

EXPLORING THE CHARACTERIZATION AND GROWTH OF ORGANIC AND SEMI-ORGANIC MATERIALS

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ABSTRACT

A new semi-organic nonlinear optical thiosemicarbazide cadmium acetate (TSCA) material has been synthesized. TSCA single crystals were grown from aqueous solution by slow evaporation method. The solubility of TSCA has been determined for various temperatures. The grown crystals were characterized by single crystal X-ray diffraction (XRD), FTIR, UV-Vis., thermal and second harmonic generation (SHG) analysis. Single crystal XRD study has been carried out to identify the lattice parameters. FTIR studies confirm the functional groups present in the grown crystal. Optical transmission studies have confirmed that the grown crystal is highly transparent. Thermogravimetric and differential thermal analyses reveal the good thermal stability of the material. The SHG conversion efficiency of TSCA was determined using Kurtz powder technique and found two times that of potassium dihydrogen orthophosphate (KDP).

Keywords: Growth from solution, Semi organic, Nonlinear optical crystal

INTRODUCTION

Organic materials have a wide range of properties and can be used in various applications, including telecommunications. With the development of novel nonlinear optical materials, it will be feasible to achieve a significantly stronger directed nonlinear optical field. Donor-acceptor compounds exhibit distinct variations in their dipole moments, excited state characteristics, and ground state features. It is worth noting that molecules with significant transition dipole moments can exhibit substantial second-order optical nonlinearities.

After reviewing the latest publications in the field, along with other articles on nonlinear optics (NLO), I have been inspired to conduct research on maleic acid and lithium sulphate monohydrate. Understanding the combination of lithium sulphate monohydrate and oxalate provides valuable insights into the use of semi-organic compounds in nonlinear optical (NLO) applications. Lithium sulphate monohydrate (LSMH) is an inorganic material that exhibits nonlinear optical (NLO) properties, which sets it apart from the organic maleic acid. When these two chemicals are combined, a remarkable semi-organic material is formed that exhibits enhanced nonlinear optical (NLO) capabilities. The primary objective of this study is to examine the suitability of two synthetic variations of lithium sulfate monohydrate for non-linear optical (NLO) purposes: lithium sulfate monohydrate with maleic acid (MLSMH) and lithium sulfate monohydrate (LSMH). In order to improve the field of photon-based transmission techniques, it's vital to identify new material with extraordinary optical characteristics. Scientists have made significant effort to develop materials with distinct features, like an extremely high threshold and a broad spectrum of transparency, In addition, ability to produce a high nonlinear coefficient. They have the potential to be used for the development in the field of

optical nonlinear (NLO) material with the capability of doubling frequencies is huge. Within the realm of nonlinear optics, semiorganic substances have attracted a great deal of focus. They are an advancement in the field of intensive optical nonlinearities. In the course of ionic bonds, an organic host and an inorganic component were bonded to create these materials. The variety of optical uses is extended by the possibilities of amino acid complexes that are made up of inorganic substances. Optic communication, computation information processing, storage of data on optical disks In addition, laser fusion reactions remote sensing using the light of lasers have a broad array of potential applications.

L-glutamic Acid is a remarkable NLO-related material due to its transparency to UV light, which makes it particularly suitable to match phase. L-Glutamic Acid plays an essential part in the operation of NLO. NLO apparatus. The chemical has an acidic carboxyl group its side chain, and has that it can accept and transfer ammonia. In the past we studied the development and examination of crystals made up of L-glutamic Acid when combined with various chemical halogens, including HCl L-glutamic acid and salts of halogen. In a recent study, Sathyalakshmi et al. studied the process of process of making and characterizing the hydrochloride l-glutamic. They studied both its unchanged structure and its association with various chemical compounds. Selvaraju et al. investigated the length of the period for induction in addition, size of metastable region within crystals of L-glutamic chloride. The study focused of crystals formed by the low temperature process of solution growth and also those that were created and

studied through sluggish Evaporation. The study of multiaxial growth of the L-glutamic chloride crystals, and an analysis of the comparative

LITERATURE REVIEW

Kai Xu [2022] Chalcone structures formed through structural alteration are a significant class of molecular organic crystals known for their valuable nonlinear optical characteristics (NLO). The study employed a technique that involved altering the structure and expanding the π -conjugation to create two unique chalcone compound crystals, namely 6MN3MPP (C₂₁H₁₈O₃, Pca21) and 6MN4MPP (C₂₁H₁₈O₃, Pn). The crystals lack symmetry in their structure. Using the provided data, gearbox spectra, and dielectric constant. In comparison to previously reported chalcone NLO crystals, the synthesised crystals exhibited superior crystal clarity ($\geq 70\%$). For a more precise understanding, let's delve into the power of SHG.

Zulfikar Noormansyah [2021] Finding a middle ground between ecological protection and economic feasibility in agriculture is the goal of organic rice growing. Environmental, social, and economic aspects are all taken into account. The transition from conventional to organic rice farming isn't without its practical and financial obstacles, however. To ease into it, think about using semi-organic agricultural practices. Comparing conventional, organic, and semi-organic farming from a technological, productional, and economic perspective is the overarching goal of this research. This study's overarching goal is to assess the potential of semi-organic agricultural practices as a stepping stone to fully organic rice production. In Priangan Timur, West Java Province, Indonesia, 75

farmers from different agricultural backgrounds (including organic, semi-organic, and non-organic farms) were surveyed for the research.

S.Devi [2020] A crystal measuring $7 \times 5 \times 3$ mm³ was successfully created through a slow evaporation method at room temperature from an aqueous solution. This crystal was later synthesised as a unique semi-organic material called potassium boro-oxalate (KBO), which has fascinating nonlinear optical properties. The single crystals are analysed to investigate Utilising advanced techniques, the crystal and molecular structure of KBO can be effectively solved. To further enhance accuracy, the SHELXL-2014 software incorporates the full-matrix least-square method for refinement purposes.

R. Manickam [2019] The LSZA single crystals were formed via a method of gradual evaporation. In addition to having semi-organic properties, these crystals exhibit nonlinear optical behaviour. The successful fabrication of a large crystal marked a key milestone after an astounding 47 days of diligent effort. The interatomic lengths were found to be 15.31 Å, 5.28 Å, and 10.84 Å, respectively, using a single crystal X-Ray diffractometer. These three angles, $\alpha = 90$ degrees, $\beta = 100$ degrees, and $\gamma = 100$ degrees, make up the crystal lattice vectors. Crystal unit cells have a volume of 807 cubic angstroms. The crystal's space group C indicates that its structure is monoclinic and non-centrosymmetric. In particular, the UV-Vis spectra show that the L-Serine Zinc Acetate crystals have excellent light transmission over the whole visible range.

Inorganic crystals

Ions are the predominant factor responsible for the cohesion of most

inorganic crystals. Producing organic compounds is often easier. Key characteristics of it include a very an unparalleled. Multiple fields of study are now investigating high-temperature oxides due to their potential use in electro-optics, piezoelectricity, and ferroelectricity, among other domains. Among the valuable crystals discovered, notable examples are LiNbO₃, LiNbO, KNbO₃, KDP, KTP, and b-Barium borate, along with other comparable crystals. These materials provide access to previously inaccessible regions of the spectrum that cannot be accessed by traditional optical crystals with nonlinear optical properties and standard laser sources.

Crystal Growth Techniques

The methods of growth are classified by the properties material that was used as starting point. By carefully evaporated solution it's possible to create distinct crystals. Imagine the amazing formation of crystals from state of vapour, but with the exacting control of conditions. It happens because the vapour gets supersaturated. By applying a scientific methodology melt expansion is one of the most popular methods to create materials that have an even melting pattern. This is because it permits fast growth rates and reaches astonishing levels of crystalline perfectness. The growth of crystals from melt is a common method, and is often thought of as being more efficient than solutions and vapour techniques.

Crystal Growth Process

A supersaturated solution occurs when there is an excess amount of solute in a solution compared to its normal capacity to dissolve at a specific temperature. A small nucleus is formed in the initial stage. Phase two involves the gradual expansion of this nucleus to create the crystal and its

distinct shape. Understanding the energy loss that occurs during compound solidification is a key concept in this field. To truly delve into the intricacies of crystal growth, one must possess a profound comprehension of the nucleation process as the fundamental starting point.

Crystal growth by chemical reaction method:

Compounds that are insoluble and break down before they reach their melting point or temperature are excellent candidates for the chemical reaction method of growth. Two reactants that can dissolve in water are meticulously arranged in layers on top of a gel using this technique. A solid byproduct is formed when carefully chosen chemicals undergo a controlled reaction, leading to the creation of a crystal that is either completely insoluble or very slightly soluble. When growing crystals in a gel, the reaction method is frequently employed. One application of this technology involves the production of monocrystals of compounds that have limited solubility in water. This enables the substances to dissolve right before they approach their melting point.

Semi-Organic Crystals

Recently, there's been an rise in interest in studying semi-organic crystals because of the distinct properties and their the reliability of their physiochemical capabilities. This is essential to the advancement of new technologies. In addition, expanding our knowledge of. Making use of more sophisticated crystals technologically offers numerous benefits which include the ease of creating three-dimensional semi-organic crystals. Utilizing this tool makes cutting and polishing samples significantly simpler. Semi-organic crystals have a variety of extraordinary properties, which include

their chemical flexibility, remarkable mechanical hardness, resistance damaging lasers, their low angle sensitivities, In addition, impressive the nonlinear optical (NLO) capabilities.

METHODOLOGY

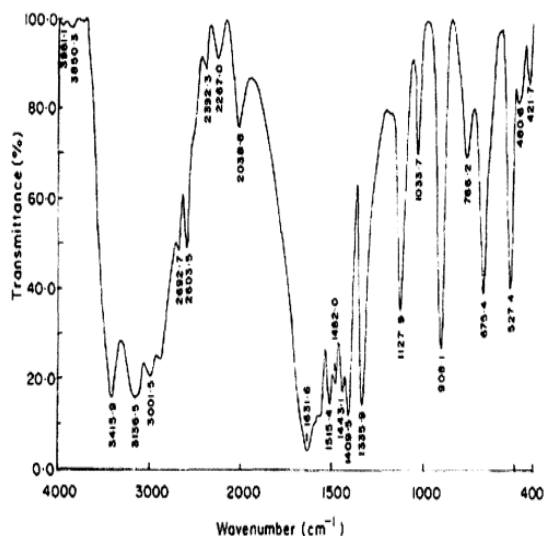
Growth of crystals is extremely important within realm of engineering and materials science. Purchasing crystals with the right dimensions and quality is crucial. Crystals like these are vital for collecting basic data developing practical tools, such integrated circuits and detectors which have multiple functions. As a physicist, I am fascinated by the ever-growing necessity for crystals in this technological age incredible technological advancements that are being made through research. Scientists have dedicated nearly 100 years to studying various methods of crystal formation. They have been captivating world for a long time. Knowing essential characteristics of crystals and other materials primary objective for crystal formation. A thorough understanding principle of science that defines properties of crystals is vital to making crystals that have their intended size and quality.

RESULTS

GLC crystal and FT-IR spectral analysis

Using a Perkin Elmer infrared probe, the Fourier transform infrared spectra of the GLC crystal were acquired under standard conditions. Spectra in the 4000-400 cm^{-1} range were obtained using the KBr pellet technique. Here is the spectrum displayed convenience. The bands observed at 675 and 908 cm^{-1} could be associated with carboxylate groups, while the peaks at 1482 and 1127 cm^{-1} indicate the presence of NH_3 groups. In glycine lithium chloride, the carboxylic acid group is

represented by a carboxylate ion, while the amino group is represented by an ammonium ion. When the C-N bond is extended, it undergoes vibrations, resulting in an absorption peak at 1033 cm⁻¹. The absorption peak observed at 1631 cm⁻¹ is attributed to the asymmetric stretching vibration of the C=O bond. The frequencies and values for pure glycine are displayed in Table 1. glycine are displayed in Table 1.



Graph 1: FTIR spectrum of glycine lithium chloride

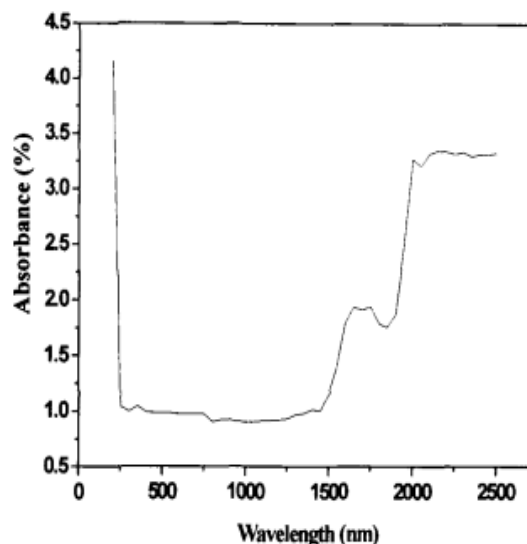
Table 1 A graph displaying the comparative vibrational frequencies (in cm⁻¹) of glycine and GLC.

FTIR glycine	FTIR GLC	Band assignment
3419	3415	(O-H) Asymmetric stretching
3282	3136	(O-H) Asymmetric stretching
1593	1631	(O-H) Asymmetric stretching
1502	1515	CH ₂ stretching vibration
	1482	COO ⁻ Asymmetric stretching
	1443	COO ⁻ Asymmetric stretching
1407	1409	NH ₃ ⁺ Scissoring vibration
1345	1335	NH ₃ ⁺ Scissoring vibration
1112	1127	NH ₃ Symmetric stretching
1034	1033	NH ₃ Symmetric stretching

892	908	stretching
766	766	CH ₂ deformation
690	675	scissoring
607	527	COO ⁻ Symmetric stretching
		CH ₂ wagging
		NH ₃ Rocking
		C-N Asymmetric stretching
		CH ₂ Rocking
		NH ₂ Rocking
		COO ⁻ scissoring
		NH ₃ twisting

UV - vis- NIR spectral studies

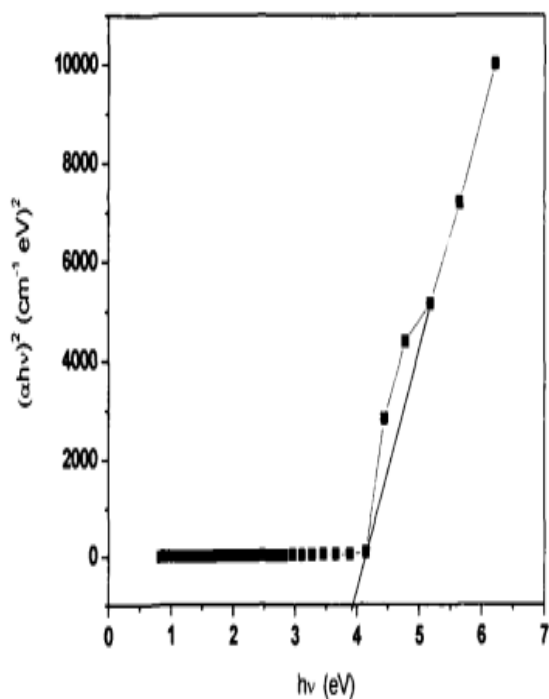
To obtain the absorption spectra, we measured the light transmission of a 3mm thick clear single crystal (Graph 2) using a Varian Cary 5E UV-vis-NIR spectrophotometer, across a wavelength range of 230-2500 nm. This crystal is ideal for frequency doubling due to its lower cutoff at 230 nm and its transparency across the entire visible spectrum. Here is the formula for the optical absorption coefficient, denoted as "a":



Graph 2: UV -vis- NIR absorbance spectrum of GLC

The symbol used to represent the energy gap is Eg. Understanding the optical band

gap (E_g) is crucial in determining the extent of light absorption in the ultraviolet (UV) spectrum. Understanding the relationship between the band gap, the energies of incoming photons ($h\nu$), and the optical absorption coefficient (α) is crucial. Graph 5.6 illustrates the examination of the correlation between the photon energy ($h\nu$) and the square of the product of the absorption coefficient (α) in order to determine the band gap energy. By extending the linear component of the curve until there is no absorption, we can determine the optical band gap value (3.9eV) for the GLC single crystal.



Graph 3: $(\alpha h\nu)^2$ vs $h\nu$ plots of GLC single crystal

CONCLUSION

Utilizing techniques such as XRD, FTIR, and NMR, we successfully characterized the crystal structures of the synthesized organic and semi-organic compounds. This in-depth analysis allowed us to determine crucial crystallographic parameters and identify functional groups, providing a comprehensive understanding of the

materials' compositions. SEM studies have enabled us to observe the surface morphology of the crystals, shedding light on their physical features and growth patterns. This aspect is crucial for understanding the relationship between crystal structure and morphology, influencing the properties and potential applications of these materials. Through systematic experiments varying parameters such as temperature, solvent composition, and concentration, we optimized the growth conditions for the crystals. This optimization is essential for achieving well-defined crystals with improved properties, in addition, for understanding the kinetics of nucleation and crystal growth.

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