

Study of Nonlinear Optical Properties of Sodium Molybdate Dihydrate Doped Hippuric Acid Single Crystal

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STUDY OF NONLINEAR OPTICAL PROPERTIES OF SODIUM MOLYBDATE DIHYDRATE DOPED HIPPURIC ACID SINGLE CRYSTAL

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ABSTRACT

The NLO single crystal organic Hippuric Acid doped with inorganic Sodium molybdate dihydrate (HS) was synthesised and grown from methanol solvent by the slow evaporation method at room temperature and also pure hippuric Acid (HA) single crystal was compared with it. SCXRD indicates that the product crystallized as HS with an orthorhombic system with lattice in the space group $P2_12_12_1$ and possessed unit cell dimensions $a, b, c = 8.876 \text{ \AA}, 10.514 \text{ \AA} \text{ \& } 9.037 \text{ \AA}$ and $V = 843.2 \text{ \AA}^3$ respectively. PXRD also confirms the crystalline nature. Fourier transform infrared (FTIR) analysis confirms the functional groups. The UV–Vis–NIR spectrum of HS was taken, which indicated that the transparency of HS is relatively high in the visible and near-infrared (NIR) wavelength region with a sharp cut-off wavelength at 318 nm. Thermal stability of the crystal has been studied using TG–DTA upto 220°C and also dielectric properties have been investigated. The laser damage threshold on crystal surface is carried out using in 1064 nm Nd:YAG laser and the value is obtained to be 3.13 GW/cm². The HS crystal shows that SHG efficiency is 0.84 times that of KDP when measured using Nd:YAG laser source which illuminated the SHG measurements. The results of the structural, optical, thermal, electrical and NLO study indicate that the HS single crystal is a potential candidate for optoelectronic and photonic devices applications.

Keywords: Single crystal growth, optical properties, TG-DTA, dielectric studies, nonlinear optics.

1 Introduction

Nonlinear optics (NLO) is an active and rapidly developing field of investigation since many years because of its various applications in laser technology, well suited for optical data storage and very useful in optical communication, electro-optical modulation as well as frequency conversion. The nonlinear optical responses of a material are greatly determined by its structural purity and physicochemical properties. Especially second-order NLO materials have been focused a lot on due to the tuneable radiation generation in region of UV, as well as their uses in parametric amplification and optical switching [1].

Eventhough there are advancement in various crystal growth methods, the slow evaporation solution method is adapted since it has control supersaturation and nucleation depth and has enabled high quality single crystal growth. Organic NLO materials have both large nonlinear optical coefficients and structural flexibility. Unfortunately, the practical realization of these materials is often compromised by poor mechanical strength, limited thermal stability, and low laser damage thresholds [2]. However, inorganic materials tend to be mechanically rigid and thermally stable, yet commonly suffer from weak NLO effects that originate from limited π -electron delocalization [3].

In order to overcome these deficiencies, the development of organic doped with inorganic materials through the combination of organic and inorganic components have been investigated. Such materials will process advantage of the high nonlinear optical properties of organic constituents as well as the good thermal, mechanical, and chemical stability of inorganic components [4-6].

In this context, organic doped with inorganic crystals typically exhibit large optical transparency, high laser-damage thresholds, and excellent physicochemical stability, which are important for photonic and optoelectronic applications. Hippuric acid is an

amide of benzoic acid that bears both carboxylic and amine functional groups; this chemical feature allows hippuric acid to form a highly intermolecular hydrogen-bonded system, enabling the crystallization of sufficiently non-centrosymmetric crystal structures while suppressing NIR blackening processes. Sodium molybdate dihydrate, an inorganic molecule is well known for its excellent thermal stability and can enhance structural integrity by forming a metal–oxygen bridged network. The combination of these two components is therefore expected to yield a semi-organic material with improved stability and desirable nonlinear optical response [7-10].

Despite extensive investigations on various NLO crystals, the combination of hippuric acid doped with sodium molybdate dihydrate with the molecular formula $C_9H_9NO_3$ has not been reported in the literature so far. In particular, no detailed studies are available on the crystal growth and comprehensive physicochemical characterization of this semi-organic system. This absence of prior reports clearly indicates a research gap and motivates the exploration of this new material. In this context, the present work focuses on the synthesis, growth, and detailed characterization of a novel organic doped with inorganic crystal using the slow evaporation solution technique. The grown crystal HS has been subjected to structural, optical, thermal, dielectric, mechanical, and nonlinear optical investigations to evaluate its potential for advanced photonic device applications [11-13].

2 Experimental work

The slow evaporation solution growth method was used to grow the HS crystals. Sodium molybdate dihydrate and hippuric acid were employed as starting materials without further purification. A stoichiometric mixture of 0.1 mol sodium molybdate dihydrate and 1 mol hippuric acid was dissolved at room temperature in methanol solvent. Since, both the starting materials are moderately soluble in methanol allowing for efficient supersaturation and controlled crystal nucleation upon cooling. The resulting solution was magnetically stirred for 24 h to obtain a clear and homogeneous solution and was filtered through Whatman filter paper to remove insoluble impurities. The filtered solution was transferred to a clean crystallization vessel which was covered with

a perforated sheet for the slow evaporation of solvent under dust free ambient conditions [14-15]. After 2 days, nucleation in the mother liquor was observed and after 7 days of growth the HS single crystals with dimensions (9 x 5 x 1) mm were obtained as shown in Fig 1. For comparison, pure hippuric acid (HA) crystals were also grown separately using a similar slow evaporation process. The obtained HS crystals were transparent, well-faceted, making them suitable for further structural and optical studies.

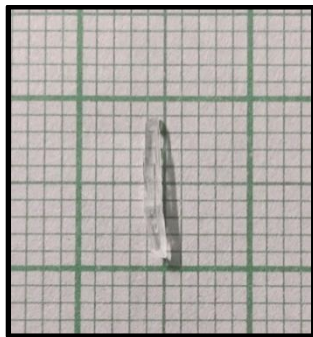


Fig 1 The picture of grown hippuric acid doped with sodium molybdate dihydrate (HS) single crystal

2.1 Characterization methods

For the grown single crystal, various characterization techniques were employed. Single-crystal X-ray diffraction data were collected at room temperature using a Bruker APEX4 diffractometer with Mo K α ($\lambda = 0.71073 \text{ \AA}$) radiation. PXRD patterns were obtained with a PANalytical X-ray diffractometer in the range of angle $10^\circ - 80^\circ$. FT-IR spectrum was performed on Shimadzu IR Affinity spectrometer (Japan). The linear optical characteristics were measured on a PerkinElmer Lambda 25 spectrophotometer, and the thermal stability behaviour was explored using a PerkinElmer Diamond STA 600 instrument. An LCR meter was used to perform dielectric measurements in a frequency range for varying temperature. The LDT was examined for 1064 nm wavelength with a Q-switched Nd:YAG laser. SHG efficiency measurements via Kurtz–Perry powder method [16].

3 Results and discussions

3.1 Single crystal X-ray diffraction (SXRD) study

The grown HS crystal was subjected for single-crystal X-ray diffraction (SCXRD) analysis using Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$), in order to assure the cell parameters, system, volume and space group of the unit cell. The evaluated parameters are presented in Table 1. The obtained values for HS show slight variations when compared with those of pure HA, confirming the incorporation of the dopant into the host lattice.

Table 1 Single-crystal XRD data of the grown crystal HS

Crystal data	Reported [17]	Present work
Empirical formula	$C_9H_9NO_3$	$C_9H_9NO_3$
Molecular weight	179.18 g/mol	179.18 g/mol
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
Unit cell dimension	$a = 8.862 \text{ \AA}$ $b = 10.594 \text{ \AA}$ $c = 9.116 \text{ \AA}$ $\alpha = \beta = \gamma = 90^\circ$	$a = 8.876 \text{ \AA}$ $b = 10.516 \text{ \AA}$ $c = 9.036 \text{ \AA}$ $\alpha = \beta = \gamma = 90^\circ$
Volume ($\text{\AA}^3$)	855.9	843.2

3.2 Powder X-ray diffractometer study

Fig 2 shows the powder X-ray diffraction patterns recorded for pure and grown crystals. Comparison of the grown crystals with the pure sample indicates their crystalline nature along with phase purity and structural stability. Subtle changes, such as slight peak shifts arising from lattice deformation or crystallite size variations due to sodium molybdate dihydrate incorporation and variations in relative peak intensities from atomic

scattering factor modifications or minor structural disorder, indicate the successful doping of the host lattice [18-19].

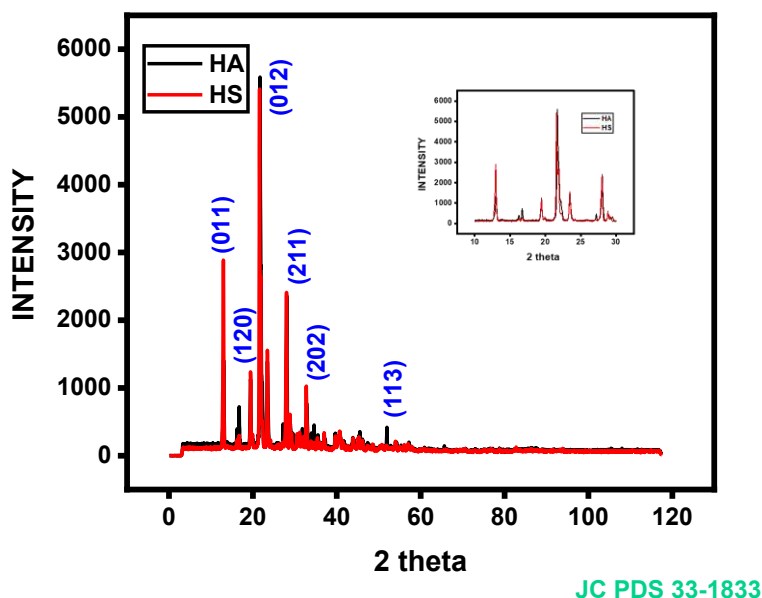


Fig 2 Powder XRD pattern of HA and HS crystals

3.3 FT-IR analysis

The FTIR spectral analysis of the grown crystals was performed to determine the functional groups and their vibrational modes. The spectra were recorded using the KBr pellet method in the range of 4000–450 cm^{-1} . The recorded spectra for HA and HS are presented in fig. 3 and 4, respectively [20-22].

The existence of a definitive chemical interaction between the organic and inorganic components was established via FTIR analysis. The addition of the inorganic sodium molybdate into the hippuric acid matrix causes shifts in the primary vibrational modes of the organic host material as shown in Table 2. Specifically, the N-H stretching vibration shifts from 3328 cm^{-1} to 3331 cm^{-1} , demonstrating a significant modification of the amide hydrogen-bonding environment. Similarly, the aromatic C-H stretching vibration shifts downward from 3080 cm^{-1} to 3051 cm^{-1} . Most importantly, the C=O carbonyl stretching

vibration shifts from 1745 cm^{-1} to 1740 cm^{-1} , which confirms the direct coordination of the oxygen lone pairs with the inorganic molybdenum centers. These combined spectral shifts provide definitive evidence of chemical bonding between the organic and the inorganic components [23-24].

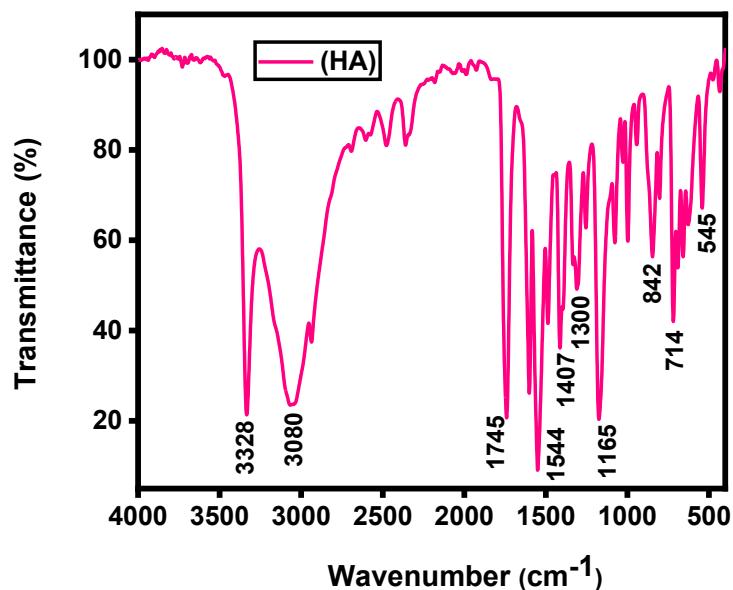


Fig 3 FT-IR spectrum of HA crystal

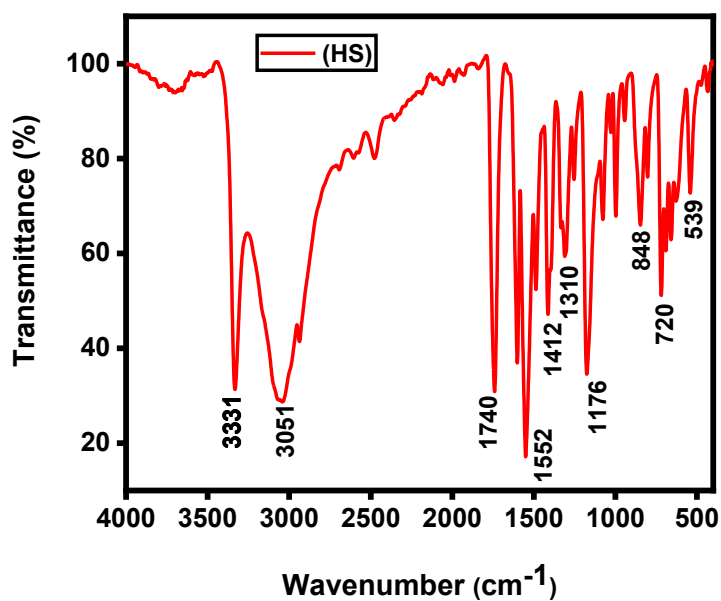


Fig 4 FT-IR spectrum of HS crystal

The observed spectral changes confirm the successful incorporation of HA into the host matrix, and the corresponding vibrational assignments are presented in Table 2.

Table 2 Functional group assignments from FT-IR spectra

Wavenumber (Cm ⁻¹)		Functional group assignments
(HA)	(HS)	
3328	3331	N – H Stretching
3080	3051	C – H Stretching
1745	1740	C = O Stretching
1544	1552	N–H Bending
1407	1412	C – C Stretching
1165	1176	C – O Stretching
842	848	C – H Bending
714	720	C – C Bending

3.4 Energy Dispersive X – Ray Analysis (EDX)

Fig 5 represents the elemental spectra of the HS sample, the spectral reconfirm the successful incorporation of the Na and Mo elements in Hippuric acid, the Table 3 represents a composition and % of elements present in the HS sample [25].

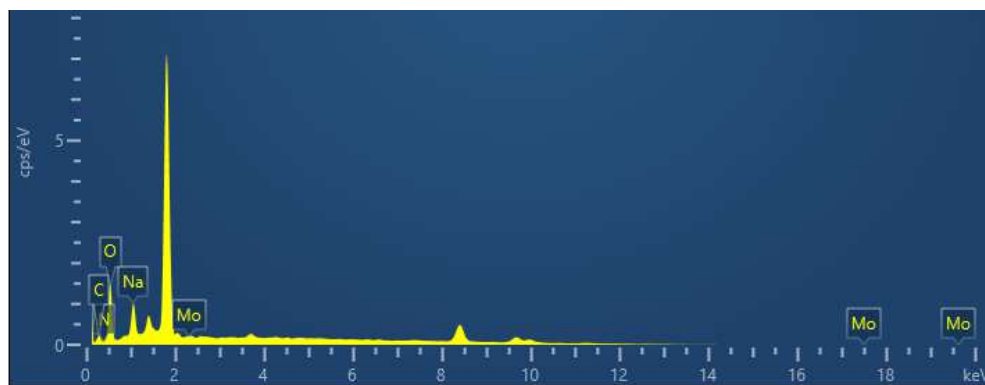


Fig 5 EDX analysis of HS

Table 3 Composition and % of element present in the sample by EDX analysis

Element	Series	Weight %	Atomic %	Weight % Sigma
C	K series	18.58	25.49	4.09
N	K series	0.41	0.49	3.56
O	K series	56.29	57.99	3.75
Na	K series	21.60	15.49	1.72
Mo	L series	3.12	0.54	1.84

3.4 Optical studies

UV–Vis–NIR spectroscopic technique was used to characterize the optical properties of pure and doped crystals of size (5 x 1 x1) mm in the wavelength region of 200–800 nm. Both samples can be considered suitable for nonlinear optical applications due to strong absorption in the UV region accompanied by very little interference in the visible region. The HA crystal has a very sharp absorption edge in the deep UV region; however, the HS crystal shows a slight red shift.

For this purpose, the HS crystal displayed significantly diminished absorption in the ultraviolet region. It is also noted that the lower cut-off wavelength of the HS crystal is 318 nm; therefore, the doped crystal still maintains good transmittance in the visible and near-IR region [26-27]. The red shift of the absorption edge upon doping indicates alteration of the electronic environment due to Na₂MoO₄ incorporation into hippuric acid. The obtained absorption spectrum for the grown crystal is presented in fig.6.

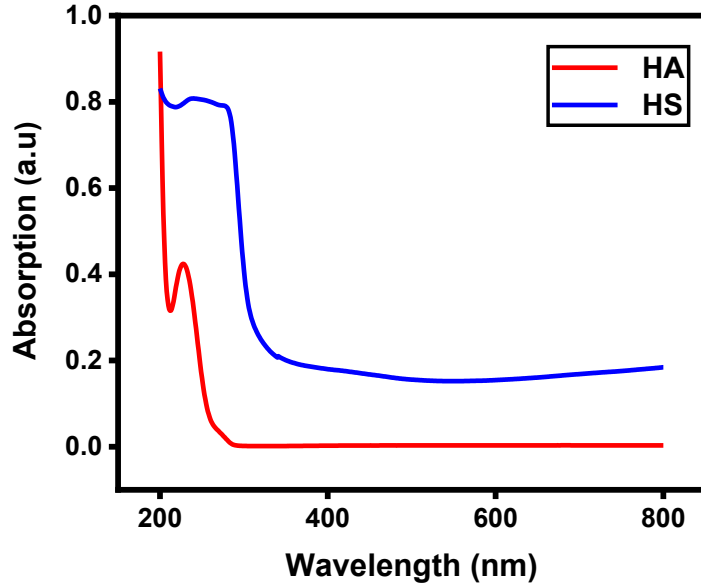


Fig 6 Absorption spectrum of HA and HS crystals

The optical absorption coefficient (α) was determined using the relation:

$$\alpha = \frac{2.3026}{t} \log_{10} \frac{100}{T} \quad (1)$$

where T is transmittance (%) and t is thickness (1mm) of the crystal.

The optical bandgap energy (E_g) of the grown crystal was calculated from the Tauc's plot using the equation:

$$\alpha h\nu = A(h\nu - E_g)^2 \quad (2)$$

Here, E_g is optical bandgap energy, A is an arbitrary constant, α is the absorption coefficient, and $h\nu$ is incident photon energy.

The band gap was calculated using Tauc's relation by plotting $(\alpha h\nu)^2$ against the photon energy ($h\nu$). The band gap values were calculated from the extrapolation of the linear region of the curve 5.18 eV for HA and 4.13 eV for HS shown in Fig 7.

The reduction in band gap upon sodium molybdate incorporation is observed since foreign atoms (sodium molybdate) introduce intermediate impurity states within the forbidden band gap. These defect states alter the host's (Hippuric acid) electronic structure, causing an upward shift of the valence band edge, a downward shift of the conduction band edge [28,29]. The narrowing of the band gap helps to better understand the greater electronic polarizability in the HS crystal and the possible generation of localized energy states after doping, which may promote optical applications as well.

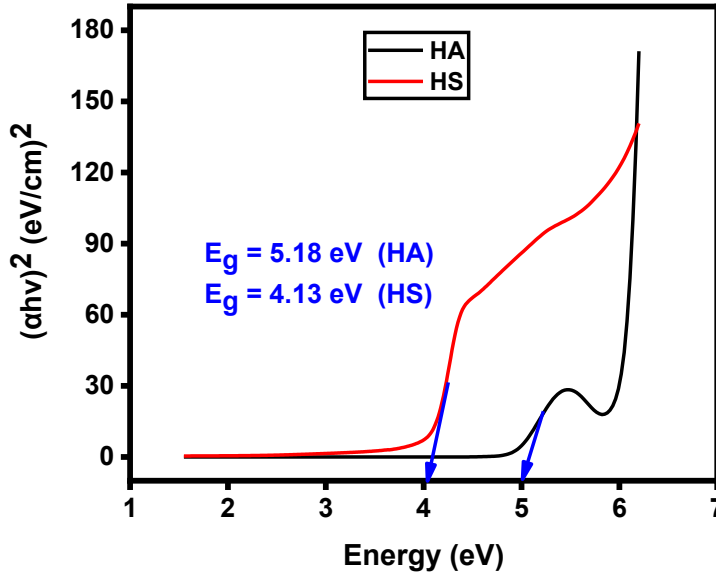


Fig 7 Tauc's plot of HA and HS crystals

Data from the absorption analyses were used to calculate the extinction coefficient (k). The extinction coefficient of the HS crystal in the visible region is low, confirming good optical transmittance and it is shown in Fig 8. The small change of k in the UV range indicates the intrinsic band gap.

$$K = \frac{\alpha\lambda}{4\pi}. \quad (3)$$

The refractive index (n) was evaluated as a function of wavelength.

$$n = -(R + 1) \pm \frac{2\sqrt{R}}{(R-1)} \quad (4)$$

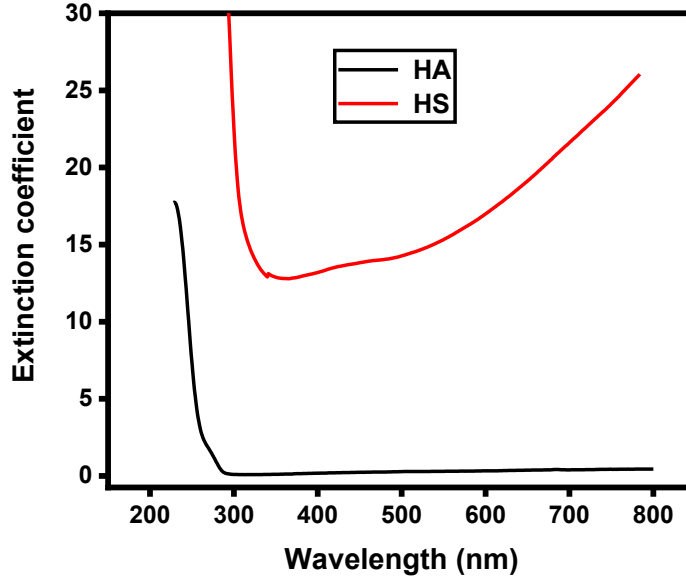


Fig 8 The plot of extinction coefficient vs. wavelength

Fig 9 represents the variation of the refractive index (n) with wavelength. The HS crystal shows normal dispersion behavior, where the refractive index decreases rapidly near the absorption edge and then tends to level off at higher wavelengths. The low refractive index in the visible region, in spite of the high optical homogeneity, suggests small reflection losses and therefore potential suitability for photonic and optoelectronic applications.

Optical studies confirm that sodium molybdate dihydrate doping of hippuric acid enhances the optical features while maintaining excellent transparency. The HS crystal illustrates its potential for nonlinear optical device applications due to its wide band gap, low extinction coefficient, and stable refractive index [30-32].

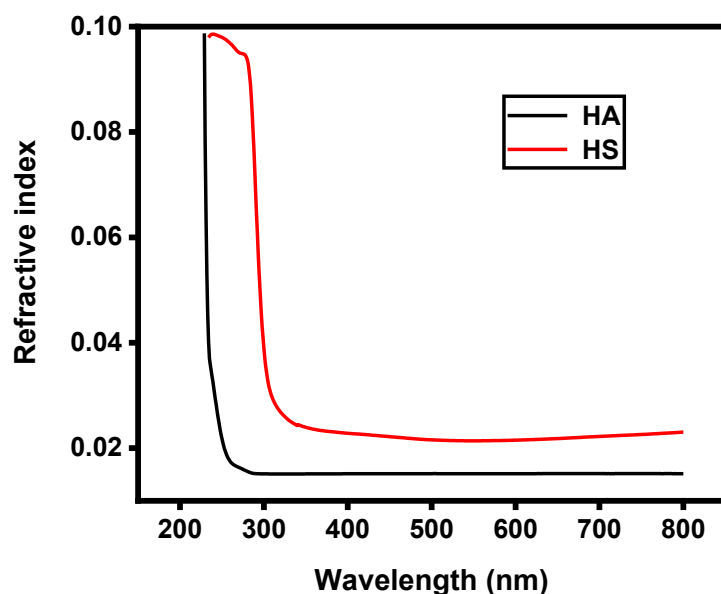


Fig 9 The plot of Linear refractive index with wavelength

3.6 Thermal studies

The thermal stability and decomposition behavior of hippuric acid doped with sodium molybdate dihydrate (HS) crystal was studied using thermogravimetric and differential thermal analyses (TGA/DTA) and compared with the pure hippuric acid thermal analysis. Measurements were carried out at a heating rate of $20\text{ }^{\circ}\text{C min}^{-1}$ under an argon atmosphere in the temperature range of $35\text{--}900\text{ }^{\circ}\text{C}$, and the corresponding TGA–DTA curves are presented in Fig. 10(a-b). The TGA curves indicate that the material undergoes multi-stage thermal decomposition.

On analyzing the HS single crystal, In the first stage, observed between $35\text{ }^{\circ}\text{C}$ and $200\text{ }^{\circ}\text{C}$, a small weight loss of about 3–5% is observed. This early weight loss may be due to the elimination of physically adsorbed moisture and volatile impurities in the crystal lattice. The second decomposition stage (in the temperature range of $200\text{ }^{\circ}\text{C}$ – $350\text{ }^{\circ}\text{C}$) was observed to be the major weight loss region [33–34].

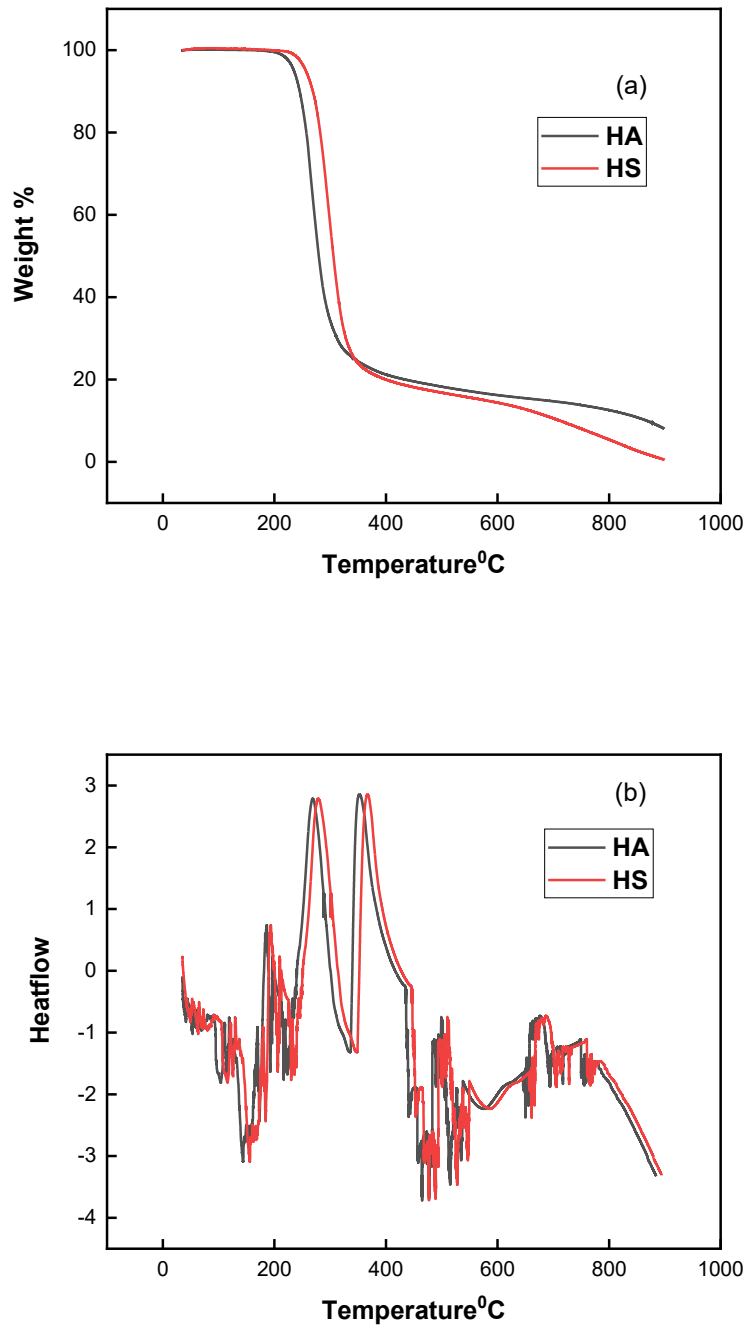


Fig 10 (a) TGA (b) DTA curves of HS crystal

In this temperature range, the TG curve shows a sudden decrease in mass due to thermal degradation of the organic component hippuric acid and partial decomposition

of the molecular skeleton of the doped crystal. The third stage from 350 °C to 900 °C shows a slow weight loss, representing gradual carbonization of residuals and the formation of stable inorganic phases. This material is further converted into a stable ash-like residue beyond this region. A same kind of weight loss was observed for the HA pure samples also but the thermal stability has been increased by 30-40°C by the HS sample.

The DTA curve shows a clear endothermic peak at ~220–230 °C, which corresponds to the melting of the crystal and the subsequent onset of decomposition. Further weak thermal events present at higher temperatures are related to sequential degradation of the material. Thus, it may be concluded from the TG–DTA results that the HS crystal is thermally stable until 220 °C about 30-40°C was thermal stability of the hippuric acid was improved due to incorporation of sodium molybdate. The moderate level of thermal stability observed is favorable for NLO applications, suggesting that this grown crystal has good thermal resistance [35-36].

3.7 Dielectric analysis

Dielectric spectra for single crystals of pure hippuric acid (HA) and hippuric acid doped with sodium molybdate dihydrate (HS) in a broad frequency range over the temperatures range of 40–100 °C are presented, leading to conclusions about dielectric behaviour and polarization mechanisms relevant in the context of potential electro-optical applications of such grown crystals. Before measurements were carried out, to guarantee enough electrical contact between the electrodes, two opposite faces of the single crystals were uniformly polished and coated with silver paste [37-39].

The variation of dielectric constant and dielectric loss with logarithmic frequency is shown in Fig 11–14. The dielectric dispersion behaviour of both crystals is normal. For all measured temperatures, ϵ' decreases with increasing frequency in each case. Factors contributing to the observed relatively large dielectric constant at low frequencies include space-charge, dipolar, ionic and electronic polarizations. At higher

frequencies, the relaxation of space-charge and dipolar components cannot keep pace with rapid reversals of the electric field so that ϵ' progressively decreases.

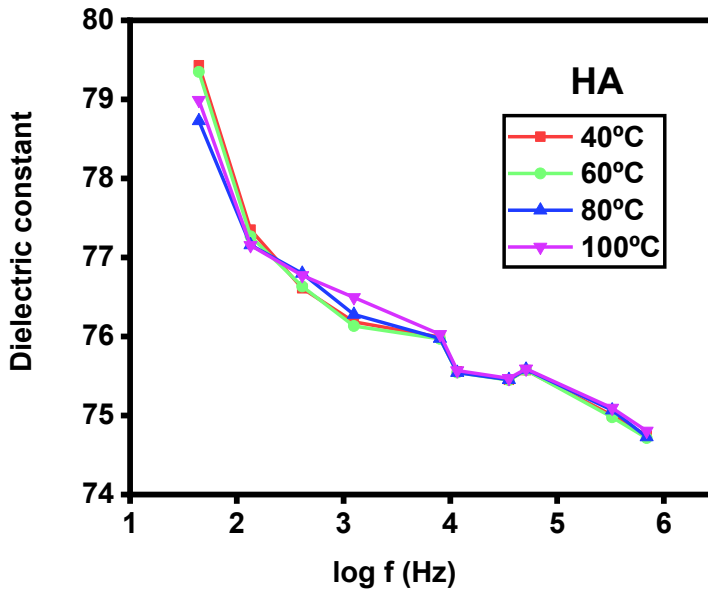


Fig 11 Dielectric constant of HA single crystal

For the HA crystal, the dielectric constant (ϵ') at 40 °C is around 80 in the low-frequency region as shown in fig 11. It decreases smoothly with increasing frequency at all measured temperatures. In the high-frequency region, ϵ' approaches an almost constant value, indicating the predominance of fast electronic polarization.

The HS crystal follows a similar decreasing pattern; however, it shows comparatively more stable behaviour at higher frequencies. The dielectric constant of HS is slightly lower about 76 at 40 °C, as illustrated in fig 12. The incorporation of sodium molybdate dihydrate into the hippuric acid lattice appears to influence the polarization mechanism by reducing space-charge accumulation and stabilizing dipolar polarization. The convergence of dielectric constant values at elevated frequencies for all temperatures confirms minimal temperature dependence and good dielectric stability. The smooth dispersion behaviour observed for both samples suggests structural homogeneity and low defect density [40-41].

The dielectric constant was evaluated using

$$\epsilon' = \frac{C_p d}{A \epsilon_0} \quad (5)$$

C_p , d , A , and ϵ_0 denotes the capacitance, thickness of the sample, the electrode area and the permittivity of free space.

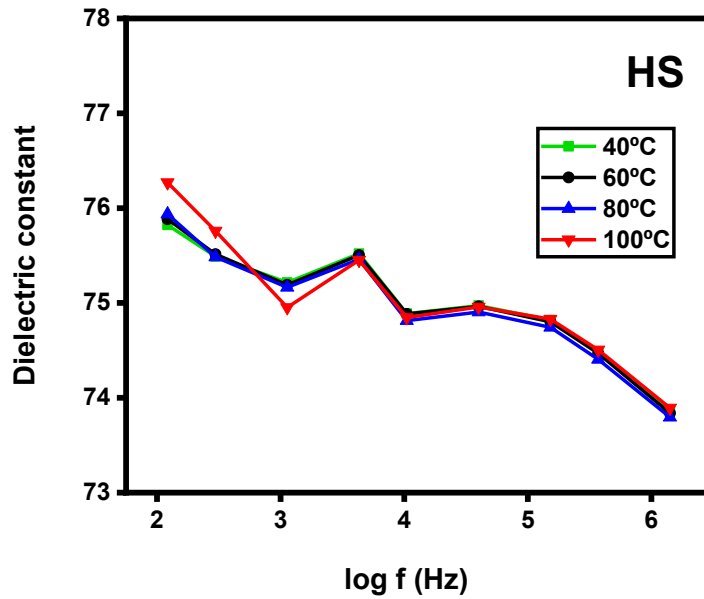


Fig 12 Dielectric constant of HS single crystal

The dielectric loss behaviour of HA and HS crystals is presented in fig 13 and 14, respectively. In both cases, the dielectric loss is relatively high in the low-frequency region and decreases rapidly as the frequency increases. For pure HA, the elevated loss at low frequencies can be attributed to space-charge polarization and charge carriers associated with defects. With the increase in frequency, $\tan \delta$ reduces steeply and attains a minimum value within mid-frequency, this being indicative of suppression of space-charge and dipolar relaxation mechanisms.

This frequency-dependent trend found for the HS crystal is analogous to that of HA, but in this case the low-frequency dielectric loss is somewhat larger than HA, possibly

because dopant-induced charge carriers and defect states [42]. At higher frequencies, the dielectric loss of HS also reduces to very low values and becomes nearly temperature independent, indicating stable dielectric behaviour.

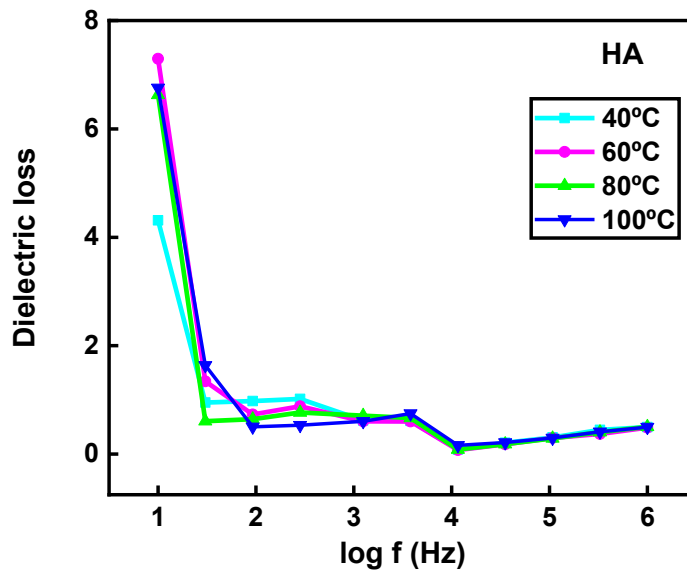


Fig 13 Dielectric loss of HA single crystal

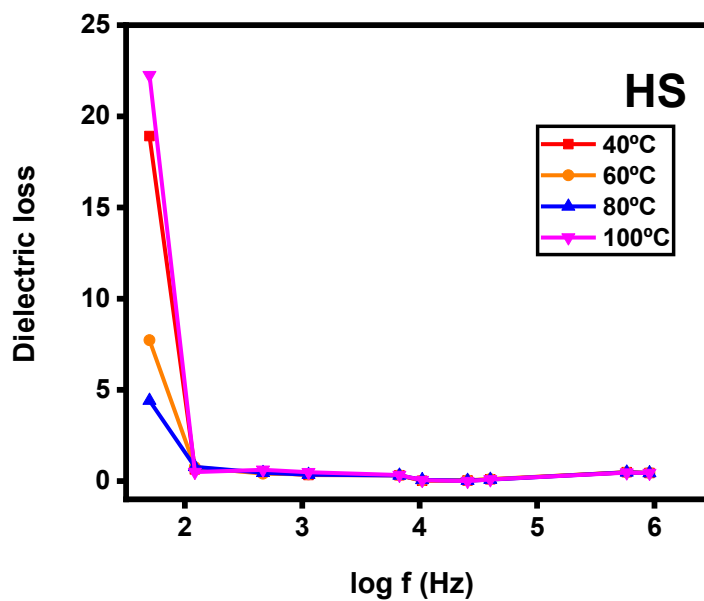


Fig 14 Dielectric loss of HS single crystal

Overall, both HA and HS crystals show typical dielectric dispersion behavior. The incorporation of sodium molybdate dihydrate improves the dielectric response without adversely affecting the intrinsic polarization characteristics of the host lattice.

3.8 Laser Damage Threshold (LDT)

Laser damage threshold is a crucial parameter for assessing the use of optical materials in high-performance laser systems, such as nonlinear optical (NLO) applications. The LDT value depends on several experimental parameters including but not limited to repetition rate of the pulse, beam diameter, irradiance, pulse length and focusing conditions [43-45]. Because NLO crystals are often subjected to high-power laser radiation, surface damage resistance of NLO materials is a critical consideration for the practical implementation of devices.

Using a Q-switched Nd:YAG laser operating in multi-shot mode at 1064 nm to produce pulses of light with a pulse width of 6 ns and a repetition rate of 10 Hz, the laser damage threshold (LDT) of the grown crystals was measured. A variable attenuator controlled the energy of the incident laser. A laser beam of 1 mm diameter was focused, using a biconvex lens with a focal length of 10 cm onto the polished flat surface of the crystal in the vicinity of the focal region [46-48]. The experiment was conducted by gradually ramping up the laser intensity until the first visible damage site formed on the surface of crystal. The corresponding input energy was recorded using an energy meter. The input energy of the laser is recorded with the help of the photo detector. The obtained input energy of the light source E_p is 8.3 mJ for HA crystal and 27.0 mJ for the HS crystals.

The radius of the laser beam waist at the focal point (ω_0) was estimated using:

$$2\omega_0 = \left(\frac{4\lambda}{\pi}\right)\left(\frac{f}{d}\right) \quad (6)$$

Where f is the focal length of the lens (10 cm) and d is the laser beam diameter (1 mm). The surface laser damage threshold was then calculated from:

$$P_d = \frac{E_p}{\tau \pi (\omega_0)^2} \quad (7)$$

where E_p is the incident pulse energy (mJ) and τ is the pulse width (ns).

From these calculations, the LDT for pure HA is determined to be 2.54 GW/cm², while 3.13 GW/cm² is obtained for HS. During laser irradiation, surface damage can be identified through visible changes on the material. The optical microscopic images were recorded before and after the passage of the laser beam of the HS crystal showing this surface damage is presented in fig. 15 and 16. The higher LDT of the HS crystal indicates that sodium molybdate dihydrate doping enhances the damage resistance of the host crystal, driven by specific mechanical, structural, and electronic modifications demonstrating its suitability for high-power NLO device applications.

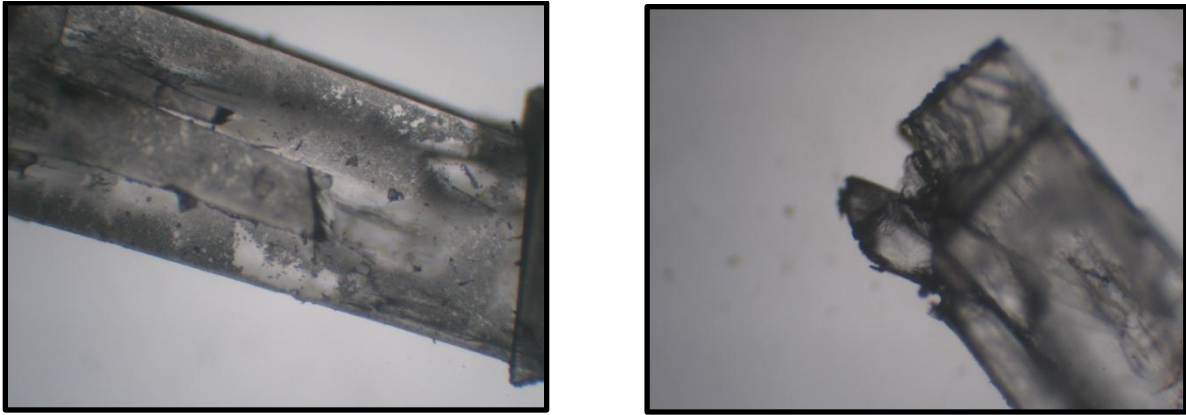


Fig 15 and 16 optical microscope image of before and after LDT of HS crystal

3.9 SHG measurement

The efficiency of the grown crystals was determined by using the second harmonic generation (SHG) according to the standard procedure reported in earlier studies. Kurtz–Perry powder technique was used, in which the relative conversion efficiency of second harmonic generation for a sample is compared with that of a reference material (potassium dihydrogen phosphate or KDP) to show the behaviors of second harmonic generation formed in the material [49-51].

A Nd:YAG laser (1064 nm, 10 ns pulse width, and 10 Hz repetition rate) was utilized as an excitation source in the present work. The powdered HA and HS samples with narrow particle size distribution were pressed on the surface of a glass slide and irradiated with a well-collimated laser beam. The input energy of the Nd:YAG laser source was 0.7 J, and for the HA, HS crystals, output values were 7.8 mJ and 5.9 mJ. The reference KDP gave 7.0 mJ for the same input. These outputs were recorded consistently over multiple trials.

The SHG efficiency of HA was found to be 1.11, whereas the doped HS crystal exhibited a lower value of 0.84. The decrease in SHG efficiency after doping may be due to slight lattice disturbance, increased absorbance, phase-matching disturbance and modification of molecular alignment within the host matrix. Although the SHG efficiency of the doped crystal is reduced when compared with the pure sample, HS still shows appreciable nonlinear optical activity [52,53].

Therefore, the grown crystal may be considered suitable for applications requiring moderate SHG response, such as low-power frequency conversion, optical modulation, and other photonic or optoelectronic device applications. The results indicate that the SHG efficiency of HS is approximately 0.84 times that of the reference KDP.

4 Conclusion

Using the slow evaporation method the hippuric acid doped with sodium molybdate dihydrate (HS) single crystals were successfully grown at room temperature and it was compared with pure hippuric acid (HA) crystals. Single-crystal X-ray diffraction and powder X-ray diffraction structural analysis showed that HS crystallizes in the orthorhombic system with space group $P2_12_12_1$, which shows little shifts of main diffraction peaks indicative of co-inclusion of sodium molybdate dihydrate into the host lattice. FT-IR analysis was performed to confirm the presence of characteristic functional groups and the creation of hydrogen-bonded interactions between dopant and host molecules. Optical characterization by UV–Vis–NIR spectroscopy showed that the films were of good optical quality, as demonstrated by their high transparency in the

visible and near-infrared regions with a sharp cut-off wavelength at 318 nm. Thermal analysis shows that HS crystal to be thermally stable upto 220 °C. Dielectric measurements also indicated normal dispersion and lower dielectric loss and temperature stability of HS compared to HA. HS shows 3.13 GW/cm² laser damage threshold which indicate excellent resistance to high-intensity laser irradiation. The SHG efficiency results of HS was 0.84 times then reference KDP sample, which indicate the presence of slight lattice distortion due to some doping, resulting in molecular alignment change in HS. Overall, the HS single crystal combines excellent structural, optical, dielectric, and thermal characteristics with moderate nonlinear optical activity for potential use in low-power photonic and optoelectronic applications such as optical modulators, signal processing, optical switches, and other NLO devices where device geometry does not require high SHG efficiency.

Author contributions

G. P. Sangeetha – carried out the synthesis and experiments and also wrote the manuscript with the input from all the authors.

G. V. Vijayaraghavan – supervision, worked out all the technical issue throughout the study and revised the manuscript critically for important intellectual concepts.

J. Priscilla – Methodology, Interpretation of data's and revised the manuscript critically for important intellectual concepts.

All the authors discussed the results and commented on the manuscript.

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Data availability

The data that support the findings of this study are available on request from the corresponding author.

Conflict of interest

No potential conflict of interest was reported by the author(s).

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