

Optical, thermal and dielectric characteristics of a novel organic nonlinear crystal have been studied. Nonahydrate single crystal of bis (2,3-dimethoxy 10-oxostrychnidinium) phthalate

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Abstract

Bis (2,3-dimethoxy-10-oxostrychnidinium) phthalate nonahydrate was synthesised, grown, and characterised for the first time in this work. The XRD examination of a single crystal demonstrates that the crystal is monoclinic in structure. Vibrational and NMR spectroscopy examinations revealed the molecule's structure and the kind of vibrations occurring inside it. It was observed that the UV absorption edge was 330 nm, with a large optical transmittance window that included the visible spectrum. Up to a temperature of 90.56 C, the crystal is physicochemically stable. The TG data was used to derive a number of thermodynamic parameters. The developed crystal's SHG efficiency was found to be phase matchable and to be 2.8 times more than that of KDP in the Kurtz powder second harmonic generation.

1. Introduction

Low birefringence suggests its appropriateness for non-linear optical (NLO) devices. Due to the carboxylic acid's supply of protons to quaternium nitrogen, there were two distinct wavelengths in the PL spectrum: 355 and 406 nm. Dielects and other modern gadgets Due to their high nonlinear coefficient, physical and chemical durability, and quick responsiveness to electro-optic effect, organic materials are becoming increasingly popular. Organic materials have been shown to be superior to traditional inorganic substances in many applications due to their higher electronic susceptibility (χ) and simplicity of device processing due to molecular hyperpolarisability ($\chi^{(2)}$) [1]. For example, optical switches, optical communications, and optical data storage have previously been implemented [2]. Host molecules with acidic groups prefer to crystallise with the host compound, which has six asymmetric carbons and no hydrogen bonding donor group. The brucine is protonated at the N (2) position after the acid-base process. Phosphoric acid (KAP) or potassium hydrogen phthalate (KHP) with mula's chemical The alkali acid phthalate salt K (C₆H₄COOHACOO) is a semi-organic salt. [3] The orthorhombic system in which KAP crystallises is Pca21. Analyzers and monochromators in high-resolution X-ray instruments rely on them extensively in the X-ray spectrum. Epitaxial growth

of orientated polymers and hierarchical development of structured materials have recently been performed on KAP crystals [4]. There are two proton-donating carboxylic groups in KHP that make Bis(2,3-dimethoxy-10-oxostrychnidinium) phthalate nonahydrate salt easily reactable to brucine. Crystal structure of Bis 2,3D10 PN was published by Krishnan et al. [5]. Hydrogen bonds between the brucinium cations and phthalate anions are NAH O and OAH O. They create ribbon structures that are head-to-tail, with the carboxy phthalate and water molecules intertwined along the 'a'-axis. For the first time, we describe the growth, structural, optical, thermal, laser damage threshold, and second harmonic generation properties of Bis 2,3D10 PN single crystals in this work.

2. Experimental

Development of crystals of Bis 2,3D10PN It was created by dissolving potassium hydrogen phthalate (Merck: 99 percent, AR grade) and brucine (Sd. Fine: 99 percent, AR grade) in a mixed solvent of ethanol and water, in a 1:1 M ratio. Figure 1 depicts the chemical process. An automated temperature-controlled motorised magnetic stirrer was used to ensure that the solubility of the Bis 2,3D10 PN salt in ethanol and water was homogenous before conducting the solubility investigations. The crystalline salt of Bis 2,3D10 PN was obtained by allowing the solution to evaporate at room temperature. The gravimetric technique was used to determine the solubility of Bis 2,3D10 PN in a 1:1 mixture of ethanol and water at a temperature range of 32–42 C. On the basis of Figure 2(a), it can be deduced that Bis 2,3D10 PN is soluble in both ethanol and water (1:1). The quality of the synthesised material was improved by re-crystallizing it five times. Continuous stirring for six hours at 30 C produced the saturated solution according to the solubility values. To prevent the solvent from evaporating too quickly, the prepared solution was poured into a beaker and filtered using Whatman filter paper. After that, a 30 C constant temperature bath was used to maintain the produced solution with an accuracy of 0.01 C. A 2,3D10 PN crystal of

considerable size (24 9 8 mm³) was formed over a period of roughly 25 days. Figure 2 is an image of the crystals that were produced (b). Characterization An APEX II CCD crystal diffraction system was used to analyse the crystal structure and cell characteristics. Using a Nicolet R3m/E four-circle X-ray diffractometer equipped with Mo K α radiation (a graphite monochromator), $k = 0.71069$, data on the X-ray diffractometer intensity of a single crystal (0.35 0.30 0.20 mm³) were acquired at 295 K. Up to 2h = 52, 12,452 distinct reflections were measured using the ω : 2 θ scan technique. An empirical adjustment was used to account for the Lorentz, polarisation, and absorption effects on the data. There were 3854 reflections that matched the $I > 2r$ (I) criterion used to solve the crystal structure and improve it using a full-matrix least-squares process based on F(000). While anisotropic displacement parameters were used to refine non-hydrogen atoms, a single weighting technique was used to incorporate hydrogen atom locations in the model at their predicted positions. A Spectrum Perkin Elmer It was necessary to use a Fourier transform infrared spectrometer to measure the infrared spectra in the region of 4000–450 cm⁻¹ at ambient temperature.

The crystal powder was pressed into a pellet shape using KBr before being used to make the sample. The FT-Raman spectra of powder were obtained using a Bruker IFS-88 spectrometer fitted with a Ge detector and chilled to liquid nitrogen temperature using a FRA-106 adapter. YAG: Nd³⁺ air-cooled diode pumped 200 mW laser was employed as an excitation source. The laser excitation line was 1064 nm at the time of incidence. Scattered light was gathered at an angle of 180 degrees in the range of 4000–50 cm⁻¹ with a resolution of 2 cm⁻¹, 256 scans. At room temperature, a Perkin Elmer Lambda 35 Spectrophotometer with a 200–800 nm wavelength range measured the transmission spectra of Bis 2,3D10 PN crystal in the UV–Vis–NIR range. Polished bis 2,3D10 PN crystal with a thickness of 1.59 mm was utilised in this test. Allowing UV–Vis rays to fall on the crystal face (0 1 0), the crystal was exposed to the whole range of wavelengths. Bis 2,3D10 PN was compared to KDP in terms of second harmonic generation efficiency utilising the Kurtz and Perry powder process and a Nd: YAG laser. Varian Cary Eclipse Fluorescence spectrophotometer with scan speed of 600 nm/s and filter size of 5 nm was used to record the photoluminescence spectrum. The generated crystal's birefringence behaviour was investigated using the modified channel spectrum technique (MCS). Even if the crystal area is as tiny as 0.004 m², this approach may be employed, and a 0.420 mm thick crystal was used in this work [6]. In

the publication [7], the experimental setting employed in this work is described. Using a Bruker AMX 400 spectrometer with tetramethylsilane as the internal standard and CDCl₃ as the solvent, NMR spectra (1 H and 13C) were collected to learn more about the molecule's carbon–hydrogen framework. A TG–DTA apparatus was used to do thermal analysis simultaneously (SDT Q 6000 V 8.2 Built 100 thermal analyzer). Temperatures ranged from ambient temperature to 1000 degrees Celsius, with a heating rate of 20 degrees Celsius per minute, N₂–gas dynamic environment, and alumina as a reference material. The sample was 2.1120 grammes of the sample without pressing. A PtAPt 13 percent Rh thermocouple was used to measure the temperature, and it was placed close to the sample pan. For the frequency and temperature-dependent dielectric measurements, we employed an HIOKI 3532-50 LCR HITESTER metre. A Bis 2,3D10 PN crystal with a thickness of 1 mm was cut in the (001) direction and polished. Electrodes were used to attach the samples to the plates.

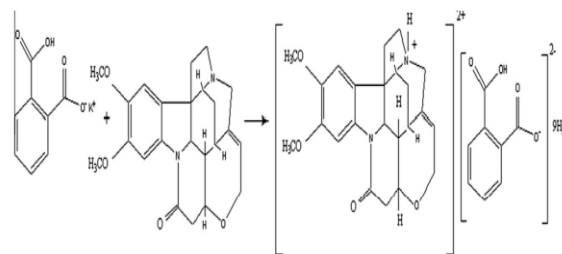
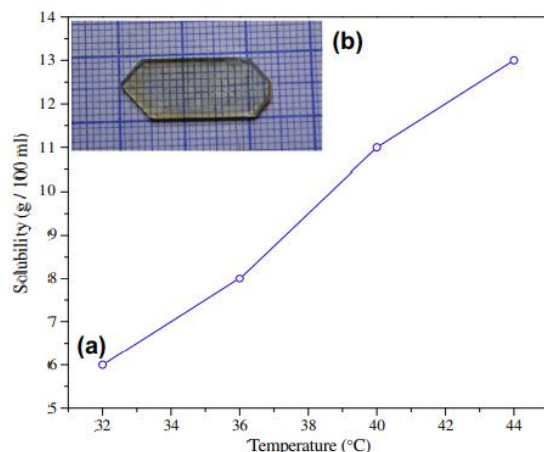


Fig. 1. Reaction scheme for Bis 2,3D10 PN compound.



Bis 2,3D10 PN single crystal as formed, with a silver coating applied to one side to make it act like a parallel plate capacitance. At room temperature, the experiment was conducted in the frequency range of 100 Hz–5 MHz.

3. Results and discussion

Structure of crystals Crystallographic analysis of the Bis 2,3D10 PN crystal reveals that it belongs to the monoclinic crystallographic system (space group C2), with lattice parameters $a = 13.939$ (five decimal places) and $Z = 2$ (five decimal places), with the latter two being the most significant. Table 1 provides more information on the crystal characteristics and the data collection for diffraction. On the 'a'-axis, Figures 3 and 4 show the Bis 2,3D10 PN molecular arrangement and projection by itself, respectively. Figures for the hydrogen bond may be found in Table 2. Table 3 contains the chosen data for bond lengths and bond angles. These hydrogen bonds hold the crystal in place.

Analyzing vibrations Understanding the chemical bonding and the microscopic mechanism of the NLO characteristics of novel materials may be gained by using vibrational spectroscopy. It is possible to validate the existence of Bis 2,3D10 PN by the use of IR and Raman spectroscopy to examine the vibrational spectra. Figures 5 and 6 show the vibrational spectra. Table 4 provides the wavenumbers of the bands, their relative intensities, and their preliminary designations. Internal vibrations are responsible for the bands shown in the measured area (4000–450 cm^{-1}).

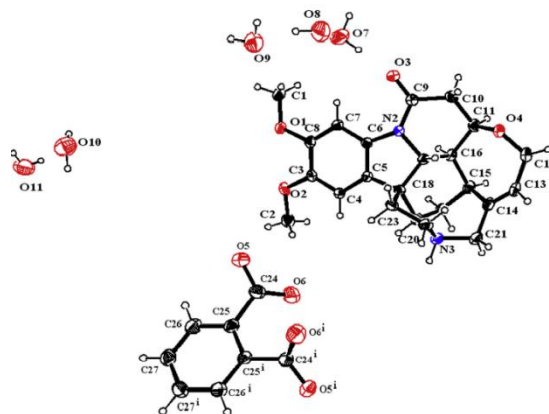
C-AH vibrations

We can see that the hetero aromatic structure demonstrates the existence of CAH stretching vibrations in the wavelength range of 3100–3000 cm^{-1} [8]. The CAH stretching modes are frequently strongly polarised and occur with a lot of intensity. The absence of Raman bands has been attributed to the high polarisation [9]. CAH stretching vibrations may be seen in the FT-IR spectra at 3068 cm^{-1} . CAH in-plane and out-of-plane bending vibrations exist in the wave number ranges of 1300–1000 cm^{-1} and 1000–750 cm^{-1} in the substituted benzenes, respectively [10,11]. When looking at the CAH in-plane bending vibrations using the IR and Raman spectral ranges, it was discovered that they occur at wavelengths of 1256 cm^{-1} and 1192 cm^{-1} , respectively. It has been determined that the infrared and Raman spectra bands at 982, 855 cm^{-1} and 980, 828 cm^{-1} correspond to vibrations of the CAH out-of-plane bending. Vibrations of the CH₃ group About 2965 and 2880 cm^{-1} [12] are typical for the CH₃ group's asymmetric and symmetric stretching modes. It's clearly visible in the IR spectrum at 2926 cm^{-1} : the methyl asymmetric stretching. At the same time,

the Raman counterpart is detected.

Table 1
Crystal data and structure refinement for Bis 2,3D10 PN.

Identification code	Bis 2,3D10 PN
Empirical formula	$2\text{C}_{23}\text{H}_{27}\text{N}_2\text{O}_4 \cdot \text{C}_8\text{H}_4\text{O}_4^{2-} \cdot 9\text{H}_2\text{O}$
Formula weight	1117.19
Temperature	295 K
Wavelength	0.71069 Å
Crystal system	Monoclinic
Space group	C2
Unit-cell dimensions	$a = 13.939$ (5) Å, $\alpha = 90.00^\circ$ $b = 12.370$ (5) Å, $\beta = 90.646$ (5) $^\circ$ $c = 15.321$ (5) Å, $\gamma = 90.00^\circ$
Volume	2641.6 (17) Å ³
Z	2
Calculated density	1.405 mg m^{-3}
Absorption coefficient	0.11 mm^{-1}
$F(000)$	1192
Crystal size	0.35 × 0.30 × 0.20 mm^3
Theta range for data	2.6–26.2 $^\circ$
Collection	
Reflections collected	12,452
Independent reflections	5094
Refinement method	Full-matrix least squares on F^2
Data/restraints/parameters	5094/16/385
Goodness of fit on F^2	1.05
R indices (all data)	$R[F^2 > 2\sigma(F^2)] = 0.049$ $wR(F^2) = 0.125$



Bis 2,3D10 PN crystal's molecular structure and atom numbering system are shown in Fig. 3. At a 30% probability level, displacement ellipsoids are sketched. The atoms of hydrogen are shown as tiny spheres of any chosen radius.

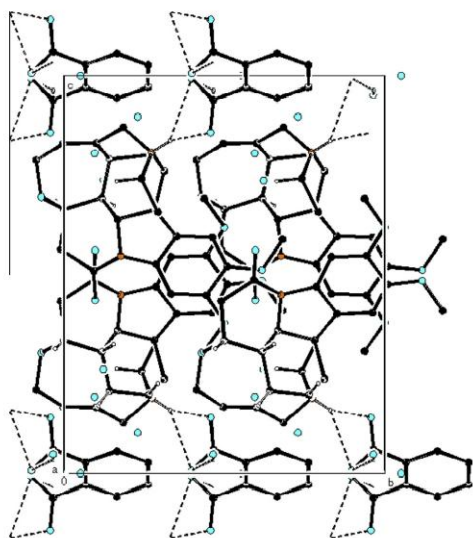


Fig. 4. View of the crystal packing showing the hydrogen-bonding interactions

intensity-packed wavenumber FT-IR and FT-Raman spectra show the same symmetric methyl stretching mode at 2891 cm⁻¹. The existence of intramolecular charge transfer is shown by the simultaneous activation of the CH₃ stretching wavenumber. In FT-IR and FT-Raman, the asymmetric bending vibrations can be seen at wavelengths of 1502 and 1503 cm⁻¹, respectively. The

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A
N3—H3...O5i	0.91 (0)	1.79 (0)	2.6
O7—H7A...O3	0.82 (1)	1.98 (2)	2.7
O7—H7B...O5ii	0.82 (1)	2.10 (4)	2.8
O9—H9A...O6iii	0.82 (1)	1.98 (2)	2.7
O8—H8B...O7	0.82 (1)	1.99 (2)	2.7
O8—H8A...O9	0.82 (1)	1.97 (3)	2.7
O9—H9B...O11iv	0.82 (1)	2.01 (1)	2.8
O10—H10C...O6v	0.82 (1)	2.29 (3)	3.0
O10—H10D...O8vi	0.82 (1)	1.99 (3)	2.7
O11—H11A...O10	0.82 (1)	2.12 (2)	2.8

Symmetry codes: (i) x + 1/2, y + 1/2, z. (ii) x + 1, y + 1, z + 1. (iii) x + 1/2, y + 1/2, z + 1. (iv) x, y + 1, z. (v) x + 1, y, z + 1. (vi) x, y + 1, z.

Table 3

Selected geometric parameters (Å, °).

Selected bonds	Bond lengths (Å)	Selected bonds	Bond angles (°)
C12—O4	1.433 (4)	O3—C9—C10	121.6 (3)
C9—O3	1.233 (3)	N2—C9—C10	115.7 (2)
C3—O2	1.365 (4)	O4—C12—H12B	109.4
C9—N2	1.358 (4)	C11—O4—C12	115.4 (2)
C8—O1	1.371 (3)	O1—C8—C7	124.4 (3)
C12—C13	1.487 (5)	O2—C3—C4	124.5 (3)
C19—H19	0.9800	C3—O2—C2	117.2 (2)
C18—C19	1.537 (4)	O2—C2—H2A	109.5
N3—C21	1.494 (4)	N3—C20—C23	105.2 (2)
N3—H3	0.9100	C21—N3—C19	113.4 (2)
C21—H21B	0.9700	C25i—C25—C26	119.28 (18)
C24—O5	1.258 (4)	C27—C26—C25	121.0 (3)
C24—O6	1.233 (4)	C7—C6—N2	128.7 (2)
C25—C25i	1.388 (6)	C4—C5—C18	129.6 (2)

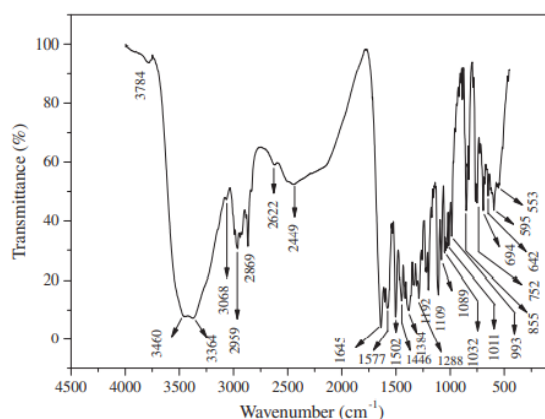


fig. 5. Powder FT-IR spectrum of Bis 2,3D10 PN

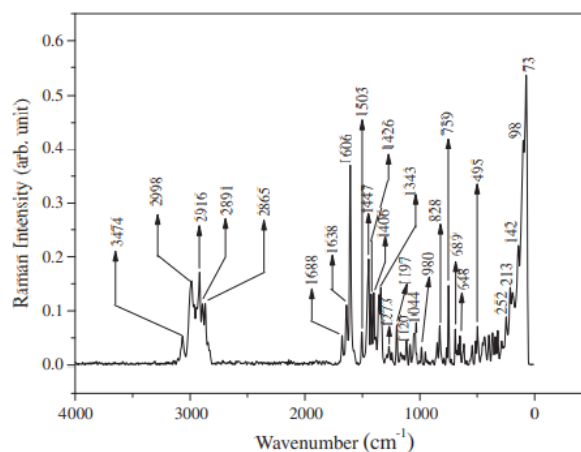


Fig. 6. Powder FT-Raman spectrum of Bis 2,3D10 PN.

FT-IR at 1336 cm⁻¹ and FT-Raman at 1356 cm⁻¹ show significant bands ascribed to the methyl symmetric bending mode, which has been seen. CH stretching and bending vibrations are linked with

other typical types of vibration (Table 4). Vibrations of the CAC and CACAC CAC stretching vibrations are responsible for the bands shown in the FT-IR and FT-Raman spectra at 1577, 1446, and 1032 cm^{-1} and 1447, 1406, and 1044 cm^{-1} respectively. In the FT-IR and Raman spectra, the CAC in-plane bending vibrations were located at 1089, 595 cm^{-1} and 1085, 613 cm^{-1} , respectively. In the infrared and Raman spectra, the out-of-plane bending vibration was identified at 855/828 cm^{-1} correspondingly. Sounds of the CAO The stretching vibration absorption zone for the alcohol CAO group was identified in the range of 1200–1000 cm^{-1} . There were Raman counterparts at 1273, 1085 cm^{-1} and these bands were moved down to 1288, 1089 cm^{-1} in the current study. Hydrogen bonding may be to blame for this change. [13] The phthalate ion's vibrational bands A deprotonated carboxylic group (COO) is found in the investigated crystal, according to crystallographic data [5]. [11] The carboxylate group contains two CAO bonds with bond strengths that are midway between CAO and C@O. The strong peak at 1645 cm^{-1} in the FT-IR spectrum is ascribed to the C@O vibration, whereas the same has been seen in the Raman band at 1638 cm^{-1} . In the asymmetric stretching, the deprotonated carboxylate group COO absorbs substantially about 1670–1550 cm^{-1} and weakly near 1440 cm^{-1} [11,14–18]. Infrared and FT-Raman bands at 1384 and 1406 cm^{-1} show that COO symmetric stretching is taking place.

These are the ionised carboxylate group's signature absorption bands. Hydrogen bonding is shown by a decrease in COO stretching wavenumber. In FT-Raman and FT-IR, the COO scissor mode shows as a medium band at 759/752 cm^{-1} . Carboxylate vibrations have been classified into wagging, rocking, and scissoring modes (Table 4). Hydrogen binds and water molecules vibrate. The analysis of vibrational spectra is greatly aided by the use of X-ray data [5] to determine hydrogen bond configuration. Ten hydrogen bonds of the OAH O and NAH O types are found in the title crystal. These two varieties have differing average lengths, which is why they're called NAH O and OAH O. The length of a NAH O type is 2.665. The infrared absorption associated with it is represented by a multicomponent wideband with a maximum wavelength of 2959 cm^{-1} . At a wavelength of 2998 cm^{-1} , the equivalent FT-Raman band may be detected. The lengths of nine OAH O kinds vary from 2.753 to 3.066, with an average of 2.822. Weak noncovalent intermolecular hydrogen bonds are the most common kind of bond found in the crystal under study. The spectral characteristic corresponding to a specific hydrogen bond is difficult to distinguish. For powder spectra,

one can only see the average image. The wide and severe absorption seen in the measured spectra in the range 3600–1800 cm^{-1} is due to weak hydrogen bond type intermolecular interactions. OH group vibrations are more prone to be affected by the surrounding environment, hence the spectra of hydrogen-bonded species display more significant alterations. In the 3700–3550 cm^{-1} range, the nonhydrogen-bonded or a free hydroxyl group absorbs substantially. If hydrogen bonds are present in the molecule, the OAH stretch band would be reduced to the 3550–2000 cm^{-1} area. Due to the presence of OAH O hydrogen bonding in the crystal, this band cannot be identified experimentally in the IR spectrum between 3700 and 3550 cm^{-1} . There were hydrogen bonds created by water molecules, and this was evident in the IR spectrum, where a wide and powerful massif covering 3400–2000 cm^{-1} with a maximum at roughly 3431 cm^{-1} was assigned to this vibration. In-plane bending vibrations of water molecules may be clearly seen at 1598/1606 cm^{-1} as a very strong band, a characteristic of water molecules. Because of the escape of water molecules, the medium and broadband at 642 cm^{-1} was detected. For a hydrogen bond with a length of 1300–1400 cm^{-1} , Novak's correlation [21] predicts a band in the 1300–1400 cm^{-1} area arising from the OAH plane bending type of vibration (dOH). Therefore, the 1320 cm^{-1} infrared band is given to this vibration. This band has a 1343 cm^{-1} Raman counterpart. In accordance with the foregoing correlation, a band at around 1000 cm^{-1} may be expected for the OAH out-of-plane bending type of OAH O hydrogen bond vibration (cOH). As a result, the 993/980 cm^{-1} band in the medium infrared was linked to this vibration. Analysis of NMR spectra The spectrum analysis methods of ^1H NMR and ^{13}C NMR are critical in the study of organic structure.

Table 4: The infrared and Raman spectra of Bis 23D10 PN powder show the following wavenumbers

(cm1) and relative intensities:

Chemical Shift (ppm)	Assignment	Relative Intensity (%)
11.8	COO	100
8.0	H	100
7.5	H	100
7.2	H	100
6.8	H	100
6.5	H	100
6.2	H	100
5.8	H	100
5.5	H	100
5.2	H	100
4.8	H	100
4.5	H	100
4.2	H	100
3.9	H	100
3.6	H	100
3.2	H	100
2.7	H	100
2.0	H	100
1.65	H	100
1.35	H	100
0.0	COO	100

compounds. Bis 2,3D10 PN has a 1 H NMR spectrum given in Figure 7. In a particularly small range of 13–10 ppm, the carboxylic proton is absorbed. In the phthalate moiety, the lack of peaks over 10 ppm indicates that there are no carboxylic protons. Directly linked hydrogen atoms, such as aromatic benzene rings, absorb between 6 and 8.5 ppm of hydrogen. There are 6.8–8.5ppm absorptions of ben-zene rings in both the brucine and phthalate groups. Shielding tends to move absorptions upward, whereas deshielding tends to move them downward. Atoms like oxygen and nitrogen, which are electron withdrawing groups like carbonyl and ethylenic double bonds, in the molecular structure, de-shield proton and shift absorptions downfield owing to electron de-shielding. Ethylenic proton is responsible for the 6.17 ppm peak. It is known that protons in water molecules absorb between 4 and 5 ppm, and this is evident in the peaks reported in the current investigation at 4.36–3.90 ppm. The benzene ring of brucine has absorption maxima at 3.91 and 3.90 ppm for the 3- and 4-methoxy groups linked to it. Chemical shift values of 3.18–3.04 ppm, 2.70, 2, 1.65, and 1.35 ppm are detected in a group of peaks. Downshield absorption peaks are seen for protons that are closer to electronegative atoms, such as oxygen and nitrogen. The rest is gone.

4. Conclusion

Slow evaporation of the solvent at room temperature resulted in the formation of single crystals of Bis 2,3D10 PN. Analysis of single-crystal X-ray diffraction revealed the crystal structure and unit cell parameters. The existence of functional groups in the formed crystal is confirmed by vibrational and NMR studies. The sample is optically transparent

throughout a broad range of wavelengths and absorbs no light in the visible spectrum, according to UV–Visible studies. Bis 2,3D10 PN's second harmonic generation efficiency was found to be 2.8 times larger than KDP crystal's. It is reasonable to assume that the crystal's low birefringence makes it appropriate for use in a harmonic generator. Stability in temperature is shown by TG–DTA. Due to the lower emission peak energies in comparison to band gap energies, the observed PL might be explained by radiative recombination of electrons and holes trapped in nearby localised states. For electro-optic applications, a low dielectric constant and low power dissipation were found in the formed crystal, as shown by dielectric measurements.

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