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Research Note

Study of crystalline growth, structural characteristics, optical behavior, thermo and dielectric properties of isoniazid single crystal

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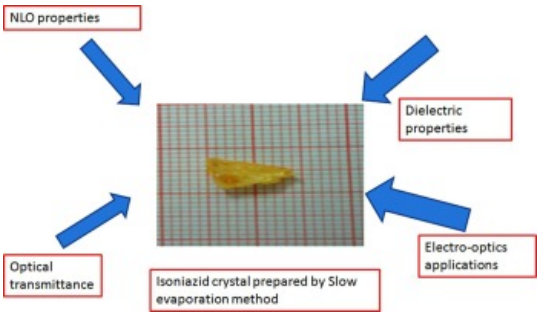
Abstract

In this study, isoniazid single crystals were synthesized using solvent mediated followed by slow solvent evaporation techniques for testing the electro-optics application. Powder XRD analysis was used to record several scattering peaks for the obtained grown material, and the presence of scattering peak positions results correlated to the reported scattering peak position of the above title compound's orthorhombic crystal structure. Further, the single crystal XRD analysis confirmed the orthorhombic crystal system based on the obtained lattice parameters of synthesized crystal. The grown crystal was scanned using an FT-IR analysis, and its chemically attached functional groups were detected in the spectrum. According to UV–visible studies, isoniazid has a transmittance value of more than 90%. In addition, the transmittance behavior of the grown compound changed significantly depending on its wavelength. The nonlinear optical property study of the grown crystal was characterized, and the results of the second harmonic generation efficiency values correlate with those of standard reference crystal. Thermal stability and melting temperature of the grown crystal were investigated using TG/DTA studies. The temperature vs weight loss plot revealed weight loss in the temperature range of 225°C to 400°C for the grown crystal. Using differential thermo gravimetric analysis (DTA), the melting temperature of the synthesized crystal was determined to be 170°C. The dielectric constant and dielectric loss responses of grown isoniazid crystals are found to be less at high frequencies and increase exponentially at low frequencies due to the presence of polarization effects.

Graphical abstract



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Introduction

Many researchers have focused in recent years on the various types of single crystal developed using different techniques for investigating the suitability of multifunctional based devices like non-linear optical and electro-optics modulation based devices; frequency shifting, optical switching, photonic devices, laser frequency conversion devices, and optical data storage, among others [1], [2], [3], [4], [5], [6], [7]. The above-mentioned multifunctional devices necessitate high optical transparency, good transmittance in the visible region, a larger optical band gap value, and good dielectric constant and dielectric loss characteristics. Further, developing such non-linear optical (NLO) activity and electro-optical characteristics in a single crystal is a difficult task in research laboratory. Isoniazid crystals and derivate compounds have been grown using different techniques, and the grown crystals have been analyzed by various instrumentation methods [8], [9], [10]. Few researchers have investigated the structural, vibrational and density functional theory (DFT) studies of isoniazid crystals and derivatives compound [1], [8], [9], [10]. In addition, the aforementioned isoniazid compounds have been tested in biomedical applications, specifically as antitubercular drugs in tuberculosis disease [8].

The aim of this work is to synthesize isoniazid single crystals using solvent-mediated followed by slow solvent evaporation techniques, and then subject the grown crystal to NLO and dielectric applications.

Section snippets

Experimental

The flow chart in Fig. 1 depicts the growing step of isoniazid crystals.

Various concentrations (15, 18, 21, 24, and 27 g) of isoniazid salt were dispersed in 100 mL of distilled water at various temperatures (25 °C to 55 °C) while stirring, and the solubility results are displayed in Fig. 2. The solubility plots clearly show that as the temperature increased from 27.5 °C to 52.5 °C, a higher concentration of isoniazid salt was dissolved, and as a result, the salt gradually became soluble in…

Results and discussion

The powder XRD analysis was used to record the diffraction angles of the grown isoniazid crystal from 10° to 60°, as shown in Fig. 4. When the diffraction angle position and corresponding diffraction peaks of the grown crystals were compared to the reported work [11], [12], [13], it was confirmed that the grown crystal was the formation of the isoniazid compound. The grown isoniazid compound's X-ray diffraction peaks and corresponding diffraction planes were indexed (CCDC No: 847197). The sharp …

Conclusion

A single crystal of isoniazid material was successfully grown using the slow evaporation technique. Various concentrations of isoniazid salt were dispersed in distilled water under magnetic stirring at different temperatures, and the saturation solution of isoniazid salt was determined using a solubility test. The observed strong diffraction peaks from the as-grown crystal's XRD pattern and lattice constant, which are closely matched with the reported XRD pattern and unit cell parameters of the …

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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References (23)

M. Buvaneswari *et al.*
Suresh Sagadevan, analysis and thermodynamic properties of vanillin isonicotinic hydrazide single crystal Synthesis, growth, structural, spectroscopic, optical, thermal, DFT, HOMO-LUMO, MEP, NBO
J. Mol. Struct. (2021)

M.I. Baig *et al.*
Influence of tartaric acid on linear-nonlinear optical and electrical properties of KH_2PO_4 crystal
Optic. Mater. (2017)

S.P. Ramteke *et al.*
, Optimizing growth, linear and 3rd order nonlinear optical traits of potassium aluminium sulfate (KAS) crystal by tuning pH for photonic device applications
Inorg. Chem. Commun. (2022)

M. Cocu *et al.*
SergiuShova, Olga Ciobanica, VictoriaGutium, Paulina Bourosh, Synthesis and structure of new mononuclear octahedral cobalt(III) dioximates derived from isonicotinic hydrazide
J. Mol. Struct. (2014)

M. Pocrnic *et al.*
SnežanaMiljanic, Zeljka Soldin, Ana Budimir, Nives Galic, Gallium(III) complexes of aroylhydrazones derived from nicotinic acid hydrazide in solid state and in solution
J. Mol. Struct. (2021)

P. Lalitha *et al.*
Sugumari Vallinayagam, Kaushik Pal, Growth dynamics and spectroscopic characterization strategies of 'L-proline' doped potassium hydrogen phthalate single crystal structural avenue
J. Mol. Struct. (2022)

M.I. Baig *et al.*
Exploring impact of Zn^{2+} on laser induced optical and electrical traits of KH_2PO_4 crystal for NLO device applications
Optik. (2021)

L.R. Keerthi *et al.*
Investigation on the growth, optical, electrical, thermal and third order NLO properties of 2-(4-methlybenzylidene) malononitrile (MBM) single crystal

Optic. Mater. (2020)

M.I. Baig *et al.*
Comparative analysis of pristine and Cd^{2+} influenced potassium acid phthalate single crystal for photonic device applications
Optik. (2020)

M. Anis *et al.*
Exploring remarkable impact of thiourea in enhancing the performance of $NH_4H_2PO_4$ single crystal for photonic device applications
Mater. Chem. Phy. (2020)

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Cited by (4)

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