure 2 shows the FTIR spectrum of the sample and table 1 shows its mode of vibrations. The functional groups like NH_3^+ , COO^- , CH, C=O, OH etc have been identified and slight shifting of absorption peaks are noticed due to doping in the sample. As an ionic salt, NaBr usually shows no discernible absorption peaks in the normal mid-infrared (mid-IR) range, which is between 4000 and 400 cm^{-1} . The vibrations of covalent bonds within a molecule are measured by standard mid-IR spectroscopy. Sodium bromide (NaBr) is an ionic compound that exists as a crystal lattice of Na^+ raised to the positive power and Br^- raised to the negative power. The sodium bromide (NaBr) monomer's basic vibration takes place in the far-infrared, more precisely in the $225\text{--}315 \text{ cm}^{-1}$ range. This falls below the usual range of the mid-IR spectrum. Impurities, such as absorbed ambient water (a large O-H band about 3400 cm^{-1} and a lesser band around 1640 cm^{-1}), would most likely be the cause of any peaks seen in a sodium bromide (NaBr) spectrum. Apart from absorbed atmospheric water, nitrate, organic pollutants such as C-H, C=O, etc., and hydroxyl groups (OH) are frequent impurities that can produce peaks in a sodium bromide (NaBr) in mid-IR spectrum. In the pure sodium bromide spectrum, no other peaks are absorbed. This peak, which is located at about 1640 cm^{-1} , is created by the addition of atmospheric water. The electrostatic interactions between the Na^+ ions and the COO^- groups and between the Br^- ions and the NH_3^+ groups may cause the peak location to slightly change. In the sodium bromide-doped L-alanine single crystal (SBLA), the FTIR peak of L-alanine shifts from about 1300 cm^{-1} to 1302 cm^{-1} . This slight shift shows that the sodium bromide has been effectively integrated into the crystal lattice, affecting the L-alanine molecule's immediate environment and vibrational modes [11-14].

2.3. EDS analysis

The Energy-dispersive X-ray spectroscopy (EDS or EDX) yields detailed elemental composition information as well as a high-resolution image of the sample's minute surface features. Carbon, oxygen, nitrogen, sodium, and bromide are the elements that are present in the sample, as shown by the recorded EDS spectrum of the SBLA crystal as in Figure 3. The weight and atomic fraction of the elements in the generated sample are listed in Table 2. Thus, it has been demonstrated that the host L-alanine crystal contains sodium and bromide components in the interstitial positions of the lattice.

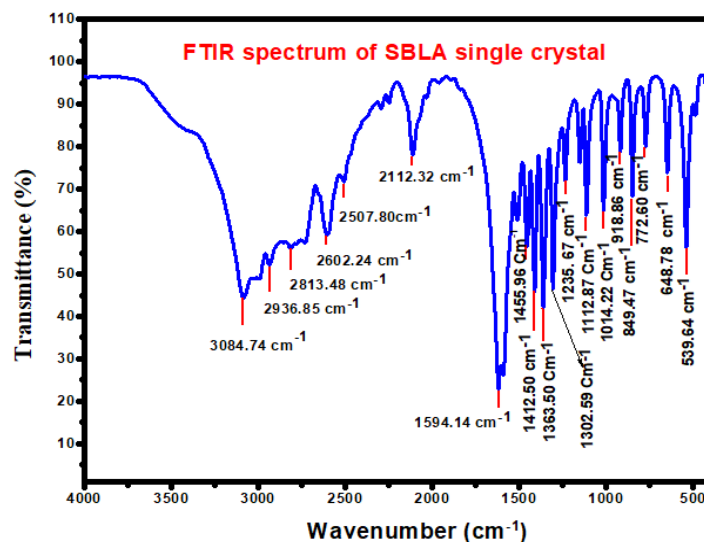


Fig. 2. FTIR spectral graph of sodium bromide-doped L-alanine (SBLA) crystal.

Table 1.

Modes of vibrations of FTIR spectrum of SBLA crystal

FTIR peaks/bands (cm ⁻¹)	Intensity	Modes of vibration
3084	W (broad)	NH ₃ ⁺ stretching
2936	W (broad)	NH stretching
2813	W (broad)	C-H stretching
2602	M	C-H stretching
2507	W (broad)	CH ₃ stretching
2112	M	Overtone& combination bonds
1594	S	NH ₃ ⁺ bending
1455	M	CH ₂ scissoring
1412	S	COO ⁻ stretching
1363	S	CH ₃ symmetric stretching
1302	S	O-H bending
1235	M	C-O stretching
1112	M	NH ₃ ⁺ rocking
1014	M	C-N stretching
918	W	C-C-N symmetric stretching
849	W	C-H out of plane bending
772	M	O-C-O deformation
648	M	COO ⁻ scissoring
539	S	CH ₃ symmetric stretching

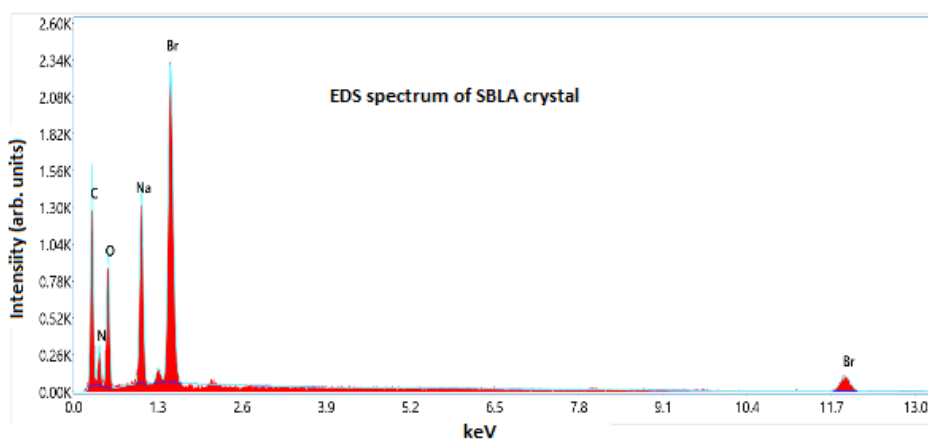


Fig. 3. EDS spectrum of SBLA crystal.

Table 2. Weight and atomic percentages of the different elements in SBLA crystal

Element and Shell	Weight %	Atomic %
C K	49.43	60.69
N K	13.42	14.13
O K	20.63	19.01
Na K	6.84	4.38
Br L	9.68	1.79

2.4. Scanning electron microscope (SEM) analysis

An strong electron beam is sent across a solid sample's surface in a raster pattern using a scanning electron microscope (SEM). The interaction of the loosely bound electrons of the surface atoms with the main electron beam on the surface, which produces secondary and back scattered electrons, is the foundation of the SEM. The sample's surface structure affects the secondary electron emission when the electron beam passes over it. An anisotropic formation of flower-shaped morphology is visible in the SEM pictures of the produced sodium bromide-doped L-alanine crystals in Figure 4 and the surface of the crystal also shows several pits. These pits, often called etch pits, are formed when a surface is exposed to a (when L-alanine react with Sodium and bromide) chemical reagent and usually indicating microscopic structural defects. The pits often reveal where defects such as grain boundaries intersect with the crystal surface. Thus, it has been demonstrated that the host L-alanine crystal contains sodium and bromide components. The surface morphology of a grown single-crystal reveals agglomeration in irregular shape, but SBLA single crystal revealed the several pits, the pits are revealed the crystal defects due to the chemical reagent of L-alanine react with Sodium and bromide [13-14].

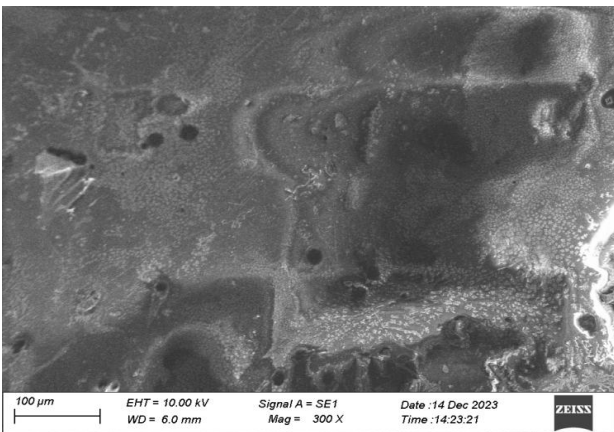


Fig. 4. SEM image of sodium bromide-doped L-alanine (SBLA) crystal.

2.5. Impedance analysis

Evaluating an object's electrical resistance, which is measured in ohms, is the main function of an impedance analysis. The sodium bromide-doped L-alanine (SBLA) crystal's resistance was measured using the Versa STAT MC-model impedance instrument at frequencies ranging from 1 Hz to 1 MHz. The two sides of the sodium bromide-doped L-alanine single crystal were painted with silver, which served as an electrode and made the crystal operate as a parallel plate capacitor [15-17]. The resistance

R and capacitance C values were used to determine the complex impedance |Z|. The complex impedance relation is given by

$$|Z| = Z' - jZ'' \tag{1}$$

where Z' and Z'' stand for the real and imaginary components of the impedance, respectively. Figure 5 shows how the impedance value drops with increasing frequency. The behavior of high impedance was seen at low frequencies. Figure 6 displays the Nyquist diagram of the sodium bromide-doped L-alanine (SBLA) single crystal. The bulk resistance (R_b) and grain boundary resistance (G_b) values are determined to be 36473.3 Ω and 20340 Ω, respectively. From figure 6, when bulk resistance (R_b) is significantly higher than grain boundary resistance (G_b), it indicates that the grain boundaries in crystal are more conductive than the grain interiors. This often occurs when defects (like vacancies or interstitials) or dopants accumulate at the grain boundaries, making them enriched with charge carriers. While grain boundaries usually act as barriers (increasing resistance), certain defects can turn them into fast conduction channels.

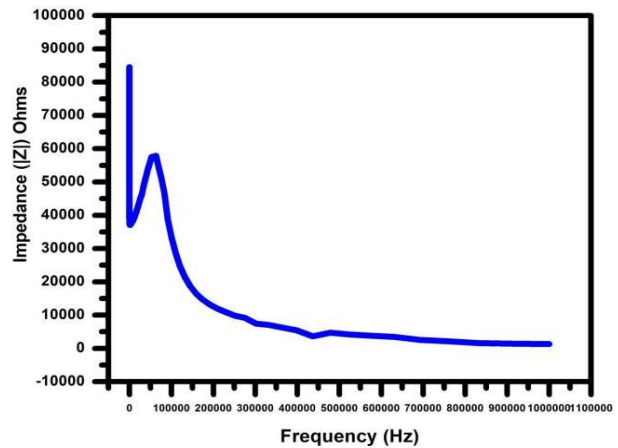


Fig. 5. Frequency versus impedance graph for SBLA single crystal.

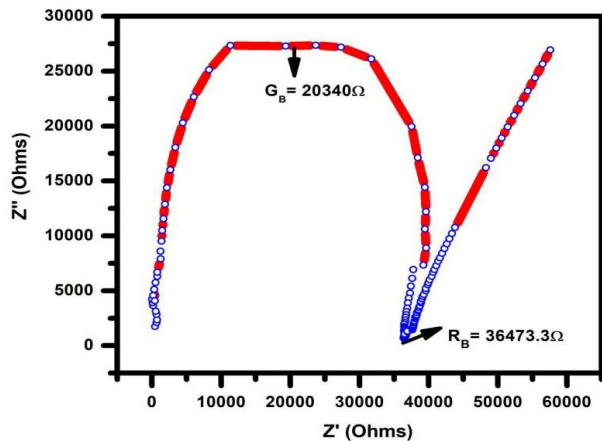


Fig. 6. Nyquist plot or complex impedance plot for SBLA single crystal.

The following relation was utilized to ascertain the sample's DC conductivity

$$\sigma_{dc} = \frac{t}{AR_b} \quad (2)$$

At normal temperature, the DC conductivity of SBLA crystal is $4.54044 \times 10^{-4} \text{ (ohm m)}^{-1}$, where t stands for crystal's thickness, A for electrolyte area, and R_b for bulk resistance [18]. In order to determine AC conductivity, the following relation was used.

$$\sigma_{ac} = \frac{t}{A|Z|} \quad (3)$$

The value of the complex impedance is shown by $|Z|$. Both resistance and capacitance are necessary for AC conductivity. Figure 7 shows how the frequency affects its AC conductivity, and it can be seen that the AC conductivity rises with frequency.

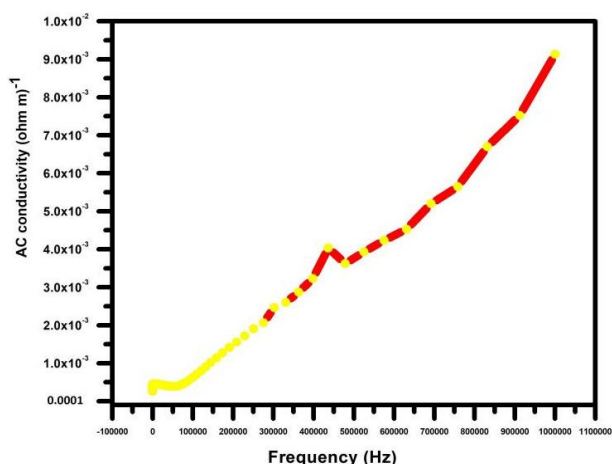


Fig. 7. AC conductivity versus frequency for SBLA single crystal.

DC Conductivity of SBLA crystal

DC conductivity value of the SBLA sample was determined to be $4.54044 \times 10^{-4} \text{ (ohm-m)}^{-1}$ for sodium bromide-doped L-alanine (SBLA) crystal and it signifies a moderately high concentration of charge carriers compared to typical pure organic amino acid L-alanine crystal [15], suggesting enhanced electrical conductivity due to the doping. In the context of organic nonlinear optical (NLO) crystals, conductivity in the range of 10^{-4} to 10^{-6} S/m indicates that the doping with sodium bromide has effectively increased the concentration of mobile ions or charge carriers, significantly enhancing the electrical conduction compared to pure L-alanine. The addition of Sodium Bromide (NaBr) introduces impurities into the L-alanine structure, creating defects. These defects, combined with the ionic nature of NaBr, increase the number of free charge carriers and DC Conductivity value of this sample is high. Pure organic crystals like L-alanine are typically excellent insulators with very low conductivity (often 10^{-10} S/m or lower). This level of conductivity, along with the reported strong UV-region absorption, indicates the material has a high sensitivity to optical stimulation (high photon response), making it suitable for applications in optoelectronic devices.

AC Conductivity of SBLA single crystal

AC conductivity of the sample was estimated to be $9.0 \times 10^{-3} \text{ (}\Omega \cdot \text{m)}^{-1}$ (or S/m) at a frequency of 10^6 Hz . In the world of crystals and semiconductors, this value is

generally considered relatively high for an organic dielectric material. Pure organic crystals are typically excellent insulators with very low conductivity and by doping L-alanine with NaBr, impurities are introduced into the lattice of L-alanine. These ions (Na^+ and Br^-) act as charge carriers, significantly boosting the conductivity at high frequencies (10^6 Hz). The AC conductivity usually increases because the high-frequency field assists the "hopping" of charge carriers across potential barriers in the crystal lattice.

2.6. Photocatalytic activity study for dye removal

The photocatalytic process using the unique properties of single crystal has been applied in a wide range of applications such as degradation of pollutants from atmosphere and water. The photocatalytic behaviour of the prepared sodium bromide-doped L-alanine (SBLA) single crystal was tested for the first time through the degradation of methylene blue (MB) and congo red dyes under visible light. Sodium bromide (NaBr) is used as the disinfectant in water treatment. A sodium bromide solution hydrolyzes when an activator (such as chlorine) is added, producing hypobromous acid (HBrO), a potent oxidizing agent and efficient bactericide that kills bacteria and algae. Microbiocides are made from sodium bromide to prevent the growth of bacteria, fungi, and algae in municipal and industrial water systems (such as cooling towers and swimming pools). It produces hypobromous acid/bromine, a potent oxidizing agent that gets rid of germs. In some situations, bromine-based treatments work better across a larger pH range and generate less hazardous byproducts than some conventional chlorine-only techniques. Sodium bromide is an effective photo-catalyst for eliminating organic dyes from waste water, according to literature reviews [19]. To establish absorbance and degradation of MB molecules and the congo red or methylene blue (MB) on the catalyst surface, 10 mg of the catalyst (sodium bromide-doped L-alanine crystal) was suspended in 10 ml of the aqueous solution of MB (10 mg L^{-1}). The suspension was then magnetically agitated in the dark for 30 minutes. The combination was then moved to a test tube and subjected to light. The degrade concentration of MB and congo red was determined by using a UV-vis spectrophotometer to measure the absorbance at 650 nm and 498 nm. The electronic transition that occurs during photo-excitation from the highest occupied energy band (VB) to lowest unoccupied energy band (CB) is primarily responsible for the photo-catalytic activity. The experiment was done for different concentrations such as 0-25 mg MB dye and congo red and the results show that bio-reduced sodium bromide doped L-alanine (SBLA) crystal could degrade and absorbance reaction of MB molecules and congo red molecules within the time of 60 min. Data in connection with the photocatalytic study for the sample are provided in the tables 3 and 4 and the corresponding data are given figures 8 and 9. From the results, it is established that sodium bromide-doped L-alanine (SBLA) crystal may work effectively as a photo-catalyst to remove the organic dyes from waste water and hence this sample could be useful for dye removal from dye solutions in textile industries [20-23].

Table 3.

Data in connection with methylene blue dye removal for SBLA single crystal

Dye concentration	Time / Methylene blue dye absorbance (arb.units) at 650 nm						
	0 min	10 min	20 min	30 min	40 min	50 min	60 min
5 mg	0.245	0.162	0.153	0.134	0.073	0.043	0.041
10 mg	0.271	0.172	0.144	0.101	0.084	0.039	0.033
15 mg	0.253	0.143	0.102	0.096	0.062	0.037	0.034
20 mg	0.285	0.134	0.108	0.074	0.043	0.016	0.015
25 mg	0.281	0.103	0.101	0.058	0.046	0.011	0.003

Table 4.

Data in connection with congo red dye removal for SBLA single crystal

Dye concentration	Time / Congo red dye absorbance (arb.units) at 498 nm						
	0 min	10 min	20 min	30 min	40 min	50 min	60 min
5 mg	0.353	0.371	0.357	0.268	0.259	0.197	0.194
10 mg	0.365	0.293	0.246	0.197	0.182	0.164	0.163
15 mg	0.32	0.298	0.301	0.201	0.174	0.171	0.156
20 mg	0.249	0.267	0.237	0.196	0.165	0.154	0.157
25 mg	0.23	0.194	0.177	0.183	0.174	0.142	0.149

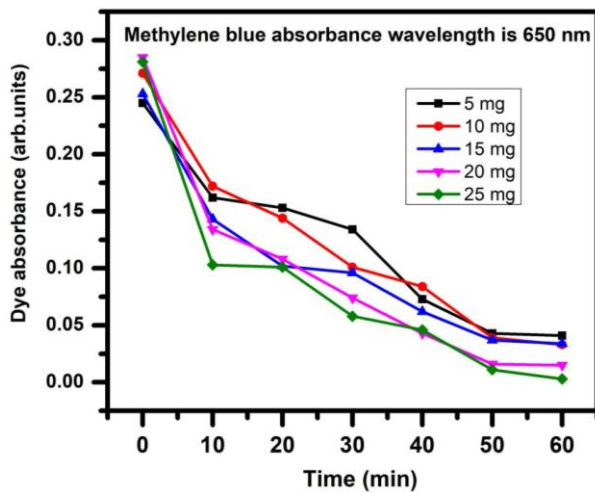


Fig. 8. Methylene blue dye removal by photocatalytic activity of SBLA single crystal.

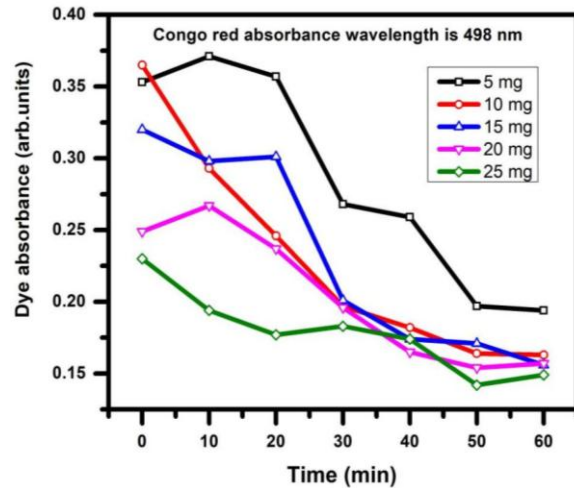
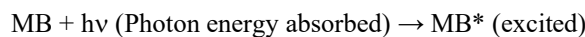
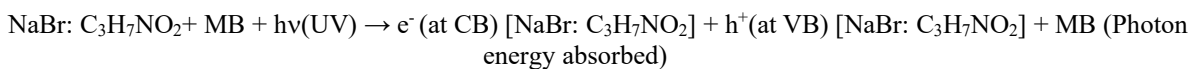


Fig. 9. Congo red dye removal by photocatalytic activity of SBLA single crystal.

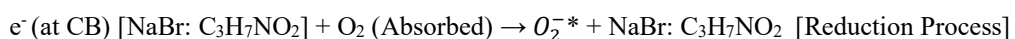
When the visible light hits the NaBr-doped crystal, electrons are promoted, creating charge carriers. The charge carriers in this mechanism are the electrons e^- at the conduction band and the holes h^+ at the valence band. These charge carriers react with adsorbed water and oxygen on the crystal surface to create highly reactive radicals. Here, the contribution of sodium bromide (NaBr) is to function as a photocatalytic enhancer, where NaBr doping enhances the absorption of visible light, reducing the bandgap to increase photoactivity. NaBr is primarily

to act as a dopant that modifies the electronic structure, it modifies the band structure of L-alanine to improve light absorption, acts as a charge trapper to prevent electron-hole recombination, and increases the production of reactive radicals HO_2 and OH necessary for the oxidative degradation of methylene blue (MB). Then this process is also similar to dye removal mechanism of congo red dye. MB dye removal mechanism for SBLA crystal is given below [24, 25].

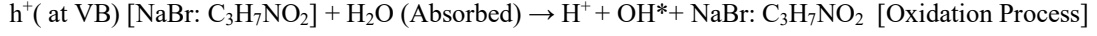
Phase 1: Photo-excitation and Charge generation



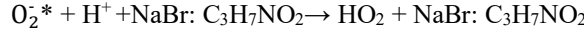
Phase 2: Formation of Reactive Oxygen Species
Formation of **Superoxide radicals**



Formation of Hydroxyl radicals

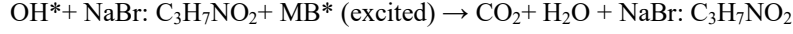
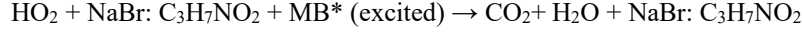


Formation of Hydroperoxyl radicals



Mineralization (Degradation)

The powerful radicals HO_2 , OH^* attack the excited Methylene Blue molecules.



2.7. Z-scan analysis

Second-order NLO study of SBLA crystal has been reported already [10] and in this paper we report the third-order NLO characterization of SBLA crystal by Z-scan approach. Nonlinear absorption coefficient, nonlinear refractive index, and nonlinear susceptibility are the crucial parameters for NLO crystals. Since SBLA crystal is a non-centrosymmetric crystal, both second-order and third-order NLO activities are possible in this sample. Z-scan measurement was performed after the crystal was experimentally sliced and polished in the Z-direction (along the thickness). A He-Ne laser with a wavelength of 632.8 nm was used to carry out the measurement. Figures 9 and 10 display the normalized transmittance for SBLA crystal in the open and closed aperture modes, respectively. The peak followed by valley in the closed aperture Z-scan curve (Fig. 10) indicates that SBLA crystal has the negative nonlinear refractive index and it is due to self-defocusing nature of the sample [26]. Using the open aperture Z-scan curve (Fig.11), the nonlinear absorption coefficient of SBLA crystal is found out.

Additionally, all of the computations were derived from the cited sources [27-29]. The quantity ΔT_{P-V} , which represents the variation between the normalized transmittance of the peak and valley, was calculated using

$$\Delta T_{P-V} = 0.406(1 - S)^{0.25} |\Delta\phi| \quad (4)$$

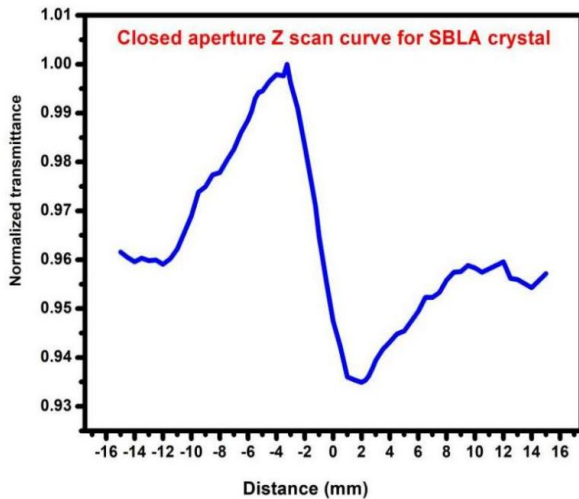


Fig. 10. Closed aperture Z-scan for SBLA single crystal.

$$S = 1 - \exp\left(\frac{-2r_a^2}{w_a^2}\right) \quad (5)$$

Here, S stands for aperture linear transmittance and r_a represents that the aperture radius and w_a stands for beam radius at the aperture. The nonlinear refractive index is given by the expression,

$$n_2 = \frac{\nabla\phi}{kl_0L_{eff}} \quad (6)$$

L is the crystal's thickness, and the linear absorption coefficient is as follows.

$$\alpha = \frac{2.303X \log(\frac{1}{T})}{d} \quad (7)$$

In this case, T is the crystal's transmittance and d is its thickness.

$$L_{eff} = \frac{1 - \alpha^{-\alpha L}}{\alpha} \quad (8)$$

From the open aperture Z-scan data, the nonlinear absorption coefficient is determined by using the relation,

$$\beta = \frac{2\sqrt{2VT}}{I_0L_{eff}} \quad (9)$$

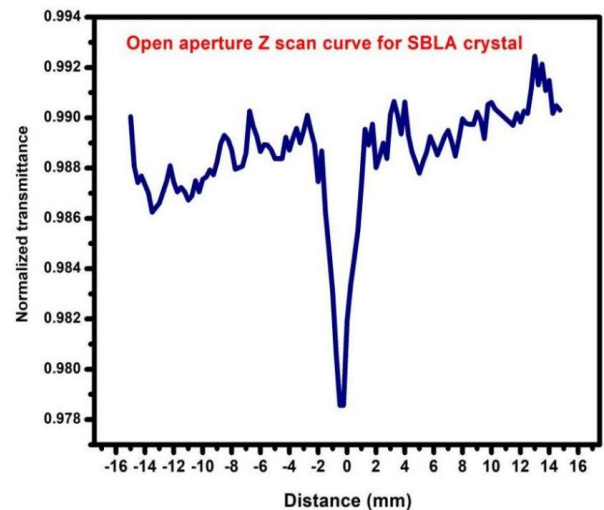


Fig. 11. Open aperture Z-scan for SBLA single crystal.

Then, T is the open aperture Z-scan curve's single valley or peak value. The third order nonlinear optical susceptibility's real and imaginary parts are ascertained from the n_2 and α values.

$$Re\chi^{(3)} = \frac{10^{-4} \epsilon_0 c^2 n_0^2 n_2}{\pi} \quad (10)$$

$$Im\chi^{(3)} = \frac{10^{-2} \epsilon_0 c^2 n_0^2 \lambda \beta}{4\pi^2} \quad (11)$$

The speed of light in vacuum is C, the linear refractive index of the crystal is n_o , and the permittivity of empty space is ϵ_o . The magnitude of the third-order nonlinear optical susceptibility of the sample is estimated by using the following relation

$$\chi^{(3)} = \sqrt{(Re\chi^{(3)})^2 + (Im\chi^{(3)})^2} \quad (12)$$

The values used for computing the third-order nonlinear optical parameters of SBLA crystal and the obtained results are provided in the table 5. The negative value of nonlinear refractive index of SBLA crystal ($-1.16807 \times 10^{-12} \text{ m}^2/\text{W}$) gives the negative nonlinearity of self-defocusing refractive index effect. The self-defocusing of the sample is due to the local variation of the refractive index with temperature and it is an important parameter for the application of the crystal in optical

sensors and night vision devices [30-32]. For comparison purpose, the values of third-order susceptibility of some of the NLO crystals are provided in the table 6 and it is observed that SBLA crystal has the high value of third-order susceptibility and it is due to -electron cloud between the donor and acceptor groups in doped amino acid (SBLA crystal). Hence, SBLA crystal could be used for optical devices like optical limiters, modulators and other third-order NLO devices [33, 34]. The presence of a self-focusing nature is indicated by the positive nonlinear refractive index of L-alanine single crystals and many of its semi-organic complexes [35]. L-alanine single crystals doped with sodium bromide have a negative nonlinear refractive index, indicating the existence of a self-defocusing tendency. This tendency proved that the sodium bromide is present in L-alanine single crystal. In table 6, third-order susceptibility value in the order of 10^{-8} esu is the good NLO behaviour compared to the other L-alanine based crystals. Sodium bromide doped L-alanine crystal (SBLA) is a high optical NLO behaviour shown by third order NLO test in terms of third-order susceptibility value. Sodium bromide doped L-alanine crystal (SBLA) is a semi-organic compound that is formed by the inorganic addition of sodium bromide. It aids in altering the crystal environment, which may have an impact on how the L-alanine molecules interact and pack. It is essential for NLO applications because it reduces conversion efficiency loss and undesired light absorption [14].

Table 5.

Values of various parameters and the computed results from Z-scan method for SBLA crystal

Parameters for SBLA crystal	Values and results
Beam diameter	0.005 m
Aperture radius (r_a)	0.002 m
Laser beam wavelength (λ)	632.8×10^{-9} m
Working laser power	12 mV
Beam radius at aperture (ω_a)	0.0045 m
Sample thickness (d)	0.001 m
Lens focal length (f)	0.200 m
Linear transmittance aperture (S)	0.3264
Phase shift ($\Delta\phi$)	0.17673
Incident intensity at the focus (Z=0) (I_o)	$15.31 \times 10^6 \text{ W/m}^2$
Effective thickness (L_{eff})	0.99581×10^{-3} m
Wave number (k)	$9.924 \times 10^6 \text{ m}^{-1}$
Linear optical absorption coefficient (α)	10.05215 m^{-1}
Nonlinear optical refractive index (n_2)	$-1.16807 \times 10^{-12} \text{ m}^2/\text{W}$
Nonlinear optical absorption coefficient (β)	$1.8155 \times 10^{-4} \text{ m/W}$
Real part of the third-order susceptibility ($Re\chi^{(3)}$)	4.00530×10^{-11} esu
Imaginary part of the third-order susceptibility ($Im\chi^{(3)}$)	3.13654×10^{-8} esu
Absolute third-order nonlinear optical susceptibility ($\chi^{(3)}$)	3.13654×10^{-8} esu

Table 6.

Values of third-order nonlinear susceptibility of some of NLO crystals

S.No.	Crystals name	Third-order susceptibility ($\chi^{(3)}$) esu	Reference
1.	Sodium bromide doped L-alanine (SBLA) crystal	3.13654×10^{-8} esu	Current study
2.	Potassium iodide-doped L-alanine	2.9169×10^{-8} esu	[36]
3.	L-alanine diglycine picrate	3.8189×10^{-8} esu	[32]
4.	L-alanine cadmium chloride	0.9134×10^{-15} esu	[37]
5.	L-alaninium oxalate	2×10^{-11} esu	[38]

2.8. Antibacterial activity

Over the past several years, a number of techniques have been utilized to investigate the antibacterial activity of different materials. The disc diffusion method was employed in this study to assess the sample's antibacterial activity [39]. Gram-positive (*Staphylococcus aureus*, *Bacillus subtilis*) and Gram-negative (*Enterobacter aerogenes*, *Klebsiella pneumoniae*, and *Pseudomonas aeruginosa*) bacterial species were tested for antibacterial activity in the grown crystal of SBLA. For 15 minutes, the media, pipette, Petri plates, and metallic borer were all sterilized in an autoclave set at 121°C. Finally, the culture media was sterilely transferred into Petri dishes. After

loading 20 µl of the SBLA sample onto the disc, the activity was examined. The control (standard sample) was 10 µg of chloramphenicol. At 37°C, each plate was incubated for 24 hours. The zone of inhibition's diameter was measured in millimeters. Figure 12 displays the schematics related to the SBLA crystal antibacterial activity investigation. Table 7 presents the zone of inhibition measurements. According to the findings, the SBLA crystalline sample has strong antibacterial activity against *Pseudomonas aeruginosa*, *Klebsiella pneumoniae*, and *Staphylococcus aureus*. Table 8 presents a comparison chart for the antibacterial activity data of SBLA crystal and other crystalline materials. Comparing SBLA crystal



(a) *Staphylococcus aureus*, (b) *Bacillus subtilis*, (c) *Enterobacter aerogenes*, (d) *Klebsiella pneumonia*, (e) *Pseudomonas aeruginosa*

Fig. 12. Area of inhibition for selected bacterial species like (a) *Staphylococcus aureus* (b) *Bacillus subtilis* (c) *Enterobacter aerogenes* (d) *Klebsiella pneumoniae* (e) *Pseudomonas aeruginosa* for SBLA crystal.

Table 7.

Values of zone of inhibition for SBLA crystal against five bacterial species

Bacteria organisms	Gram reaction	Zone of inhibition (mm)	
		Sodium bromide doped L-alanine (SBLA)	Standard
<i>Staphylococcus aureus</i>	+ve	26	25
<i>Bacillus subtilis</i>	+ve	22	28
<i>Enterobacter aerogenes</i>	-ve	15	18
<i>Klebsiella pneumonia</i>	-ve	30	35
<i>Pseudomonas aeruginosa</i>	-ve	26	22

Table 8.

Comparison of antibacterial activity of SBLA crystal with other crystalline materials

Bacteria organisms	Gram reaction	Crystals	Zone of inhibition (mm)	References
<i>Staphylococcus aureus</i>	+ve	SBLA (Sodium bromide doped L-alanine)	24	Current study
		L-threoninum sodium bromide	12	[41]
		L-alanine sodium nitrate	14	[42]
		L-alanine added nickel sulphate hexa hydrate	13 ± 0.1	[43]
		L-alanine added copper sulphate penta hydrate	17 ± 0.4	[43]
<i>Bacillus subtilis</i>	+ve	SBLA (Sodium bromide doped L-alanine)	22	Current study
		L-alanine sodium nitrate	14	[42]
		L-alanine added nickel sulphate hexa hydrate	13 ± 0.3	[43]
		L-alanine added copper sulphate penta hydrate	16 ± 0.3	[43]
<i>Enterobacter aerogenes</i>	-ve	SBLA (Sodium bromide doped L-alanine)	15	Current study
<i>Klebsiellapneumoniae</i>	-ve	SBLA (Sodium bromide doped L-alanine)	30	Current study
		L-alanine sodium nitrate	17	[42]
<i>Pseudomonas aeruginosa</i>	-ve	SBLA (Sodium bromide doped L-alanine)	26	Current study
		L-Threoninum sodium bromide	13	[41]
		L-alanine sodium nitrate	18	[42]

to other types of crystals, the results show that it works very well against both positive and negative gram bacterial organisms and has efficiently ensured good behavior antibacterially [40]. From table 8, the sodium bromide doped L-alanine single crystal (SBLA) is a better antibacterial activity when L-alanine added other crystalline materials such as sodium nitrate, nickel sulphate hexahydrate and copper sulphate pentahydrate and L-threonine. The antibacterial action of pure L-alanine single crystals is particularly effective against gram-negative bacteria such as E. coli [8]. L-alanine crystals doped with sodium bromide (NaBr) act against bacteria through a combination of biochemical interference with cell wall structures and physical disruption of cellular integrity. NaBr-doped L-alanine crystal acts by damaging the bacterial cell wall via electrostatic interaction and inhibiting metabolic processes due to the presence of the dopant, making it an effective antibacterial material. While pure L-alanine crystals have limited efficacy against gram-negative bacteria [8], the addition of sodium bromide enhances their biological activity, particularly against pathogens like *Staphylococcus aureus* (gram-positive) and *Pseudomonas aeruginosa* (gram-negative).

Conclusions

Slow evaporation was used to generate sodium bromide-doped L-alanine (SBLA) crystals, which were found to be clear, colorless, stable, and non-hygroscopic. The functional groups have been identified by using FTIR analysis to SBLA single crystal. To determine whether elements were present, the SBLA crystal's EDAX spectrum was recorded. From SEM analysis, SBLA single crystal revealed the several pits and also tiny anisotropic formation of flower-shaped morphology, the pits are revealed the crystal defects due to the chemical reagent of L-alanine react with sodium and bromide. The bulk resistance (R_b) and grain boundary resistance (G_b) values of SBLA crystal are determined to be 36473.3 Ω and 20340 Ω , respectively and the DC conductivity value is 4.54044×10^{-4} ($\Omega \cdot m$)⁻¹. AC conductivity value is 9.0×10^{-3} ($\Omega \cdot m$)⁻¹ (or S/m) at a frequency of 10^6 Hz. The ions (Na^+ and Br^-) act as charge carriers, significantly

boosting the conductivity. SBLA crystal may function well as a photo-catalyst to remove various organic dyes from waste water, so this sample could be useful for dye removal from dye solution in textile industries. The degrade concentration of methylene blue and congo red was measured using a UV-vis spectrophotometer to measure the absorbance at 650 nm and 498 nm. Here, NaBr doping enhances the absorption of visible light, reducing the bandgap to increase photoactivity and increases the production of reactive radicals HO_2 , OH necessary for the oxidative degradation of Methylene Blue and congo red dyes. According to Z-scan measurement, the SBLA sample's third-order nonlinear optical susceptibility value is 3.13654×10^{-8} esu, and the material is guaranteed the self-defocusing property of negative nonlinear refractive index. As a result, it may be more advantageous for NLO and laser opto-electronic applications. The produced SBLA crystal has strong antibacterial activity against all gram-pathogenic bacterial strains, both positive and negative, and can be used in biomedical applications. By this work, for industrial applications, sodium bromide-doped L-alanine (SBLA) crystal contributions may be better in compared to the other crystalline elements in terms of high conductivity, good antibacterial activity, good photocatalytic activity and high third order NLO activity behaviour.

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- [1] J. Uma and V. Rajendran, *Growth and characterization of γ -glycine single crystals from cadmium chloride for optoelectronic applications*, *Optik*, 125(2), 816 (2014); <https://doi.org/10.1016/j.ijleo.2013.07.067>.
- [2] J.F. Nicoud, R.J. Twieg, *In Nonlinear Optical Properties of Organic Molecules and Crystals*, D.S. Chemla, J. Zyss(Eds.), (Academic Press, New york), 227 (1987).
- [3] K.D. Parikh, D.J. Dave, B.B. Parekh and M.J. Joshi, *Growth and characterization of L-alanine doped KDP crystals*, *Cryst Res. Technology*, 45(6), 603 (2010); <https://doi.org/10.1002/crat.201000019>.
- [4] T. Fernando Loretta, Josephine Rani, S. Perumal, S. Ramalingom, *Growth, Structural, Spectral and Optical Studies of Glycine Sodium Nitrate Doped Potassium Dihydrogen Phosphate Single Crystals*, *AIP Conf. Proc.*, 1391, 143 (2011); <http://dx.doi.org/10.1063/1.3646805>.
- [5] T. Retnakumar, Ilangovan, K.C Bright, K. Sankaranarayan, T.H Freeda, and S. Vinu, *Growth, Spectroscopic, Dielectric and Non Linear Optical Studies of Strontium Metal Ion Doped Novel Semi-Organic L-Alanine Cadmium Chloride*, *International Journal of Engineering Research and Technology (IJERT)*, 4(01), (2015); <https://doi.org/10.17577/IJERTV4IS010347>
- [6] Priya Merline, Mangalaraj Chitra, *Investigation on optical, thermal, dielectric and mechanical properties of antimony potassium tartrate on l-alanine single crystals*, *Journal of Materials Science: Materials in Electronics*, 29(7), 1 (2018); <https://doi.org/10.1007/s10854-018-8519-0>.

- [7] Shi Ping Gai, Ting Zhang, Ming Yang Sun, Chen Wang, Yu Xian Chi, Yong Heng Xing, Feng Ying Bai, *A smart L-alanine modified Cd-NDI metal-organic framework crystalline material: Photochromic properties and photocatalytic degradation dye applications*, Applied Organometallic Chemistry, (2024); <https://doi.org/10.1002/aoc.7548>.
- [8] D. Jini, M. Aravind, L. Jothi Nirmal, S. Ajitha, *Structural, optical, and biological properties of L-alanine single crystal by slow evaporation method*, Materials Today: Proceedings, 43(15), 2032 (2021); <https://doi.org/10.1016/j.matpr.2020.11.736>.
- [9] C. Karnan, A. R. Prabakaran, M. Prabhakaran, G. Vinitha, *Growth, Optical, Thermal, Mechanical, Laser Damage Threshold and Electrical Polarizability of Cadmium Chloride Doped L-Alanine (LACC) Single Crystal for Optoelectronic Applications*, Journal of Electronic Materials, 50, 3757 (2021); <https://doi.org/10.1007/s11664-021-08891-y>.
- [10] S. Usha, P. Selvarajan, S. Lincy Mary Ponmani, S. Gracelin Juliana, *Investigation on crystallization, spectroscopic, SHG and thermal studies of sodium bromide-doped L-alanine single crystals*, Journal of materials science: Materials in electronics, 36, 95 (2025); <https://doi.org/10.1007/s10854-024-14159-y>.
- [11] P. Balaji Bhargav, V. Madhu Mohan, A. K. Sharma, V. V. R. N. Rao., *Structural and electrical properties of pure and NaBr doped poly (vinyl alcohol) (PVA) polymer electrolyte films for solid state battery applications*, Ionics, 13(6), 441 (2007); <https://doi.org/10.1007/s11581-007-0130-y>.
- [12] T. Vela, P. Selvarajan, T.H. Freeda, K. Balasubramanian, *Growth and characterization of pure and semiorganic nonlinear optical Lithium Sulphate admixed L-alanine crystal*, Physica Scripta, 87(4), (2013); <https://doi.org/10.1088/0031-8949/87/04/045801>.
- [13] K. Seethalakshmi, S. Perumal, P. Selvarajan, *Growth, Morphology, Spectral and mechanical properties of some doped, L Alanine family of single crystals*, IJCRR. 04(19), 53 (2012); https://ijcrr.com/uploads/1656_pdf.pdf.
- [14] D. Jini, M. Aravind, L. Jothi Nirmal, S. Ajitha, *Structural, optical, and biological properties of L-alanine single crystal by slow evaporation method*, Materials Today: Proceedings, 43(2), 2032 (2021); <https://doi.org/10.1016/j.matpr.2020.11.736>.
- [15] D. Shanthi, P. Selvarajan, S. Perumal, *Growth, Mechanical and Impedance Studies of BETA- Alanine Single Crystals*, (IJIRSE) International Journal of Innovative Research in Science &Engineering, (2018); <https://www.researchgate.net/publication/329443624>.
- [16] D. Shanthi, P. Selvarajan, S. Perumal, *Growth, SHG, THG and Impedance Analysis of Urea Admixed L-Alanine (ULA) Single Crystals*, International Journal of ChemTech Research. 6(13), 5329 (2014); <https://www.researchgate.net/publication/285136740>.
- [17] S.V. Ashvin Santhia, B. Aneeba, S. Vinu, R. Sheela Christy, Al-Mohaimed, M. Amal, Al Farraj, A. Dunia, *Studies on physicochemical and antibacterial deeds of amino acid based L-Threonine sodium bromide*, Saudi Journal of Biological Sciences; 27(11), 2987 (2020); <https://doi.org/10.1016/j.sjbs.2020.09.020>.
- [18] T. Jayanalina, G. Rajarajan, S. Parthiban, S.C. Mojumdar, *Thermal, mechanical, and optical studies of NaBr-added L-alanine crystal*, Journal of Thermal Analysis and Calorimetry; 112(2), 1025 (2013); <https://doi.org/10.1007/s10973-013-3058-7>.
- [19] M.W. Fitch, *Comprehensive Water Quality and Purification*, Constructed Wetlands, 268 (2014); <https://doi.org/10.1016/B978-0-12-382182-9.00053-0>.
- [20] Amr Nada, Yasser Moustafa and Amal Hamdy, Saad Abd El-Wahab and Dena Yahea, *Synthesis and Photocatalytic Activity of Single Crystal Titanate: Part-1*, Chemistry and Materials Research, 6(10), (2014); <https://www.iiste.org/Journals/index.php/CMR/article/view/16428/16758>.
- [21] Shiwen Kou, Qiaonan Yu, Lixiang Meng, Feng Zhang, Guoqiang Li and Zhiguo Yi, *Photocatalytic activity and photocorrosion of oriented BiVO₄ single crystal thin films*, Catalysis Science &Technology, 10(15) (2020); <http://dx.doi.org/10.1039/D0CY00920B>.
- [22] Chen Wang, Siyao Luo, Changyan Liu, Xiaoyan Liu, Chuansheng Chen, *Photocatalytic performance of single crystal ZnO nanorods and ZnO nanorods films under natural sunlight*, Inorganic Chemistry Communications, 114, 107842 (2020); <https://doi.org/10.1016/j.inoche.2020.107842>.
- [23] Haisheng Huang, Qi Kong, Xin Yue, Kunlei Wang, Zhishun Wei, and Ying Chang, *Fabrication and Photocatalytic Activity of Single Crystalline TiO₂ Hierarchically Structured Microsphere*, Catalysts, 13(1), 201 (2023); <https://doi.org/10.3390/catal13010201>.
- [24] L. Chellappan, B. Thangaraj, N. Muthukurumban, *Investigations on Chemically Synthesized Pure and Doped Manganese Dioxide Nanoparticles for Dye Removal and Photocatalytic Applications*, Journal of Fluorescence, 35(3); 1549 (2025); <https://doi.org/10.1007/s10895-024-03605-z>.
- [25] Z. Kalaycioglu, B. Ozgur Uysal, O. Pekcan, &F.B Erim, *Efficient Photocatalytic Degradation of Methylene Blue Dye from Aqueous Solution with Cerium Oxide Nanoparticles and Graphene Oxide-Doped Polyacrylamide*, ACS Omega, 8(14), 13004 (2023); <https://doi.org/10.1021/acsomega.3c00198>.
- [26] D.S. Ajisha, Ramki Chakaravarthy, R. Ezhil Vizhi, *Structural, optical, mechanical, dielectric and nonlinear optical studies of rubidium hydrogen oxalate dihydrate (RbC₄H₇O₁₀) single crystal*, Materials Chemistry and Physics, 283, 125952 (2022); <https://doi.org/10.1016/j.matchemphys.2022.125952>.

- [27] Paul Burkins, Robinson Kuis, Isaac Basaldua, Anthony M. Johnson, Siva Ram Swaminathan, Dajie Zhang, and Sudhir Trivedi, *Thermally managed Z-scan methods investigation of the size-dependent nonlinearity of graphene oxide in various solvents*, Journal of the Optical Society of America B, 33(11) (2016); <http://dx.doi.org/10.1364/JOSAB.33.002395>.
- [28] S. Azhagiri, P. Vasudevan, D. Jayaraman, A. Vichithra, *Studies on Third Order Nonlinear Optical Property and Biological Activity of DL-Methioninium Maleate for the Applications in Optoelectronics and Biomedical Field*, Bulgarian Journal of Physics, 51, 160 (2024); <https://doi.org/10.55318/bgjp.2024.51.2.160>.
- [29] P. Karuppasamy, T. Kamalesh, K. Anitha, S. Abdul Kalam, Muthu Senthil Pandian, P. Ramasamy, Sunil Vermad, S. Venugopal Rao, *Synthesis, crystal growth, structure and characterization of a novel third order nonlinear optical organic single crystal: 2-Amino-4,6-Dimethyl Pyrimidine 4-nitrophenol*, Optical Materials, 84, 475 (2018); <https://doi.org/10.1016/j.optmat.2018.07.039>.
- [30] M. Parishani, M. Nadafan, & R. Malekfar, *Z-scan investigation to evaluate the third-order nonlinear optical properties of cauliflower-like VS₂ structures*, JOSA B, 38(5), 1586 (2021); <https://doi.org/10.1364/JOSAB.418182>.
- [31] Self-focusing phenomena and applications in optical fibers, <https://www.gohecho.com/self-focusing-phenomena-and-applications-in-optical-fibers>, 2024 (accessed 14 May 2024).
- [32] R. Suganthi, K. Balasubramanian, *Functional Profiling of L-Alanine Diglycine Picrate (LADGP) Single Crystal for Nonlinear Optical Enhancement*, Tuijin Jishu/Journal of Propulsion Technology, 45(3) (2024); <https://doi.org/10.52783/tjjpt.v45.i03.7702>.
- [33] Y.R. Shen, *Self-Focusing and Filaments of Light: Past and Present*. In: Boyd, R.W., Lukishova, S.G., Shen, Y. (eds), *Self-focusing: Past and Present. Topics in Applied Physics*, 114, Springer, New York, 2009; https://doi.org/10.1007/978-0-387-34727-1_1
- [34] He-Liang Fan, Quan Ren, Xin-Qiang Wang, Ting-Bin Li, Jing Sun, Guang-Hui Zhang, Dong Xu, Gang Yu, Zhi-Hua Sun, *Investigation on Third-Order Optical Nonlinearities of Two Organometallic Dmit2- Complexes Using Z-Scan Technique*, Natural Science, 1(2), p.136-141(2009); <http://dx.doi.org/10.4236/ns.2009.12017>
- [35] T. Thilak, M. Basheer Ahamed, G. Marudhu, G.Vinitha, *Effect of KDP on the growth, thermal and optical properties of l-alanine single crystals*, Arabian Journal of Chemistry, 9(5), p.676-680 (2016); <https://doi.org/10.1016/j.arabjc.2013.04.022>
- [36] G.S. Kumar, J.M.S. Gnanaraj, V. Kathiravan, et al., *Growth of potassium iodide-doped L-alanine nonlinear optical single crystals: investigation of physico-chemical properties*, J Mater Sci: Mater Electron; 33, 26764 (2022); <https://doi.org/10.1007/s10854-022-09342-y>.
- [37] P. Kalaiselvi and Raj, S. Alfred Cecil and N. Vijayan, *Linear and nonlinear optical properties of semiorganic single crystal: L-Alanine cadmium chloride (LACC)*, Optik. 124 (24), 6978 (2013); <https://doi.org/10.1016/j.ijleo.2013.05.183>.
- [38] K.J. Arun, S. Jayalekshmy, *Third order nonlinear optical constants of L-alaninium oxalate*, Photonics letters of poland, 7(3), 81 (2015); <https://doi.org/10.4302/photon.%20lett.%20pl.v7i3.596>.
- [39] Alaa Baazeem, Abdulaziz Almanea, Palanisamy Manikandan, Mohammed Alorabi, Ponnuswamy Vijayaraghavan, Ahmed Abdel-Hadi, *In vitro antibacterial, antifungal, nematocidal and growth promoting activities of Trichoderma hamatum FB₁₀ and its secondary metabolites*, Journal of Fungi, 7(5), 31 (2021); <https://doi.org/10.3390/jof7050331>.
- [40] Mysoon M Al-Ansari, Ahmed M.I. Andeejani, Eman Alnahmi, Reem H. AlMalki, Afshan Masood, Anas Abdul Rahman., Ponnusamy Vijayaraghavan, Ki Choon Choi, *Insecticidal, antimicrobial and antioxidant activities of essential oil from Lavandula latifolia L. and its deterrent effects on Euphoria leucographa*, Industrial Crops and Products, 170, 113740 (2021); <https://doi.org/10.1016/j.indcrop.2021.113740>.
- [41] S.V. Ashvin Santhia, B. Aneeba, S. Vinu, R. Sheela Christy, Amal M. Al-Mohaimeed, Dunia A. Al Farraj, *Studies on physicochemical and antibacterial deeds of amino acid based L-Threoninum sodium bromide*, Saudi Journal of Biological Sciences, 27, 2987 (2020); <https://doi.org/10.1016/j.sjbs.2020.09.020>.
- [42] M. Shanmuga Sundaram, V. Vijayalakshmi, P. Dhanasekaran, O.N. Balasundaram and S.Palaniswamy, *Synthesis, Crystallization, Non Linear Optical and Anti-bacterial Activity of L-Alanine Sodium Nitrate Single Crystals*, Journal of Physics: Conference Series, 1172, 012072 (2019); <https://doi.org/10.1088/1742-6596/1172/1/012072>.
- [43] P. Sagunthala, V. Veeravazhuthi, P. Yasotha and P. Hemalatha, *Anticancer and Antimicrobial activities of single crystals of L alanine added nickel (ii) and copper (ii) sulphates*, World Journal of Pharmaceutical Research SJIF, 6(13), 672 (2017); <https://doi.org/10.20959/wjpr201713-9844>.

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Z-сканування, антибактеріальна активність та фотокаталітичні дослідження монокристалів L-аланіну, легованих бромідом натрію

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Методом повільного випаровування при кімнатній температурі отримано монокристали L-аланіну, легованого бромідом натрію (SBLA). Для їх дослідження використано рентгеноструктурний аналіз монокристалів (XRD), FTIR-спектроскопію, енергодисперсійну рентгенівську спектроскопію (EDS/EDX), сканувальну електронну мікроскопію (SEM), імпедансний аналіз, метод Z-сканування, а також дослідження фотокаталітичної та антибактеріальної активності.

Встановлено, що кристали SBLA мають орторомбічну структуру. FTIR підтверджує наявність характерних функціональних груп, тоді як EDS та SEM дозволяють визначити елементний склад і морфологію поверхні. Імпедансний аналіз використано для визначення об'ємного опору, внеску меж зерен та електропровідності (AC і DC). Фотокаталітичну активність оцінено за деградацією барвників конго червоного та метиленового синього. Методом Z-сканування визначено нелінійний показник заломлення (n_2), коефіцієнт нелінійного оптичного поглинання (β) та сприйнятливості третього порядку. Також встановлено антибактеріальну активність зразків SBLA.

Ключові слова: монокристал; FTIR; EDS; SEM; фотокаталітична активність; Z-сканування; антибактеріальна активність.