

Synthesis and Characterization of Semi-Organic Sodium Thiocyanate Potassium Sulphate (STPS) Crystal using Slow Evaporation Method

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In recent times, the Semi-organic crystals have high impact over optical communication, laser technology and electro-optic modulation, with its consumption of versatile Nonlinear Optical (NLO) application. Many efforts have been taken by the researchers to synthesize crystals with better optical nonlinearity and stability. Conventional techniques for growing single crystals often suffer from defects such as impurities and dislocations, which compromise the electrical and structural stability of the crystals. Furthermore, non-uniform growth conditions hinder the repeatability and reliability of these methods in specific applications. The primary aim of this research is to synthesize and investigate the growth and development of a highly proficient nonlinear semi-organic crystal known as Sodium Thiocyanate Potassium Sulphate (STPS). The STPS crystal is grown using a slow solvent evaporation method at ambient temperature, employing double-deionized water as the solvent. Extensive characterization of the STPS crystal is conducted using various techniques: X-ray diffraction (XRD) provides insights into the crystal structure and atomic plane spacing, Fourier-transform infrared spectroscopy (FTIR) identifies functional groups, UV-Vis spectroscopy reveals electronic transitions, scanning electron microscopy (SEM) detects material flaws, and microhardness testing verifies the crystal quality. The STPS crystal exhibits a microhardness value of 30.01, indicating significant mechanical strength. The UV-Vis-NIR investigations demonstrate that the STPS crystal has high optical quality, with 100% transmittance in the visible region and a cutoff wavelength below 250 nm, making it suitable for second harmonic generation (SHG) applications. Additionally, the STPS crystals display notable antibacterial properties, suggesting potential applications in medicinal fields. The comprehensive characterization confirms the improved structure and properties of the synthesized STPS crystals, highlighting their potential for advanced photonic and antimicrobial applications.

Keywords: Slow evaporation method, Scanning electron microscopy, Potassium sulphate, Sodium thiocyanate, Antimicrobial activity, UV-visible spectra

1 Introduction

The field of Optical Communication faces significant advancements in recent times, due to the introduction of organic and inorganic based Non-linear Optical (NLO) crystals. As NLO possess better advantages like high second harmonic generation efficiency, quick response times and better mechanical robustness, it is crucial to use single crystals for the nonlinear optical device production. The organic materials, generally has good non-linear co-efficient and also has the capability to associate with the various structures, however has limitations like reduced thermal behaviour and less effective mechanical strength. Besides, inorganic materials possess better mechanical and thermal properties, but due to less electron de-localization, the NLO property in it lags. Therefore, by preparing a semi-organic

crystal that gathers the positive features of both organic and inorganic components, it is possible to develop a novel crystal with better NLO properties^{1,2}. Synthesizing novel crystals using organic and in-organic materials known as Semi-organic materials, gives out better physical property and is possible to be used in applications like optical data storage, frequency conversions, telecommunication, photonics, opto-electric switches and in optical information processing^{3,4}. The introduction of single crystals with NLO properties provides higher Second Harmonic Generation (SHG) efficiency and better optical transparency. Compared to inorganic materials with NLO properties, the organic properties with NLO properties show better hyperpolarizability, optical susceptibility and significant laser damage threshold⁵.

As NLO based semi-organic crystals possess stable physiochemical properties and intriguing

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characteristics, there is lag in conducting researches over it^{6,7}. As the semi-organic materials possess high mechanical hardness, non-linearity and resistance, it is used in many applications⁸. Besides, the involvement of metal and ligand choices, makes the semi-organic materials provide different molecular architecture. If the semi-organic crystal grows well in all three dimensions, then it enables better growing process, which further assists in better device fabrication with ease in cutting and polishing; this becomes the main benefit for the use of novel crystals in technological applications^{9,10}. The formation of crystal incorporates different processes namely Gel crystallization, Solution cooling and Slow evaporation. Among the different processes, the slow evaporation process is considered to be the most significant and user-friendly technique and it promotes the nucleation and regulation of growth of the crystals, giving out better effective crystal with less limitations. Moreover, the slow evaporation process gives better control over the crystal, in terms of purity, shape and size, thereby making it suitable for the production of better-quality crystals that is necessary for detailed studies^{11,12}.

In order to identify the unique behavioral and unique properties of the crystal, wide range of investigations are carried out and their effectiveness in various technological domains are analyzed and this plays a comprehensive role in enhancing the NLO field. One of the most significant methods used for characterizing the semi-organic crystals is the X-ray diffraction (XRD) and it gives detailed and appropriate information's about the structure of the crystal, arrangement of atoms within the lattice, symmetry, and also about the unit cell dimensions¹³. The molecular architectures attained from different organic and inorganic component combinations are revealed effectively with the aid of the XRD analysis. For evaluating the vibrational modes of semi-organic crystal molecules, methods namely Fourier-transform infrared spectroscopy (FTIR) and Raman spectroscopy are used along with XRD analysis¹⁴. These techniques provide a wider knowledge about the bonding, chemical composition, and the functional groups existing in the crystals. Moreover, the use of FTIR better aids in detecting the appropriate organic and inorganic components, meanwhile, the Raman spectroscopy gives out information regarding the crystal symmetry and vibrations in the crystal.

To get an in-depth information about the characteristics of semi-organic crystals in non-linear

optics application, optical characterization is considered. To study the optical properties of the crystals, along with absorption the transmission characteristics, UV-Vis spectroscopy is employed and it aids in identifying the electronic transitions inside the crystal lattice and the transparency range of the crystal. Besides, the key factor in technological applications, (i.e.) the SHG efficiency gives the valuable data necessary for the understanding of optical behaviour of crystals^{15, 16}. As only one molecule arrangement is involved in semi-organic single crystal growth, it is very sensitive with respect to the temperature variations, also requires a reduced operating temperature.

Various single crystals have been synthesized using the slow evaporation technique, each demonstrating unique structural and optical properties. However, several limitations hinder their practical applications. L-alanine single crystals, despite their orthorhombic structure and notable photoluminescence, exhibit irregular morphology and limited antibacterial efficacy against gram-negative bacteria, restricting their potential in wastewater treatment. Similarly, 2-Amino-5-methylpyridinium phosphate (2A5MPP) crystals, though possessing well-defined functional groups and optical characteristics, face challenges due to limitations in nonlinear refractive index and third-order susceptibility, which impact their effectiveness in advanced photonic applications. Additionally, while pure and picric acid-doped KDP crystals show improved mechanical properties and second-harmonic generation efficiency, they exhibit a decreased form of micro-hardness with increasing load and significant hardness anisotropy, leading to mechanical instability. Further, the conventional crystal growing methods suffer from issues like impurities and dislocations that further has impact over the reliability and repeatability of the crystal. These drawbacks highlight the need for further optimization in crystal growth techniques to enhance structural uniformity, mechanical robustness, and functional efficiency for targeted applications.

Therefore, when compared to conventional nonlinear optical crystals, the research developed a Sodium Thiocyanate Potassium Sulphate (STPS) crystal that exhibits superior optical nonlinearity, high mechanical strength, and excellent transmittance making it highly suitable for photonic applications. Its enhanced structural stability and defect-free growth further improve its reliability in laser and electro-optic modulation technologies. In the medical field, STPS

crystals demonstrate notable antibacterial properties, which are used for biomedical coatings and antimicrobial treatments. Their high optical transparency and stability also enable potential applications in bio-imaging and laser-assisted medical diagnostics. Further modifications in doping and surface engineering could enhance their biocompatibility and efficacy in targeted therapeutic applications.

1.1 Contribution of the Paper

Besides, the non-uniform growth of the crystals leads to reduction in reliability and repeatability in case of different applications. Hence, the main contributions corresponding is stated below.

- To develop a unique single-crystal known as Sodium Thiocyanate Potassium Sulphate (STPS) using slow evaporation technique, for rectifying the issues such as impurities and dislocations of crystals, existing in the conventional crystal structures.
- To evaluate its characteristics, chemical composition, structure and imperfections, it is analyzed under XRD Diffraction, FTIR, UV-visible spectra, SEM, Photoluminescence, Micro hardness, and antimicrobial studies.

The related works concerned with the crystal studies are discussed in section 1.2 and it gives a clear and detailed view about the conventional crystal structures, along with its pros and cons.

1.2 Related Works

Chinnasamy *et al.*¹⁷ detailed the synthesis and characterization of Cadmium Nitrate p-nitro phenol (CNPN) single crystals for nonlinear optical applications. The CNPN was created by dissolving cadmium nitrate tetrahydrate and p-nitro phenol in methanol at a 2:1 ratio and mixing the solution at room temperature. FT-IR analysis was used to study the various functional groups in the CNPN molecule. The UV-visible spectrum showed that CNPN is highly transparent in the visible range, with a cut-off wavelength of 386 nm. The optical direct bandgap was estimated at 3.10 eV. Dielectric properties such as dielectric constant, dielectric loss, and AC conductivity were measured, revealing that impedance components decrease with increasing frequency. However, the crystal's unpredictable behavior affected its overall effectiveness. Devi *et al.*¹⁸ synthesized a single crystal of potassium hydrogen oxalate, a semi-

organic nonlinear optical material, from aqueous solutions of potassium hydroxide and oxalic acid in a 1:1 stoichiometric ratio using the slow evaporation method at room temperature. The crystals were characterized for their structural, thermal, and optical properties for potential optoelectronic applications. Single-crystal X-ray diffraction revealed a monoclinic structure with a non-centrosymmetric space group P21/c. FTIR spectra confirmed the presence of functional groups, while UV-Vis-NIR spectra showed optical transparency. TG-TDA analysis indicated thermal stability up to 295 °C, though further TG-TDA investigation is needed.

Priya *et al.*¹⁹ utilized slow evaporation to generate high-quality Bis (L-alaninato) zinc (II) (BLALZ) crystals, which were then characterized using a variety of analytical techniques. Single crystal XRD was used to estimate lattice parameters, while FT-IR spectroscopy confirmed the existence of different functional groups in BLALZ. The thermal behavior of BLALZ was investigated using TGA and DSC analysis. The synthesized crystals were transparent in the visible area (300 nm-1000 nm) and had a significant band gap, as evidenced by the UV spectra. BLALZ also showed moderate NLO efficiency and LDT values. However, the complexity should be reduced. Palani *et al.*²⁰ focused on slow evaporation, to successfully form a semi-organic crystal of L-Histidine Cadmium Bromide (LHCdBr). Single crystal X-ray diffraction revealed a triclinic structure in the produced crystal. Fourier Transform Infrared spectroscopy confirmed the presence of several functional groups. The crystal's optical quality was enhanced with fewer imperfections, making it ideal for non-linear optical device production due to low dielectric loss and high frequency. The impedance of charge carriers at electrodes generates space charge and macroscopic distortion, leading to higher dielectric constant values at lower frequencies. However, achieving consistent and reproducible crystal development is difficult, resulting in differences in crystal quality and characteristics.

Reis *et al.*²¹ synthesized and characterized a semi-organic crystal made from the amino acid L-histidine and hydrofluoric acid. The L-histidine bis (fluoride) crystal was created using slow solvent evaporation and analyzed using X-ray diffraction (XRD), crystallography, thermogravimetric (TGA), and differential thermal (DTA) studies. The TGA-DTA tests showed that the crystal remained thermally

stable up to 191 °C. The DTA curve indicated no phase transitions, which XRD analysis confirmed across temperatures. The orthorhombic phase exhibited significant anisotropic behavior, indicating that temperature variations greatly affect the crystallographic axes. Akilandeswari *et al.*²² synthesized single crystals of nonlinear alanine and hippuric acid (AH) through gradual evaporation at room temperature. FT-IR and FT-Raman analyses identified the vibrational modes and functional groups. UV-VIS-NIR transmission spectra showed high transparency and a reduced cut-off wavelength of 300 nm, with lower absorption in the visible range. The fluorescence spectrum revealed a 574 nm emission peak, indicating green radiation. Microhardness testing classified the AH single crystals as soft materials. However, the optical transparency of the crystals needs improvement.

Natarajan *et al.*²³ used the slow solvent evaporation solution growth method to produce high-quality single crystals of L-asparagine monohydrate potassium dichromate (LAMPDC). Single-crystal XRD analysis revealed the cell properties and crystal structure, while SEM showed a smooth, flower-like surface. EDAX analysis examined the elemental composition. LAMPDC demonstrated a second-harmonic signal with 0.59 times higher NLO efficacy than KDP. Vickers's microhardness test categorized LAMPDC as a soft material, with Meyer's plot confirming a reverse indentation size effect. However, the orthorhombic phase exhibited strongly anisotropic behavior, meaning the crystal's properties vary along different crystallographic axes. Karuppasamy *et al.*²⁴ used the solvent evaporation method to generate high-quality single crystals of piperazinium tetrachlorozincate monohydrate (PTCZ). The crystal structure and morphology were investigated using single-crystal XRD with WinX Morph software. The functional groups of the current systems were recognized. The crystal possesses high optical transmittance across the visible and UV regions, and the lower cut-off was found to be around 180 nm. The optical band gap energy was measured to be 6.2 eV. PTCZ has a thermal stability of 70 °C and is considered mechanically soft. Nevertheless, the method of crystal formation is not superior.

Yasothea *et al.*²⁵ utilized the slow evaporation approach, and single crystals of zinc sulfate monohydrate doped with L arginine were produced. Powder X-ray diffraction investigation demonstrates

the crystalline form of L-arginine-doped zinc sulfate monohydrate. The existence of functional groups was verified by the FTIR spectrum. The L-arginine doped zinc sulfate monohydrate crystal had a low cut-off wavelength of about 228 nm and a wide range of transparency in the UV, visible, and infrared regions, according to the UV-visible absorption spectra. L-arginine was present in the formed crystal, according to EDAX analysis. The formed crystal falls into the soft material group, according to the microhardness investigation. Nevertheless, the unpredictability of a single crystal reduces its efficacy.

Rimple Saini and David Joseph²⁶ have discussed the Rhodamine B-dye doped sulphamic acid single crystals and Sulphamic acids that are grown under a slow evaporation process. From the XRD, the Orthorhombic structure of the crystal is confirmed and by combining dye along with the crystal, the changes in the peaks in FTIR and spectroscopy are identified. Further, with Tauc plot, the value of bandgap is computed and is about 5.09eV and 5.13eV for pure, as well as doped crystals. The analysis results show that the dye-doped crystal shows high stability, which makes it efficient to be used in optoelectronic applications. Ravisankar *et al.*²⁷ utilized the slow-evaporation approach, and glycine sodium nitrate (GSN) crystals were produced. Group Cc in the monoclinic system is where the GSN crystals were located. The various functional groups were detected qualitatively using the FTIR spectrophotometer. The evaluation of the GSN crystal's third-order nonlinear optical quality using the Z-scan approach revealed an improvement in the material. Relatively defect-free crystals were what the low dielectric loss behavior in the dielectric investigation indicated about the formed crystal. The crystal was found to have a negative photoconducting character upon photoconductivity research. It was seen from the Temperature I-V characteristic that conductance rises with temperature.

Sivasubramani Vedyappan *et al.*²⁸ have presented an NLO third-order single crystal known as 2A5NPTCA (2-amino-5-Nitropyridinium Trichloroacetate), which is grown successfully with the aid of conventional Slow Evaporation Solution Technique (SEST). To identify the crystal structure, X-ray diffraction analysis is carried out and the results achieved indicate that the crystal grown is monoclinic and the multiple functional groups in the crystal is identified using FTIR spectroscopy analysis. The

results attained from UV-Vis NIR results indicate that the crystal grown has transmittance of about 60% and the wavelength ranges between 405 and 1100nm. Then, for computing the third-order NLO parameters, a solid-state laser with wavelength 532nm is employed. Further, the parameters of the title molecule are determined using quantum chemical calculations. Furthermore, the influence of intermolecular interactions over the crystal grown is evaluated using Hirschfeld Surface Analysis. The analysis results show that the crystal developed has better utilization in third-order NLO and Optoelectronic applications. However, it is identified that the output transmittance increases only at reduced input intensity. Kiran N Vijayan^{etal.}²⁹ discussed about the single crystal GBS (Guanidinium Benzenesulfonate) for NLO application and is processed using SEST for achieving better quality crystals. For studying the structure of the crystal, powder XRD and single crystal X-ray diffraction were carried out. Then, the functional groups in the crystal are evaluated using FT-IR spectra and then using UV-visible spectroscopy, the transmittance, as well as the optical band gap of the crystal are computed. To identify its emission spectrum, the sample was excited at a wavelength of about 260nm. Then, the activation energy was estimated using thermogravimetric data, and third-order non-linearity in the crystal was determined using the Z-scan technique. With the increase in pulse repetition rate, the LDT value decreases using Nd:YAG laser, and the analysis results show that the developed crystal shows self-defocusing nature.

Problem Statement: From the literature survey, it is clear that in¹⁷ a single crystal's unpredictable behavior lowers the crystal's effectiveness, in¹⁸ further investigation into TG-TDA is also necessary, in¹⁹ the complexity needs to be reduced, in²⁰ achieving consistent and reproducible crystal development is difficult, in²¹ temperature variations affect the crystallographic axes significantly, in²² the optical transparency of the crystal needs to be enhanced, in²³ it is problematic to have an orthorhombic phase with strongly anisotropic behavior, in^{24, 25} the method of crystal formation is not superior, in²⁶ the crystal is used only for optoelectronic applications and in²⁷, the unpredictability of a single crystal reduces its efficacy, while in^{28, 29}, the output transmittance and the LDT varies with the analysis results. For it to create better crystals, new semi-organic crystals have

to fulfill all of the physiochemical requirements. This is done by developing the crystals gradually through evaporation and then characterizing them using effective techniques like XRD, FTIR, UV-Vis, SEM, microhardness, and antimicrobial studies.

In this paper, a novel semi-organic NLO material, Sodium Thiocyanate Potassium Sulphate (STPS) is introduced and synthesized using a slow evaporation process, which assists in addressing the shortcomings of existing single-crystal growth methods by investigating the growth physicochemical properties of this semi-organic crystal. It describes the synthesis of STPS single crystals, their growth by slow evaporation technique, and their characterization using XRD, FTIR, and UV-visible spectroscopy. These findings highlight the superior quality and potential applications of the defect-free STPS crystal. Moreover, the results of the compound's X-ray diffraction and antibacterial activity are briefly reviewed. It is also explored for potential applications in the medical field.

2 Materials and Methods

Single crystal synthesis is the process of creating a material with a single, continuous crystal lattice structure that lacks the grain boundaries and imperfections that are typical of polycrystalline materials. This method is critical in many scientific and technological domains, including electronics, photonics, and materials research, where the distinct features of single crystals are used for specialized purposes. The quality and properties of the crystal are compromised by the shortcomings of existing single-crystal growth methods. Defects like impurities and dislocations are frequently encountered problems that endanger the crystal's electrical and structural stability. Variations in growth circumstances also result in non-uniform crystal quality, which affects the material's repeatability and dependability for specific purposes. To overcome the drawbacks associated with existing single-crystal growth methods, a novel approach is implemented by synthesizing and exploring the growth of physiochemical properties of a semi-organic crystal called Sodium Thiocyanate Potassium Sulphate using the slow evaporation technique. The goal of this approach is to reduce flaws like impurities and dislocations that are frequently present in traditional growth methods. The gradual development of the crystal is encouraged by the slow evaporation process,

which lowers the possibility of structural flaws. By addressing growing condition fluctuations and ensuring a more consistent crystal quality, the semi-organic compound selection further enhances electrical and structural stability.

A complete analysis of the structural, optical, and functional characteristics of the STPS crystal is conducted using a variety of characterization techniques such as XRD, FTIR, UV-visible, SEM, microhardness, and antimicrobial activity. Crystal defects that result from insufficient control over growth circumstances are examined; these include inclusions and mechanical stress. FTIR is used to detect functional groups, SEM is used to evaluate surface morphology, and XRD is used to analyze crystal structure. The optical transmission and absorption are examined using UV-Vis-NIR spectroscopy, and the crystal's resistance to localized deformation is evaluated using a microhardness test. Antimicrobial research also examines antifungal and antibacterial activities, offering information on possible uses and safety. Combining these methods provides a comprehensive understanding of the characteristics of STPS crystals, which is essential for a variety of applications in materials research and device fabrication. The two provided components Sodium thiocyanate and Potassium Sulphate are initially combined and stirred at room temperature. After that, the solution is slowly evaporated to create a semi-organic crystal named STPS crystal, which is created. Several characterization techniques, including XRD, FTIR, UV-visible, SEM, microhardness, and antimicrobial activity, are used to examine the generated STPS semi-organic crystal in this work to obtain a better crystal.

2.1 Experimental Data Specifications

A well-defined methodology is essential to ensure the reproducibility of experimental results. This section provides detailed insights into the data collection process, equipment configurations, and specific experimental procedures followed in the study. By maintaining precise control over these aspects, the quality and consistency of the synthesized STPS crystals are optimized.

2.1.1 Data Collection

The data collection process involves systematically recording observations and measurements at each stage of STPS crystal synthesis and characterization. During the crystal growth phase, parameters such as temperature, evaporation rate, and solution

concentration are monitored to ensure consistency. Optical, structural, and mechanical properties are assessed through multiple characterization techniques, including XRD, SEM, FTIR, UV-Vis spectroscopy, and micro-hardness testing. The antifungal and antibacterial activities are also recorded by measuring the inhibition zones against microbial strains, ensuring accurate biological evaluation.

2.1.2 Equipment Settings

To ensure precise and reproducible results, specific instrument settings are maintained during characterization. XRD analysis is conducted using a radiation source with a scan step size optimized for high-resolution structural analysis. SEM imaging is performed under controlled vacuum conditions, using an electron beam voltage appropriate for surface morphology analysis. FTIR spectroscopy is conducted in the mid-infrared range of 4000-400 cm^{-1} with a set resolution to capture distinct functional group vibrations. UV-Vis spectroscopy is performed within the 200-800 nm wavelength range to analyze optical absorption and transmission properties. Micro-hardness measurements are carried out with a fixed load and settle time to assess mechanical stability.

2.1.3 Specific Procedures

The STPS crystal synthesis follows a slow evaporation method at room temperature of 30°C to promote controlled growth. Sodium thiocyanate and potassium sulfate are dissolved in double-deionized water, ensuring high-purity solutions. The solutions are filtered using 11 μm pore-sized Whatman filter paper to remove impurities before being transferred to beakers with perforated covers for gradual evaporation. Over 26 days, solvent evaporation leads to the formation of single crystals with improved structural integrity. The crystallized samples are then subjected to multiple characterization techniques, ensuring a comprehensive evaluation of their properties for potential applications.

2.2 Synthetization of Materials

The slow evaporation method is used for single-crystal growth in the synthesis of compounds such as sodium thiocyanate, and potassium sulphate. To ensure purity, the compounds are first dissolved in a solvent and the resulting solutions are then carefully filtered. After that, the filtered solutions are put into sanitized containers, and a seed crystal is placed at the bottom of the container to start the crystal growth process. The controlled and organized crystal

formation made possible by this method is crucial for in-depth structural and analytical investigations.

2.2.1 Sodium Thiocyanate-Potassium Sulphate

The Sodium Thiocyanate Potassium Sulfate (STPS) crystal is a novel semi-organic material synthesized using a slow evaporation technique at room temperature. This crystal combines sodium thiocyanate and potassium sulfate, offering unique properties. Sodium thiocyanate and Potassium Sulphate are synthesized through equip-molar stoichiometric relation. Using double-deionized water, Sodium thiocyanate is first dissolved, and then the quantity of the Potassium Sulphate is mixed in Sodium thiocyanate by constant stirring. Crystal growth is generated by a slow evaporation technique and the results are based on room temperature (30°C). The structure of Sodium Thiocyanate-Potassium Sulphate is shown in Fig. 1(a) and Extracted Sodium Thiocyanate-Potassium Sulphate Crystal images are presented in Fig. 1(b).

Crystal growth is induced by employing a slow evaporation technique at room temperature (30°C). The saturated solutions are prepared using recrystallized salt at the same ambient temperature. These solutions were then filtered through Whatman

filter paper with an 11 μm pore size, and the obtained crystal grain size was on average of (5-7) mm. Figure 1 (b) displays STPS crystals of varying sizes, demonstrating the effectiveness of the slow evaporation growth technique. Each crystal is placed on a calibrated grid background to provide a visual reference for size comparison. The dimensions range from 5 mm to 6.9 mm, indicating controlled and slightly varied growth under identical conditions. The hexagonal morphology suggests uniform crystallization, influenced by the optimized saturation and evaporation parameters. This visual representation validates the reproducibility and quality of the synthesized crystals, essential for further characterization and application analysis. Further, to facilitate crystallization, the filtered saturated solutions are transferred to beakers with perforated covers, maintaining the beaker at room temperature for 26 days to allow for the gradual evaporation of the solvent. After this period, single crystals are obtained through the slow evaporation process. The described methodology ensures the successful synthesis of the specified chemical compounds with controlled crystal growth. Further, environmental factors such as temperature and humidity are important in STPS crystal growth,

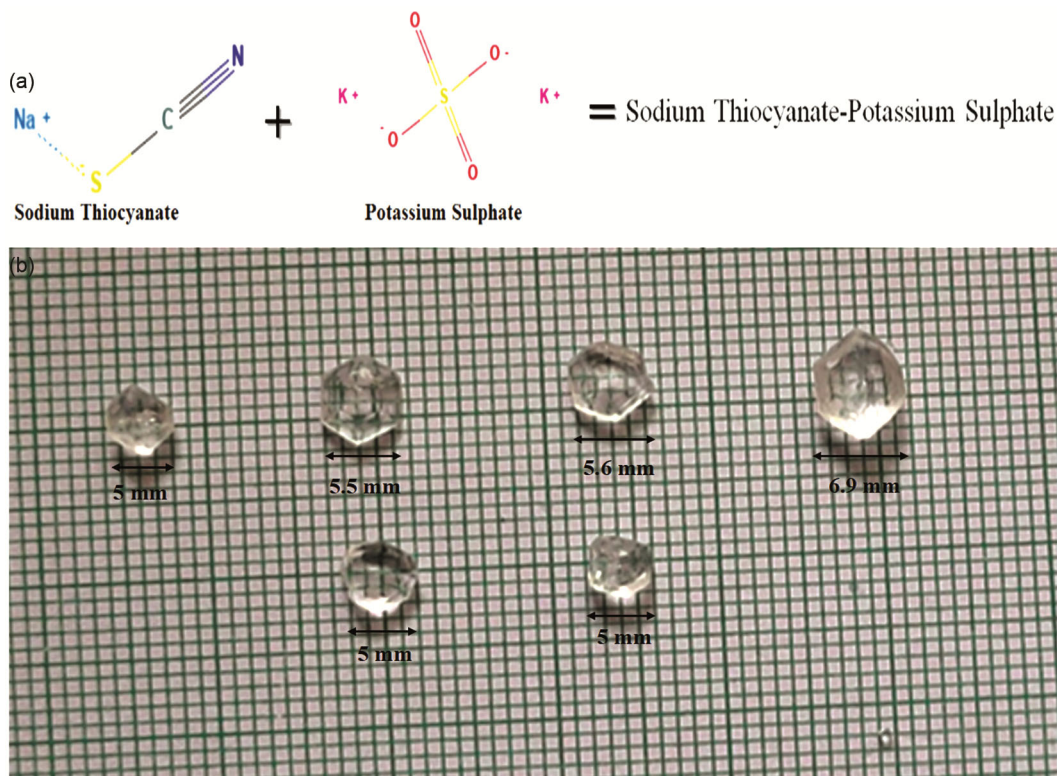


Fig. 1 — (a) Sodium Thiocyanate-Potassium Sulphate, and (b) Extracted Sodium Thiocyanate-Potassium Sulphate Crystal

influencing nucleation rate, solubility, and overall crystal quality. Fluctuations in temperature alter super-saturation levels, potentially leading to defects or irregular morphology, while variations in humidity affect solvent evaporation rates, impacting crystal size and transparency. Maintaining stable ambient conditions is essential for achieving uniform growth and minimizing structural inconsistencies. Optimizing these parameters ensures better reproducibility and enhances the optical and mechanical properties of STPS crystals. Therefore, the methodical use of the slow evaporation technique improves the quality and reproducibility of the synthesized crystals.

2.3 Characterization Studies of STPS

The structural, optical, and functional features of STPS crystal were studied by a thorough analysis using various kinds of characterization techniques. The study of crystalline flaws includes defects resulting from incorrect control of crystal development conditions, such as inclusions and mechanical stress. Common methods for characterizing defects include optical, thermal, spectral, structural, and nonlinear optical studies, among others. The assessment of optical attributes includes the examination of the crystal's optical transmission and absorption, SHG conversion efficiency, NLO values, electro-optical coefficients, and the structural dependence of these characteristics.

To thoroughly investigate the properties of the proposed STPS crystal, various characterization techniques such as XRD, SEM, FTIR, UV-Vis-NIR, Antimicrobial studies, and Microhardness Tests are used. A D8 Phaser Bruker Powder diffractometer is used to examine the crystal structure, as demonstrated by STPS. X-ray diffraction patterns are used in XRD, an effective technique that clarifies the crystal structure. The arrangement of atoms in the crystal lattice is determined by measuring the angles and intensities of diffracted X-rays, which provides vital information on the structural properties of the crystal. SEM is used to analyze the crystals' surface morphology. This method produces high-resolution pictures by employing electron beams. This made it possible to see the crystal's exterior characteristics in great detail and gave information on its size, topography, and any flaws. The SPECTROMRX1 FTIR Spectrometer is used to determine which functional groups are present in the crystal. This approach uses the KBr pellet technique to record the FTIR spectrum and disclose the vibrational modes of

the chemicals that make up the crystal. To fully characterize the composition of the crystal, FTIR is essential for identifying the different kinds of chemical bonds and functional groups. A Perkin Elmer k35 model UV-Vis-NIR double beam spectrometer is implemented to record the optical transmission and absorption spectra of the crystals, which covered the wavelength range of 190 nm to 790 nm. This method yields important details regarding the transparency, absorbance, and electronic transitions of the crystal in the visible, near-infrared, and ultraviolet wavelength ranges. Using a microhardness test, the crystal's resistance to localized deformation is assessed. This method of controlled indentation provides numerical information on the hardness of the crystal. Comprehending the crystal's mechanical characteristics is crucial for applications in fields like materials science and device manufacturing. Analyzing crystals' antimicrobial qualities, such as their antibacterial and antifungal activity, provides important details regarding their safety and efficacy along with potential future application possibilities. STPS surpasses traditional materials like potassium dihydrogen phosphate (KDP) in various performance aspects, and to obtain a high-quality crystal, many characterization methods are used, including XRD, SEM, FTIR, UV-Vis-NIR, Antimicrobial studies, and Microhardness Tests. Hence, evaluation of the STPS crystal observations is covered in section 4 which follows.

3 Results and Discussion

This section presents the findings from a crystal of potassium sulfate and sodium thiocyanate. The crystals that were created are predicted to be highly stable both chemically and physically, according to the results.

3.1 UV-Vis-NIR Spectra

The UV-Vis-NIR spectral analysis of Sodium Thiocyanate Potassium Sulfate (STPS) crystals provides crucial insights into their suitability for nonlinear optical (NLO) applications. The transmission and absorption spectra, measured between 190 and 790 nm, reveal a lower cutoff wavelength of 250 nm, indicating that the crystal exhibits high transparency in the visible region. This transparency, with 100% transmission in the visible spectrum, underscores the high optical quality of the STPS crystal and its potential for Second Harmonic Generation (SHG) applications. The absence of

absorption in the visible range confirms that the STPS crystal is a viable candidate for optoelectronic devices. Additionally, compared to conventional KDP crystals, the STPS crystal demonstrates superior transparency, enhancing its attractiveness for advanced optical applications. The UV-Vis-NIR spectra confirm the crystal's effectiveness in absorbing ultraviolet light and its optimal performance for various NLO processes.

The above Fig. 2 shows the UV spectrum of Sodium Thiocyanate Potassium Sulphate crystal. The UV-Vis-NIR transmission and absorption spectra were captured between 200 and 800 nm for the STPS crystal. The spectra that a lower cutoff wavelength is 250 nm, which supports the absence of absorption in the visible area. The UV-visible spectra demonstrate that the crystal structure effectively absorbs ultraviolet light, as indicated by the lower cutoff wavelength at 250 nm. Hence, the optimal bandgap of the developed STPS crystal is computed as 4.96eV and as it is within the standards, the STPS crystal is identified to be a pure one.

3.2 FTIR Spectral Analysis

The recognition of functional groups is performed using FTIR spectrum analysis. When compared to other available electronic data, the FTIR spectrum delivers more trustworthy information about the molecule. When establishing which functional groups exist in the harvested crystal, the presence or absence of certain absorption bands is critical. The FTIR spectrum is evaluated by comparing it to the exact information now available about KDP and the produced crystal. The FTIR spectra of the crystal formed utilizing the KBr pellet technique were

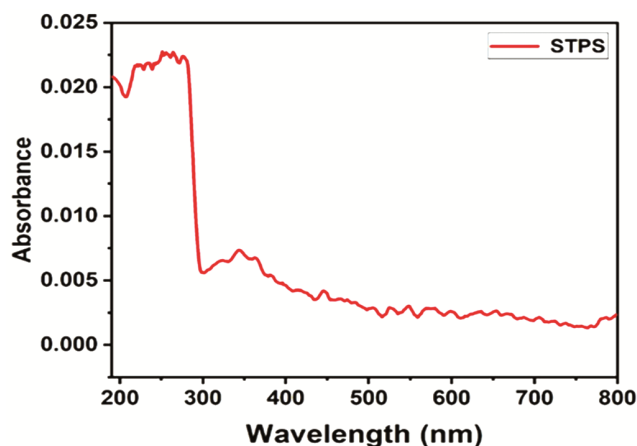


Fig. 2 — UV spectrum of Sodium Thiocyanate Potassium Sulphate crystal (STPS)

recorded using a Perkin Elmer spectrometer with a range of 400-4000 cm^{-1} .

Figure 3 shows the FTIR spectrum of STPS crystal. A strong band with multiple peaks was found between 1610 and 1187 cm^{-1} due to the NH_3 stretching frequencies. The C-H stretching of STPS is visible as a weak absorption band at 999 cm^{-1} . The presence of the metal bond is confirmed by the peak at 447 cm^{-1} , which also suggests that it may be the cause of the carboxylic group's C=O stretching. The metal linkage N of the amino acid group causes the peak disappearance at 618 cm^{-1} .

The comparative analysis of STPS with that of other crystals like Pure KDP (Potassium Dihydrogen Phosphate)³⁰, DL-Alanine-KDP³⁰, PTCZ (Potassium Chloride Doped-Potassium Dihydrogen Phosphate)³¹, GBS²⁹ and 4DME (1-[4-(4-(Dimethylaminophenyl) Ethynyl) Phenyl] Ethanone)³² have been illustrated in Table 1. The analysis results show that the proposed STPS crystal has NH_3 Stretching of about 1187 cm^{-1} , while pure KDP has 1099 cm^{-1} and DL-Alanine KDP has 1098. In case of C-H Stretching, the STPS has 999 cm^{-1} , while the other crystals like Pure KDP, DL-Alanine KDP, PTCZ, GBS and 4DME has 2800 cm^{-1} , 2600 cm^{-1} , 2782 cm^{-1} , 998 cm^{-1} and 2896 cm^{-1} respectively. Similarly, the C-O Stretching, the vibration occurs at 447 cm^{-1} peak and for 4DME, the vibration is at the peak 1671 cm^{-1} . From the above analysis, the characteristics of the STPS crystal grown using SEST technique is better compared to other crystals.

3.3 X-Ray Diffraction

The crystalline nature and structure of the generated STPS crystal have been determined using

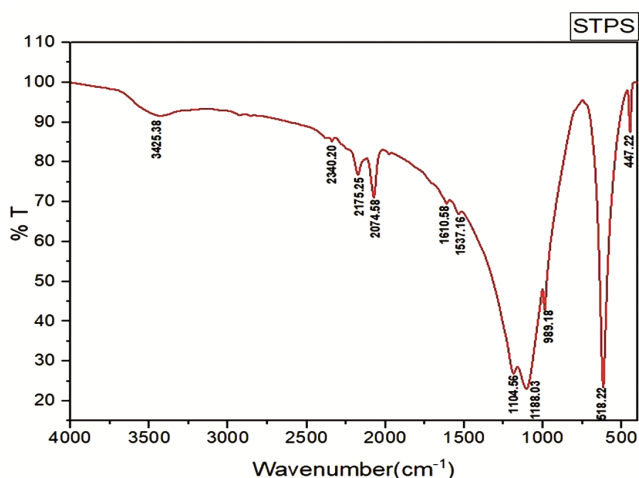


Fig. 3 — FTIR Spectrum of STPS crystal

Table 1 — Comparative Analysis of STPS crystal and Other Crystals

Assignment	Proposed STPS (cm ⁻¹)	Pure KDP (cm ⁻¹)	DL-Alanine-KDP (cm ⁻¹)	PTCZ (cm ⁻¹)	GBS (cm ⁻¹)	4DME (cm ⁻¹)
NH ₃ Stretching	1187	1099				
C-H Stretching	999	2800	2600	2782	998	2896
C-O Stretching	447				4DME (cm ⁻¹)	1671

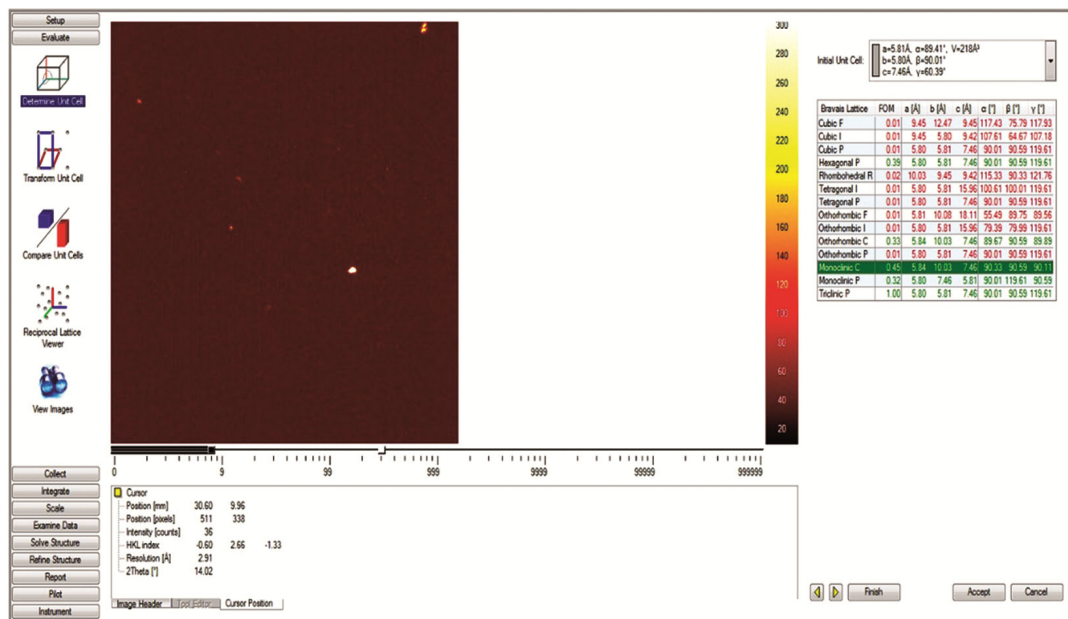


Fig. 4 — X-ray diffraction pattern of STPS

X-ray powder diffraction. The crushed powder sample is exposed to a high-intensity X-ray beam with a wavelength of 1-5418Å and a scanning speed of 1/min. The XRD pattern is indexed using the Rietveld Index program.

The measured X-ray diffraction spectrum for STPS crystal is shown in Fig. 4. The presence of distinct, well-defined peaks, with the relevant peaks indexed, attests to the good crystalline quality of the STPS crystal. The strong intensity peak was located at 34° with the crystal faces of the (138) plane. From the diffraction method, it is identified that the new crystal formed comes under Monoclinic C crystal family-lattice system. The Figure of Merit (FOM) which measures the phase quality of every single reflection is about 0.45. The unit cell, which is the building block of the crystal structure possess six lattice parameters namely α , β and γ , which are the angles in-between them; a , b and c are the cell edge lengths. From the analysis, the length of the edges is identified to be 5.84nm, 10.03nm

and 7.46nm; the angles in-between them are 90.33°, 90.59° and 90.11°, respectively.

3.4 Micro Hardness

A crystal's hardness is determined by how resistant it is to local deformation; determining a crystal's hardness is crucial to comprehend the composition of the crystalline substance. Microhardness is calculated by using Vickers Number. Microhardness investigations were performed on STPS crystals along the (1 0 0) plane using an HMV SHIMADZU microhardness tester equipped with a diamond Vickers pyramidal indenter to evaluate mechanical properties. Static indentations were conducted at room temperature with a consistent indentation time of 10 to 15 seconds for all tests. The measurements were taken using moderate loads ranging from 10 grams to 50 grams, yielding hardness values between 150 and 300 HV.

The mechanical strength of the Sodium Thiocyanate Potassium Sulfate (STPS) crystal,

essential for its NLO applications, is assessed through its microhardness, as shown in Fig. 5. During testing, a force of 0.05 Kgf is applied to press a Vickers indenter into the crystal's surface, with indentations spaced approximately 19.3 μm apart. The resulting Vickers microhardness value of 30.01 indicates that the STPS crystal possesses significant strength and flexibility. This robust mechanical property is advantageous for maintaining structural integrity and reliability in various NLO applications, such as frequency conversion and optical switching, where durability under operational conditions is crucial.

3.5 Scanning Electron Microscopy

An investigation of an STPS crystal's surface morphology was conducted using SEM. With the use of a concentrated electron beam, this potent imaging method creates three-dimensional, high-resolution pictures of the specimen's surface. SEM gave precise insights into the semi-organic crystal's microstructure, enabling the investigation of surface characteristics, crystal shape, and any flaws.

The top and cross views of the catalytic pervaporation method used for the slow evaporation method in STPS are shown in Fig. 6. Three layers such as the support layer, separation layer, and catalytic layer are found in the cross-sectional view of the STPS crystal. The STPS crystal has a thickness of approximately 100 μm . Compared to the catalytic membrane prepared by mixing, which has a denser catalytic layer, the catalytic membrane made through immersion phase inversion has a more porous structure. In addition to increasing catalyst exposure and the number of active sites available for the reaction, an improved porosity structure decreases diffusion resistance, facilitating the transfer of constituents from the bulk to the active sites.

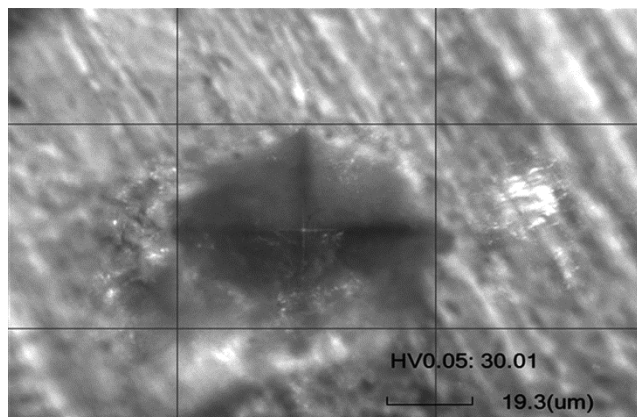


Fig. 5 — Micro hardness of STPS

Moreover, there were no discernible changes in the morphology of the membrane, suggesting that its structure remained stable.

3.6 Antimicrobial Activity

The antimicrobial activity of STPS crystals was assessed to evaluate their potential as a functional material in biomedical and environmental applications. The presence of antibacterial and antifungal properties makes STPS a promising candidate for use in medical devices, such as wound dressings, coatings for implants, and surfaces of medical equipment, where bacterial contamination poses a significant risk.

3.6.1 Anti-Bacterial Activity

STPS crystal tested against *Staphylococcus aureus* and *Pseudomonas aeruginosa* bacteria strains which are shown in Fig. 7. The observed zones of inhibition are shown in Table 2. Based on these results, it concludes that STPS is active toward both bacterial strains in a concentration-dependent manner. The zone of inhibition was evaluated at various STPS concentrations such as 500 $\mu\text{g}/\text{ml}$, 250 $\mu\text{g}/\text{ml}$, 100 $\mu\text{g}/\text{ml}$, and 50 $\mu\text{g}/\text{ml}$, and compared to a positive control (PC) using kanamycin as a reference antibiotic. The results for STPS with *Staphylococcus aureus* express that at 500 $\mu\text{g}/\text{ml}$, there is a zone of inhibition of 12.5 ± 0.7071 mm, while for 250 $\mu\text{g}/\text{ml}$ and 100 $\mu\text{g}/\text{ml}$ the test organism shows an inhibition zone of 4.25 ± 0.35 mm, 3.25 ± 0.3 mm respectively. Moreover, there is no inhibition dosages found for the test organism *Pseudomonas aeruginosa*. These results show that the STPS compound is considered active towards selected bacterial strains. Hence, the antibacterial activity of STPS against *Staphylococcus aureus* includes a potential mechanism involving cell wall disruption, leading to increased membrane permeability and eventual bacterial cell death. The stronger inhibition observed against Gram-positive bacteria compared to Gram-negative strains like *Pseudomonas aeruginosa* is due to differences in cell wall composition, with the thicker peptidoglycan layer in Gram-positive bacteria being more susceptible to interaction with STPS. Additionally, the presence of thiocyanate and sulfate ions contributes to antimicrobial action by interfering with bacterial metabolic processes and disrupting the ion homeostasis. The absence of significant inhibition against *Pseudomonas aeruginosa* indicates that the outer membrane of Gram-negative bacteria may act as a barrier, reducing STPS's efficacy. Further studies on

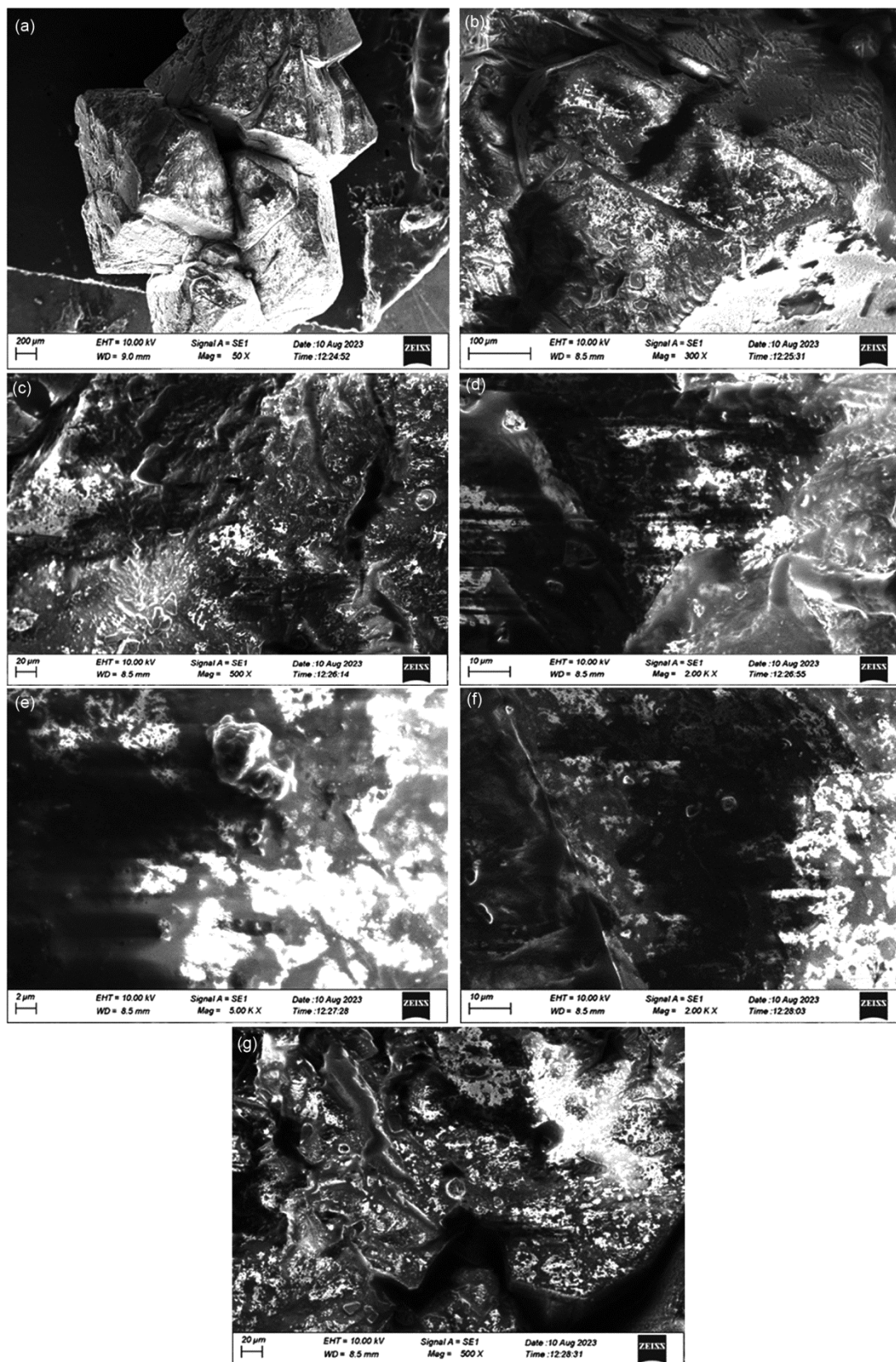


Fig. 6 — SEM images of various structures of STPS (a) Top View of the Crystal STPS (b-g) Cross-sectional view of the crystal STPS

S. No	Name of the test organism	Name of the test sample	Zone of inhibition (mm) SD ± Mean				PC
			500 µg/ml	250 µg/ml	100 µg/ml	50 µg/ml	
1.	<i>Staphylococcus aureus</i>	STPS	12.5±0.7071	4.25±0.35	3.25±0.3	0	15.25±0.35
2.	<i>Pseudomonas aeruginosa</i>	STPS	0	0	0	0	15.5±0.707

Name of the test organism	Name of the test sample	Zone of inhibition (mm) SD ± Mean				PC
		500 µg/ml	250 µg/ml	100 µg/ml	50 µg/ml	
<i>Candida albicans</i>	STPS	4.25±0.35	0	0	0	15.5±0.7

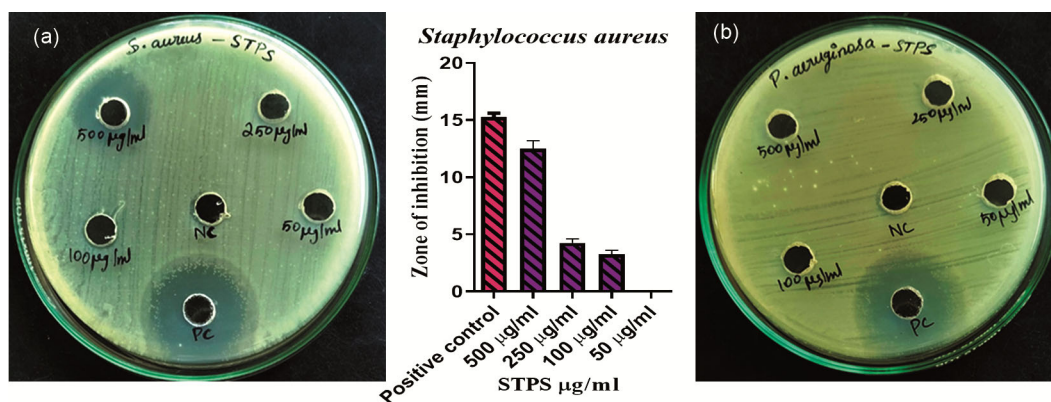


Fig. 7 — Effect of STPS in a) *Staphylococcus aureus*, and b) *Pseudomonas aeruginosa*

the structural and biochemical interactions of STPS with bacterial cells provide deeper insights into its precise antibacterial mechanism.

3.6.2 Anti-Fungal Activity

Effect of STPS crystal against *Candida albicans* is represented in Fig. 8. The antifungal activity of the recently synthesized STPS crystal against yeast strain *C. albicans* was determined using the diffusion method. The antifungal activity of substances was compared to nystatin, and the findings are summarized in Table 3. The results for STPS show that at 500 µg/ml, there is a zone of inhibition of 4.25±0.35 mm, whereas there is no inhibition found at lower dosages of 250 µg/ml, 100 µg/ml, and 50 µg/ml. The positive control (PC) nystatin has an inhibitory zone of 15.5±0.7 mm. The antifungal activity of STPS against *Candida albicans* at higher concentrations presents a potential mechanism involving disruption of the fungal cell membrane, through interference with ergosterol synthesis or ion imbalance. The lack of inhibition at lower doses indicates a concentration-dependent effect, where a threshold concentration is required to exert significant antifungal action. Compared to nystatin, STPS exhibits moderate efficacy, which is attributed to weaker membrane permeability effects or reduced binding affinity to fungal cell components. Further

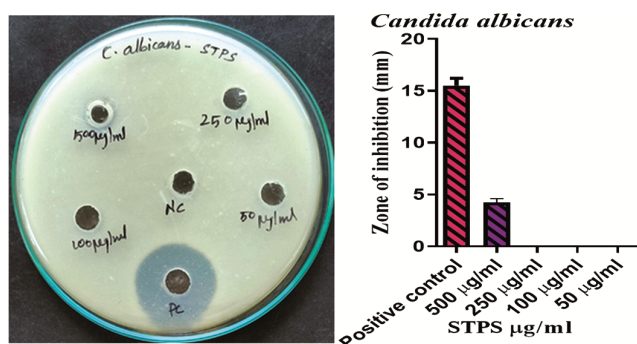


Fig. 8 — Effect of STPS crystal against *Candida albicans*

investigation into its interaction with fungal structures and metabolic pathways could help to enhance its antifungal potential.

Overall, the STPS single crystal is characterized using XRD, FTIR, UV-visible spectra, SEM, microhardness, and antimicrobial activity. The discovery of the best-quality crystal demonstrates its potential for use in a wide range of applications that require high-performance materials with superior structural and functional properties. The results showed that the STPS crystal's structure outperformed the previous KDP crystal in terms of quality. The antimicrobial activity results of STPS crystals demonstrate that STPS can be used in medical, environmental or industrial applications.

4 Conclusion

Developing a defect-free semi-organic crystal is crucial for achieving superior quality and enhanced performance in nonlinear optical applications. Sodium Thiocyanate Potassium Sulphate (STPS) has been synthesized using the slow evaporation process at an ambient temperature of 30°C, exhibiting superior stability and making it a reliable candidate for various optical and electro-optic applications. Its high transparency ensures effective light transmission, essential for photonic applications, while mechanical strength testing revealed a micro-hardness value of 30.01, indicating robustness and durability. The structural and chemical composition of STPS was analyzed using FTIR spectroscopy, confirming the presence of fundamental functional groups in the range of 400-4000 cm⁻¹. Further UV-Vis spectroscopy validated its optical properties, revealing a lower cut-off wavelength of around 250 nm, enhancing its potential for SHG and laser applications. The STPS crystal was examined under an SEM, which confirmed its stable structure across all layers. Notably, STPS exhibits strong antimicrobial activity, including both antibacterial and antifungal properties, with a significant zone of inhibition against *Staphylococcus aureus*, demonstrating superior antibacterial efficacy compared to conventional KDP crystals. This makes STPS highly suitable for biomedical applications, including antimicrobial coatings and pharmaceutical advancements, while its high optical quality and structural stability further support its use in precision optics and electro-optic modulation. However, challenges remain in optimizing growth conditions to produce larger, defect-free crystals, and enhancing its biocompatibility for direct medical applications requires further research and refinement. Addressing these challenges will improve its effectiveness in both optical and medicinal fields, making it an effective material for advanced technologies. With continued development, STPS significantly contributes to both photonics and biomedical engineering applications, paving the way for future innovations in these fields.

Applications of STPS Crystals

The STPS single crystal-synthesized in this study presents a range of potential applications due to its unique combination of structural and functional properties. These crystals, owing to their high purity and well-controlled growth, can be utilized in various fields including optoelectronics, nonlinear optics, and

materials science. Specifically, STPS crystals can be employed in the development of high-performance optical devices such as laser modulators, optical switches, and sensors, as well as in the fabrication of high-efficiency photovoltaic cells. The stability of the crystal structure also enhances its potential in electronics and photonics applications, where precise control over material properties is essential. Due to their semi-organic nature, STPS crystals are expected to exhibit excellent mechanical and electrical properties, making them suitable for advanced applications in sensor technologies and memory devices. Moreover, STPS crystals exhibit notable antibacterial properties, making them efficient usage for medicinal applications such as antimicrobial coatings for medical devices, wound dressings, and drug formulations to combat bacterial infections. Their efficacy against *Staphylococcus aureus* suggests potential use in preventing hospital-acquired infections, while their crucial antifungal activity indicates possible applications in antifungal treatments. Further optimization could enhance their biocompatibility and effectiveness, expanding their role in pharmaceutical and biomedical fields. Their potential use in these fields can be attributed to their ability to maintain high structural integrity under varied conditions, which is critical for their reliability in long-term applications.

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