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## Research Article

# Halogen Substituted Indeno Quinoxaline Derivative Crystal: A Spectroscopic Approach

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## Abstract

**Background and Objective:** Quinoxaline derivatives shown antibacterial, antiviral and anticancer properties which have received considerable interest due to their biological properties. Thus the halogen substituted indeno quinoxaline derivative hetero cyclic compound of 6'-(3-bromo phenyl)-7'-nitro-1', 6', 7', 7a'-tetrahydro-3' H-spiro[indeno[1, 2-b]quinoxaline-11, 5'-pyrrolo[1,2-c]thiazole] (BPNTSIPT) has been crystallized by slow evaporation method and characterized by FT-IR, FT-Raman and UV-Visible spectroscopy analyzes.

**Materials and Methods:** Colourless block shaped crystals were obtained from slow evaporation method by recrystallization of synthesized compound with ethanolic solution. Benzene-1, 2-diamine, 1H-indene-1, 2, 3-trione, thiazolidine-4-carboxylic acid, methanol, chloroform and trans- $\beta$ -bromo nitrostyrenes are the raw materials used for this crystallization. **Results:** The complete vibrational FT-IR and FT-Raman spectra were interpreted in terms of functional group wavenumbers. The optical property of the title compound was analyzed by UV-Visible spectroscopy study. The crystal has the maximum absorbance peaks at 267, 347 and 369 nm. **Conclusion:** The FT-IR and FT-Raman spectra were studied and the functional group assignments of title compound have been seen to be in good agreement with the corresponding results in the literature. The title crystal has 4.3 eV optical band gap, this showed that it is a predictable dielectric material. Due to the wide variety of biomedical applications of modified quinoxaline structure in biological and pharmaceutical fields, it was taken to study and analyzed in this present work.

**Key words:** Slow evaporation, FT-IR, FT-Raman, UV-Visible spectroscopy

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**Competing Interest:** The authors have declared that no competing interest exists.

**Data Availability:** All relevant data are within the paper and its supporting information files.

## INTRODUCTION

Quinoxaline derivatives are an important class of benzohetero cycles which has been investigated in the recent years to discover new compounds owing to their both biological properties and pharmaceutical applications<sup>1,2</sup>. These derivatives showed an antimicrobial, anticancer, antimalarial, antiinflammatory, antinociceptive, antitubercular, anthelmintic, antidiabetic and antiepileptic property<sup>3-8</sup>. Spiro compounds are the naturally occurring substances characterized by highly pronounced biological properties<sup>9</sup>. Also, the thiazole with indole heterocyclic derivatives can be found in a variety of biologically active compounds that make them some of most extensively studied for heterocycles<sup>10</sup>. The substitution of bromine to these classes of heterocyclic compounds provides medicinal benefits. So in the present work, the halogen substituted indeno quinoxaline derivative crystal was synthesized and recrystallized by slow evaporation method due to its biological potential. The crystal structural data of title compound is recently reported by Muthuselvi *et al.*<sup>11</sup>. Several studies have been reported on the vibrational analysis of substituted indeno quinoxaline derivatives<sup>12-17</sup>. Recently, Muthuselvi *et al.*<sup>12</sup> has made spectroscopic investigation on 7'-nitro-6'-phenyl-1', 6', 7', 7a'-tetrahydro-spiro[indeno[1,2-b]quinoxaline-11, 5'-pyrrolo[1,2-c][1,3]thiazole] crystal. In the present work, the second series of the closely related compound has been investigated by spectroscopy approach. In order to investigate the assignments of the vibrational spectra of have been studied using FT-IR, FT-Raman and UV-Visible spectroscopy techniques in order to establish its conformation.

## MATERIALS AND METHODS

Benzene-1, 2-diamine, 1H-indene-1, 2, 3-trione, thiazolidine-4-carboxylic acid, methanol, chloroform and trans- $\beta$ -bromo nitrostyrenes are the raw materials used for this crystallization which were purchased from Sigma Aldrich Company through local scientific companies in Tamil Nadu, India. Initially an equimolar amount of benzene-1, 2-diamine, 1H-indene-1, 2, 3-trione and thiazolidine-4-carboxylic acid were dissolved in 20 mL of methanol in a round bottom flask and refluxed under water bath for 5 min. Then equimolar amount of substituted trans- $\beta$ -bromo nitrostyrenes added to the reaction mixture and continued for refluxing until completion of the reaction. The reaction progress was monitored intermittently using TLC. As evident from the TLC the reaction attained completion after 5 h of continuous refluxing. The precipitated solid was filtered and washed

with methanol to obtain the title compound in good yields (92-96%). Colourless block shaped crystals were obtained from slow evaporation method by recrystallization of synthesized compound with ethanolic solution. The FT-IR vibrational spectrum was recorded by PERKIN ELMER SPECTRUM1FT-IR spectrometer in the range 4000-400  $\text{cm}^{-1}$ . Also, the FT-Raman spectrum was recorded using the BRUKER: RFS 27 Raman spectrometer in the wave number range 4000-400  $\text{cm}^{-1}$ . The optical absorbance spectrum of title compound has been recorded with SHIMADZU-UV1800 double beam spectrometer in the wavelength range 200-1100 nm insteps of 1 nm. This research work was completed within two months in the year of 2017 by us.

## RESULT AND DISCUSSION

**Vibrational analyzes:** To identify the vibrational modes, bonding and structural features of BPNTSIPT organic molecular compound, it was analyzed by FT-IR and FT-Raman spectroscopic techniques. It has ring groups such as bromo phenyl, pyrrolo thiazole, indeno quinoxaline and nitro group with associated functional groups C-H, C-Br,  $\text{CH}_2$ , C-N, C=N, C-S, C-C, C=C,  $\text{NO}_2$  and C- $\text{NO}_2$ . The chemical diagram of BPNTSIPT crystal was depicted in Fig. 1 which was taken from the recently published X-ray paper of Muthuselvi *et al.*<sup>11</sup>. Also, the FT-IR and FT-Raman spectra of title compound were depicted in Fig. 2 and 3. The detailed wavenumber assignments for these functional groups were shown in Table 1.

**Vibrations of indeno quinoxaline ring:** The C-H stretching, C-H in-plane bending C-H out-of-plane bending, C-C, C=C, C-N

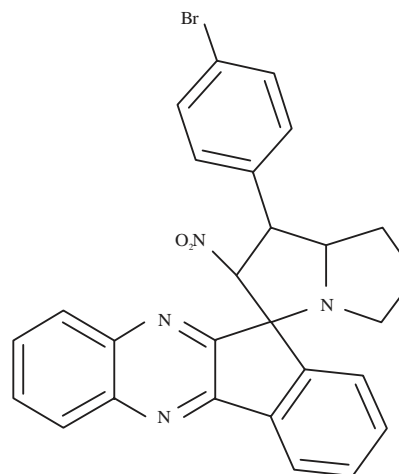


Fig. 1: Chemical diagram of BPNTSIPT crystal

Table 1: FT-IR and FT-Raman wavenumbers and their assignments for BPNTSIPT crystal

FT-IR (cm <sup>-1</sup> )	FT-Raman (cm <sup>-1</sup> )	Assignment
3434 (br)	-	$\nu(\text{O-H})_{\text{Trace of water}}$
-	3164 (w)	$\nu(\text{C-H})_{\text{Pyrrolo thiazole}}$
3057 (m)	3060 (m)	$\nu(\text{C-H})_{\text{BromoPhenyl}}; \nu(\text{C-H})_{\text{Pyrrolo thiazole}}; \nu(\text{C-H})_{\text{Indeno quinoxaline}}$
2975 (m)	2974 (m)	$\nu(\text{C-H})_{\text{BromoPhenyl}}$
2929 (m)	2942 (m)	$\nu_{\text{as}}(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
2871 (m)	2867 (m)	$\nu_{\text{s}}(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
1616 (w)	1610 (m)	$\nu(\text{C=C})_{\text{Bromo Phenyl}}; \nu(\text{C=N})_{\text{Indeno quinoxaline}}; \nu(\text{C=C})_{\text{Indeno quinoxaline}}$
1571 (m)	1580 (s)	$\nu(\text{C=C})_{\text{Bromo Phenyl}}; \nu(\text{C-C})_{\text{Pyrrolo thiazole}}; \nu_{\text{as}}(\text{NO}_2)_{\text{Nitro group}}$
1544 (s)	1544 (w)	$\nu(\text{C=C})_{\text{Bromo Phenyl}}; \nu(\text{C-C})_{\text{Pyrrolo thiazole}}; \nu(\text{C-NO}_2)_{\text{Nitro group}}; \nu(\text{C=C})_{\text{Indeno quinoxaline}}$
1508 (m)	1507 (m)	$\nu(\text{C=C})_{\text{Bromo Phenyl}}; \nu(\text{C-C})_{\text{Pyrrolo thiazole}}; \nu(\text{C-C})_{\text{Indeno quinoxaline}}$
1478(m)	-	$\nu(\text{C-C})_{\text{Bromo Phenyl}}$
1463 (m)	1469 (m)	$\nu(\text{C-N})_{\text{Pyrrolo thiazole}}; \nu(\text{C-C})_{\text{Indeno quinoxaline}}; \nu(\text{C-C})_{\text{Bromo Phenyl}}; \nu(\text{C-C})_{\text{Pyrrolo thiazole}}; \rho(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
-	1390 (s)	$\nu(\text{C-C})_{\text{Bromo Phenyl}}$
1372 (s)	-	$\nu(\text{C-C})_{\text{Bromo Phenyl}}; \nu(\text{C-C})_{\text{Pyrrolo thiazole}}; \omega(\text{CH}_2)_{\text{Pyrrolo thiazole}}; \nu_{\text{s}}(\text{NO}_2)_{\text{Nitro group}}$
1336 (s)	1337 (w)	$\nu(\text{C-C})_{\text{Bromo Phenyl}}; \omega(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
1277 (m)	1265 (w)	$\beta(\text{C-H})_{\text{Bromo Phenyl}}; \beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Indeno quinoxaline}}; \tau(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
1200 (m)	1225 (w)	$\beta(\text{C-H})_{\text{Indeno quinoxaline}}; \beta(\text{C-H})_{\text{Pyrrolo thiazole}}$
1172 (m)	1180 (m)	$\beta(\text{C-H})_{\text{Indeno quinoxaline}}; \beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Bromo Phenyl}}$
1124 (w)	1131 (w)	$\beta(\text{C-H})_{\text{Indeno quinoxaline}}; \beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Bromo Phenyl}}; \nu(\text{C-N})_{\text{Indeno quinoxaline}}$
1101(s)	-	$\beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Bromo Phenyl}}; \beta(\text{C-H})_{\text{Indeno quinoxaline}}$
1072 (s)	-	$\beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Bromo Phenyl}}; \beta(\text{C-H})_{\text{Indeno quinoxaline}}$
1052 (m)	1025 (w)	$\beta(\text{C-H})_{\text{Pyrrolo thiazole}}; \beta(\text{C-H})_{\text{Bromo Phenyl}}; \beta(\text{C-H})_{\text{Indeno quinoxaline}}$
1010 (w)	1001 (w)	$\beta(\text{C-H})_{\text{Bromo Phenyl}}$
972 (w)	970 (w)	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \gamma(\text{C-H})_{\text{Indeno quinoxaline}}$
940 (w)	937 (w)	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \text{Five membered ring breathing mode}$
886 (w)	-	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \gamma(\text{C-H})_{\text{Pyrrolo thiazole}}; \gamma(\text{C-H})_{\text{Indeno quinoxaline}}$
847 (w)	842 (w)	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \gamma(\text{C-H})_{\text{Indeno quinoxaline}}; \gamma(\text{C-H})_{\text{Pyrrolo thiazole}}; \rho(\text{NO}_2)_{\text{Nitro group}}$
796 (m)	785 (w)	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \gamma(\text{C-H})_{\text{Indeno quinoxaline}}; \nu(\text{C-S})_{\text{Pyrrolo thiazole}}; (\text{Ring breathing mode})_{\text{Bromo Phenyl}}; \omega(\text{NO}_2)_{\text{Nitro group}}$
752 (s)	755 (w)	$\gamma(\text{C-H})_{\text{Bromo Phenyl}}; \gamma(\text{C-H})_{\text{Indeno quinoxaline}}; \tau(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
717 (w)	718 (w)	$\tau(\text{CH}_2)_{\text{Pyrrolo thiazole}}$
696 (w)	-	$\gamma(\text{C-H})_{\text{Indeno quinoxaline}}; \nu(\text{C-S})_{\text{Pyrrolo thiazole}}$
675 (w)	678 (w)	$\gamma(\text{C-H})_{\text{Indeno quinoxaline}}; \delta(\text{C-C-N})_{\text{Indeno quinoxaline}}$
650 (w)	-	$\delta(\text{C-C-N})_{\text{Indeno quinoxaline}}$
632 (w)	-	$\delta(\text{C-C-N})_{\text{Indeno quinoxaline}}; \beta(\text{C-C-C})_{\text{Bromo Phenyl}}$
569 (w)	551 (w)	$\delta(\text{C-C-N})_{\text{Indeno quinoxaline}}; \gamma(\text{C-C-C})_{\text{Bromo Phenyl}}$
538 (w)	548 (w)	$\tau(\text{NO}_2)_{\text{Nitro group}}; \nu(\text{C-Br})_{\text{Bromo Phenyl}}; \delta(\text{C-C-N})_{\text{Indeno quinoxaline}}$
465 (w)	-	$\gamma(\text{C-C-C})_{\text{Bromo Phenyl}}$

s: Strong, w: Weak, m: Medium, br: Broad,  $\nu$ : Stretching,  $\nu_{\text{s}}$ : Sym. stretching,  $\nu_{\text{as}}$ : Anti sym.stretching,  $\delta$ : Bending,  $\gamma$ : Out-of-plane bending,  $\beta$ : In-plane bending,  $\tau$ : Rocking,  $\omega$ : Wagging,  $\rho$ : Scissoring,  $t$ : Twisting

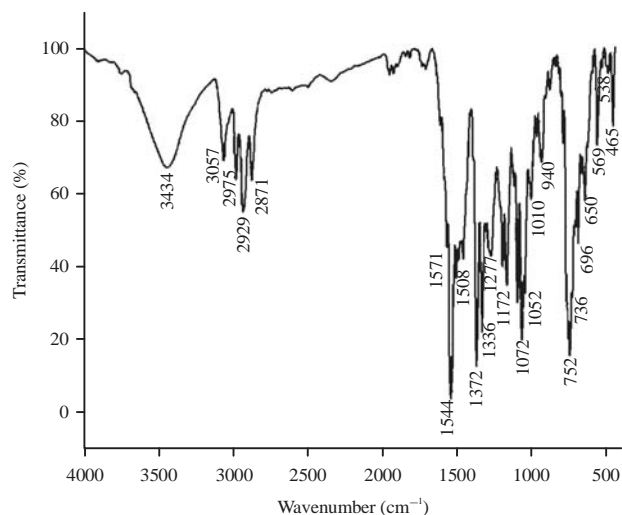


Fig. 2: FT-IR spectrum for BPNTSIPT crystal

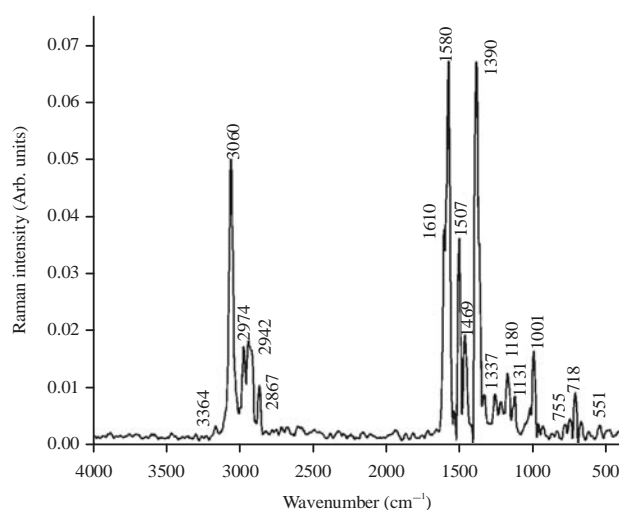


Fig. 3: FT-Raman spectrum for BPNTSIPT crystal

and C=N stretching vibrations occurred in indeno quinoxaline moiety. The C-H stretching vibration normally appeared in the region of 3100-3000  $\text{cm}^{-1}$  <sup>13-15</sup>. By using B3LYP method, Subramanian *et al.*<sup>16</sup> reported the C-H stretching vibration of quinoline ring at 3062, 3052, 3038, 3029 and 3026  $\text{cm}^{-1}$ . In the present work, the C-H stretching vibration for indeno quinoxaline ring was observed at 3057  $\text{cm}^{-1}$  in FT-IR and at 3060  $\text{cm}^{-1}$  in FT-Raman spectra for title compound respectively. The in-plane and out-of-plane aromatic C-H deformation vibrations occur in the region 1300-1000  $\text{cm}^{-1}$ <sup>15</sup>. The theoretically predicted C-H in-plane bending vibrations by Babu *et al.*<sup>17</sup> were at 1406, 1394, 1344, 1308, 1293, 1278, 1259, 1231, 1164, 1128, 1117  $\text{cm}^{-1}$ . For the title compound,  $\beta$ (C-H) mode was identified at 1277, 1200, 1172, 1124, 1101, 1072, 1052  $\text{cm}^{-1}$  in IR and at 1265, 1225, 1180, 1131, 1025  $\text{cm}^{-1}$  in Raman spectra respectively. The out-of-plane bending mode of C-H group appeared in the region 900-667  $\text{cm}^{-1}$ <sup>14</sup>. Li and Zhang<sup>18</sup> reported C-H out-of-plane bending mode at 816  $\text{cm}^{-1}$  and also calculated by using DFT/B3LYP method at 960, 934, 835 and 803  $\text{cm}^{-1}$ . The vibration due to  $\gamma$ (C-H) mode was assigned at 886, 847, 796, 752, 696, 675  $\text{cm}^{-1}$  in IR spectrum and the same mode was observed at 842, 785, 755, 678  $\text{cm}^{-1}$  in Raman spectrum for title compound.

The ring C-C stretching vibrations observed in the region 1625-1430  $\text{cm}^{-1}$  <sup>14</sup>. Rofouei *et al.*<sup>19</sup> the C-C stretching modes have been noticed at 1589, 1516  $\text{cm}^{-1}$  in FT-IR and at 1596, 1541  $\text{cm}^{-1}$  in FT-Raman spectra. For the title compound, wave numbers were observed in IR spectrum at 1508, 1463  $\text{cm}^{-1}$  and at 1507, 1419  $\text{cm}^{-1}$  in Raman spectrum was assigned to C-C stretching modes. The appearance of C=C stretching mode normally seen in the range 1674-1504  $\text{cm}^{-1}$  <sup>14</sup>. In the present study it was observed as medium bands at 1616, 1544  $\text{cm}^{-1}$  in IR and at 1610, 1544  $\text{cm}^{-1}$  in Raman spectra respectively.

The appearance of C=N stretching frequencies were identified as strong absorption bands in the region 1630-1600  $\text{cm}^{-1}$ . Also, the bands appeared in the region 1150-1130  $\text{cm}^{-1}$  were assigned to  $\nu$ (C-N) vibration<sup>20,21</sup>. Al-Jibouri and Hasun<sup>22</sup> reported the (C=N) mode at 1610  $\text{cm}^{-1}$  for amide pyrazine compound. Gulluoglu *et al.*<sup>20</sup> reported the C-N stretching mode at 1135  $\text{cm}^{-1}$  for piperidine molecule. Based on these literature data, the C=N and C-N stretching modes of indeno quinoxaline ring were attributed at 1616, 1610  $\text{cm}^{-1}$  and at 1124, 1131  $\text{cm}^{-1}$  in both spectra respectively in the present work. Generally the strong band in the region nearly around 500  $\text{cm}^{-1}$  was due to C-C-N group deformation mode<sup>23</sup>. Gunasekaran and Anitha<sup>24</sup> reported the deformation mode for C-C-N group due to the bands at 669, 612, 601  $\text{cm}^{-1}$  and 565  $\text{cm}^{-1}$  for piperazine compound. In the present

analysis, the weak bands observed at 675, 650, 632, 569, 538  $\text{cm}^{-1}$  in IR and at 678, 551, 548  $\text{cm}^{-1}$  in Raman spectra respectively were attributing to C-C-N deformation mode.

**Vibrations of nitro group:** The wavenumbers that arise between 1570-1485 and 1370-1320  $\text{cm}^{-1}$ , respectively were attributed to anti symmetric and symmetric stretching vibrations of aromatic nitro compound ( $\text{NO}_2$ )<sup>25-28</sup>. Gobinath and Xavier<sup>29</sup> have assigned the bands at 1570  $\text{cm}^{-1}$  (IR), 1598  $\text{cm}^{-1}$  (DFT) to anti symmetric stretching modes of  $\text{NO}_2$  group of 2-bromo-5-nitrothiazole compound. Also, the symmetric stretching mode for the same compound was assigned by Gobinath and Xavier<sup>29</sup> at 1365  $\text{cm}^{-1}$  (Raman), 1379  $\text{cm}^{-1}$  (DFT). In the present study, the observed medium IR band at 1571  $\text{cm}^{-1}$  and strong Raman band at 1580  $\text{cm}^{-1}$  were attributed to the anti symmetric stretching mode of  $\text{NO}_2$  group. Also, the band identified at 1372  $\text{cm}^{-1}$  in IR spectrum has been assigned to the symmetric stretching mode of  $\text{NO}_2$  group.

The appearance of bands due to bending modes of aromatic nitro compounds were usually seen at  $855 \pm 40 \text{ cm}^{-1}$  ( $\text{NO}_2$  scissoring),  $760 \pm 30 \text{ cm}^{-1}$  ( $\text{NO}_2$  wagging),  $540 \pm 30 \text{ cm}^{-1}$  ( $\text{NO}_2$  rocking) and  $70 \pm 20 \text{ cm}^{-1}$  ( $\text{NO}_2$  torsional)<sup>30</sup>. The  $\text{NO}_2$  scissoring, wagging and rocking modes were reported by Panicker *et al.*<sup>31</sup> at 800, 724, 534  $\text{cm}^{-1}$  (theoretically) and at 809, 727, 717, 524  $\text{cm}^{-1}$  (experimentally). For 2-(p-fluorobenzyl)-6-nitrobenzoxazole molecule, Sheena Mary *et al.*<sup>30</sup> observed the bands for  $\text{NO}_2$  scissoring modes at 778  $\text{cm}^{-1}$  (DFT), 773  $\text{cm}^{-1}$  (IR) 773  $\text{cm}^{-1}$  (Raman) and the wagging mode at 692  $\text{cm}^{-1}$  (DFT) respectively. Also, the rocking mode of  $\text{NO}_2$  group for the same compound was assigned at 533  $\text{cm}^{-1}$  (DFT), 522  $\text{cm}^{-1}$  (IR), 528  $\text{cm}^{-1}$  (Raman) and torsional mode at 61  $\text{cm}^{-1}$  (DFT)<sup>30</sup>. In the present work, the scissoring, wagging and rocking modes of  $\text{NO}_2$  group were identified at 847, 796 and 538  $\text{cm}^{-1}$  in IR and at 842, 785 and 548  $\text{cm}^{-1}$  in Raman spectra respectively with the support of literature data of relative compound. For 5-bromo 2-nitropyridine molecule, Arivazhagan and Jeyavijayan<sup>27</sup> reported C- $\text{NO}_2$  stretching mode theoretically at 1540  $\text{cm}^{-1}$  and experimentally at 1545  $\text{cm}^{-1}$  in FT-Raman spectrum. The bands corresponding to the stretching vibration of C- $\text{NO}_2$  appears at 1544  $\text{cm}^{-1}$  in both spectra for the title compound.

**Vibrations of pyrrolothiazole ring:** The C-H stretching bands for furans, pyrroles and thiophenes appeared in the region 3180-3090 and 3120-3060  $\text{cm}^{-1}$ , respectively<sup>14,32</sup>. The C-H stretch for 2-thiophene carboxylic acid compound, Magdaline and Chithambarathanu<sup>33</sup> predicted theoretically in the range 3117-3080  $\text{cm}^{-1}$  by B3LYP method. In the present work, a

weak band observed at  $3164\text{ cm}^{-1}$  in Raman spectrum was assigned to C-H stretch for pyrrole ring and the same mode was attributed at  $3057\text{ cm}^{-1}$  and at  $3060\text{ cm}^{-1}$  in both spectra for thiazole ring.

Naturally, the C-H in-plane and out-of-plane bending wave numbers appeared in the region between  $1300\text{-}1000$  and  $1000\text{-}750\text{ cm}^{-1}$ <sup>34</sup>. The bands at  $1283, 1105, 1041\text{ cm}^{-1}$  in FT-IR and at  $1114\text{ cm}^{-1}$  in FT-Raman were reported by Magdaline and Chithambarathanu<sup>33</sup> to C-H in plane bending modes and the C-H out-of-plane bending vibrations were assigned at  $910, 858\text{ cm}^{-1}$  in FT-IR and at  $862\text{ cm}^{-1}$  in FT-Raman for the 2-thiophene carboxylic acid molecule<sup>33</sup>. Based on 2-thiophene carboxylic acid molecule literature data reported by Magdaline and Chithambarathanu<sup>33</sup>, the  $\beta(\text{C-H})$  mode was attributed at  $1277, 1200, 1172, 1124, 1101, 1072, 1052\text{ cm}^{-1}$  in IR and at  $1265, 1225, 1180, 1131, 1025\text{ cm}^{-1}$  in Raman spectra respectively for the title compound. The  $\gamma(\text{C-H})$  mode was assigned as medium bands at  $886, 847\text{ cm}^{-1}$  in IR and at  $842\text{ cm}^{-1}$  in Raman spectra respectively.

Many researchers observed the  $\text{CH}_2$  antisymmetric stretching vibrations were exist in the region  $3000\text{-}2900\text{ cm}^{-1}$ , while the  $\text{CH}_2$  symmetric stretch will appeared between  $2900$  and  $2800\text{ cm}^{-1}$ <sup>35-37</sup>. Babu *et al.*<sup>17</sup> described the  $\text{CH}_2$  symmetric stretching vibration for Irinotecan molecule at  $2943\text{ cm}^{-1}$  in IR spectrum. Also, the intended wavenumbers of  $\text{CH}_2$  anti symmetric and symmetric stretching vibrations for Irinotecan molecule were seen in the range  $3008\text{-}2951\text{ cm}^{-1}$  and  $2948\text{-}2903\text{ cm}^{-1}$ , respectively. In the present work, bands were identified at  $2929\text{ cm}^{-1}$  in IR and at  $2942\text{ cm}^{-1}$  in Raman spectra for antisymmetric stretching mode of  $\text{CH}_2$  group respectively. Also, the symmetric stretching mode of the  $\text{CH}_2$  group of five membered rings was assigned at  $2871, 2867\text{ cm}^{-1}$  in both spectra for the title compound. The bending modes wavenumber assignment orders for the  $\text{CH}_2$  group were given as follows:  $\text{CH}_2$  scis> $\text{CH}_2$  wag> $\text{CH}_2$  twist> $\text{CH}_2$  rock<sup>17</sup>. Theoretically reported values of  $\text{CH}_2$  scissoring mode fall in the range  $1482\text{-}1437\text{ cm}^{-1}$  and also observed FT-IR and FT-Raman bands at  $1435$  and  $1449\text{ cm}^{-1}$ , respectively for Irinotecan molecule<sup>17</sup>. It is attributed as medium bands at  $1463\text{ cm}^{-1}$  and  $1469\text{ cm}^{-1}$  in both spectra respectively in the present work.

Generally, the wagging and twisting vibrations of  $\text{CH}_2$  group were observed in the region  $1390\text{-}1180\text{ cm}^{-1}$ <sup>14</sup>. These modes were assigned by Babu *et al.*<sup>17</sup> at  $1373, 1323, 1233, 1222\text{ cm}^{-1}$  (B3LYP),  $1373, 1329\text{ cm}^{-1}$  (IR),  $1376, 1236, 1223\text{ cm}^{-1}$  (Raman) respectively. The absorption bands at  $1372, 1336, 1277\text{ cm}^{-1}$  (IR),  $1337, 1265\text{ cm}^{-1}$  (Raman) on pyrrolo thiazole ring of title compound have been interpreted as due to  $\text{CH}_2$  wagging and twisting vibrations respectively.

The rocking vibration of cyclopentane group splitting due to crystallinity and appears at  $730$  and  $720\text{ cm}^{-1}$ <sup>14</sup>. The rocking mode of  $\text{CH}_2$  group calculated by B3LYP method at  $968, 914\text{ cm}^{-1}$ <sup>17</sup>. In this present work, the existing bands at  $752, 717\text{ cm}^{-1}$  in IR spectrum and at  $755, 718\text{ cm}^{-1}$  in Raman spectrum was assigned to the rocking modes of  $\text{CH}_2$  group of pyrrolo thiazole ring. The ring breathing mode for pyrrolidine five membered rings appears at  $902\text{ cm}^{-1}$ <sup>14</sup>. This mode was recognized at  $940\text{ cm}^{-1}$  in IR spectrum and at  $937\text{ cm}^{-1}$  in Raman spectrum for pyrrolo thiazole ring in the present study.

The C-C stretching vibrations arised generally in the region  $1600\text{-}1350\text{ cm}^{-1}$ . For 2-substituted thiophenes, the C-C band was observed in the regions between  $1532\text{-}1514, 1454\text{-}1430$  and  $1367\text{-}1347\text{ cm}^{-1}$ . For five membered heterocyclic rings, wide wavenumber variation can occur due to position and intensity of the bands was more sensitive than the corresponding bands of benzene in the substituent<sup>32</sup>. Xavier *et al.*<sup>32</sup> observed in the FT-IR spectrum at  $1528$  and  $1352\text{ cm}^{-1}$  were assigned to C-C stretching vibrations. Magdaline and Chithambarathanu<sup>33</sup> theoretically predicted the C-C stretching vibrations at  $1526, 1410$  and  $1356\text{ cm}^{-1}$  by DET/B3LYP method. In the present work, the stretching of C-C bonds in the pyrrolo thiazole ring was identified at  $1544, 1508, 1463, 1372\text{ cm}^{-1}$  in IR and at  $1580, 1507, 1469\text{ cm}^{-1}$  in Raman spectra respectively which shows good agreement with the reported spectral data<sup>32,33</sup>. The C-S stretching mode was observed between region  $710\text{-}687\text{ cm}^{-1}$ <sup>38,39</sup>. Magdaline and Chithambarathanu<sup>33</sup> observed theoretically the stretching of C-S bond in the thiophene ring at  $852, 649\text{ cm}^{-1}$  but only one peak was observed at  $647/637$  in the experimental FT-IR/FT-Raman spectra. For the title compound, a strong band occurs at  $796, 696\text{ cm}^{-1}$  in IR and at  $785\text{ cm}^{-1}$  in Raman spectra were assigned to C-S stretching mode of thiazole ring. The mixing of pyrrolo ring and substituent of  $\text{NO}_2$  group affecting the stretching wavenumber of C-S group and gets upshifted. Xavier *et al.*<sup>32</sup> observed bands at  $1425, 1440\text{ cm}^{-1}$  for C-N stretching vibration of 1,2,4triazole ring. In the present study, N stretching mode of pyrrolo thiazole ring was identified in both spectra at  $1463$  and  $1469\text{ cm}^{-1}$ .

The strong peak that occurred at  $3434\text{ cm}^{-1}$  in the IR spectrum was due to incorporation of water molecule during KBr pellet preparation. The corresponding Raman band was so weak that it is hardly noticeable.

**Vibrations of bromo phenyl ring:** For 1, 4 di-substituted benzene, the C-H stretching modes were found in the region  $3105\text{-}3000\text{ cm}^{-1}$ <sup>40</sup>. Zainuri *et al.*<sup>41</sup> reported theoretically, the phenyl C-H stretching modes in the range  $3103\text{-}3075\text{ cm}^{-1}$  by DFT method and experimentally observed at  $3081\text{ cm}^{-1}$  in IR

spectrum for (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one molecule. For the title compound, the bands at 3057, 2975  $\text{cm}^{-1}$  in IR and at 3064, 2974  $\text{cm}^{-1}$  in Raman spectra were assigned to the bromo phenyl C-H stretching mode in the present work. The in-plane bending vibrations of C-H modes for 1,4-disubstituted benzenes were expected in the range 1315-1015  $\text{cm}^{-1}$ . The out-of-plane deformations of aromatic C-H were usually observed between 995 and 720  $\text{cm}^{-1}$ . These vibrations were reported theoretically by Zainuri *et al.*<sup>41</sup> to bands at 1268, 1189, 1165, 1037  $\text{cm}^{-1}$  and at 975, 942, 858, 806  $\text{cm}^{-1}$ , respectively. In IR spectrum, in plane and out of plane vibrations of aromatic C-H group are observed at 1256, 1178, 1031, 1006 and 834, 813  $\text{cm}^{-1}$ , respectively for (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one molecule<sup>41</sup>. In the present work, the  $\beta$ (C-H) mode was attributed at 1277, 1172, 1072, 1052, 1010  $\text{cm}^{-1}$  in IR spectrum and at 1265, 1180, 1025, 1001  $\text{cm}^{-1}$  in Raman spectrum. Also,  $\gamma$ (C-H) mode has been found at 972, 940, 886, 847  $\text{cm}^{-1}$  and at 970, 937, 842  $\text{cm}^{-1}$  in both spectra for the title compound. The in-plane and out-of-plane C-C-C bending vibrations have been identified by Varsanyi<sup>13</sup> at 610  $\text{cm}^{-1}$  and at 590, 500, 350  $\text{cm}^{-1}$  in FT-IR respectively. For the title compound these modes were attributed at 632  $\text{cm}^{-1}$  and at 569, 538, 465  $\text{cm}^{-1}$  in the IR spectrum respectively. The out-of-plane bending mode has corresponding wavenumber at 551, 548  $\text{cm}^{-1}$  in Raman spectrum.

The C=C stretching mode of benzene ring is normally occurs in the range 1660-1580  $\text{cm}^{-1}$  while the theoretically computed C=C vibrations are in the range 1674-1504 and 1437-1428  $\text{cm}^{-1}$  as suggested by Anbarasan *et al.*<sup>42</sup>. The wave numbers observed by Babu *et al.*<sup>17</sup> in the FT-IR spectrum at 1687, 1612, 1435  $\text{cm}^{-1}$  and in FT-Raman spectrum at 1669, 1614, 1566  $\text{cm}^{-1}$  have been assigned to C=C stretching vibrations of Irinotecan molecule. For the title compound  $\nu$ (C=C) vibrations was observed at 1616, 1571, 1544, 1508  $\text{cm}^{-1}$  (IR), 1610, 1580, 1544, 1507  $\text{cm}^{-1}$  (Raman). In all substituted benzenes, C-C stretching mode is usually observed in the region 1650-1400  $\text{cm}^{-1}$ . For 4-chlorotoluene molecule this mode was assigned by Anbarasan *et al.*<sup>42</sup> at 1605, 1477, 1390  $\text{cm}^{-1}$ . In the present work, this mode was identified at 1478, 1463, 1336  $\text{cm}^{-1}$  in IR and at 1469, 1390, 1337  $\text{cm}^{-1}$  in Raman spectra for title compound.

The ring breathing modes of para-substituted benzenes were usually observed in the interval 840-680  $\text{cm}^{-1}$ . The ring breathing modes were assigned by Zainuri *et al.*<sup>41</sup> at 792  $\text{cm}^{-1}$  for phenyl ring theoretically and observed at 790  $\text{cm}^{-1}$  in the IR spectrum for (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one molecule. This mode was observed in IR and Raman spectra at 796  $\text{cm}^{-1}$  and at 785  $\text{cm}^{-1}$  for title compound of p-bromo phenyl ring.

The C-Br bond shows lower absorption frequency as compared to C-H bond due to the decreased force constant and increase in reduced mass. Literature reports showed that aromatic C-Br stretching vibrations occur strongly at 650-395  $\text{cm}^{-1}$  in the IR spectrum<sup>43</sup>. For the (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one compound, bands calculated at 513  $\text{cm}^{-1}$  and observed a peak at 524  $\text{cm}^{-1}$  in the IR spectrum was due to the C-Br stretching vibration. The weak bands observed at 538 and 548  $\text{cm}^{-1}$  in both spectra were assigned to the C-Br stretching mode of title compound.

**Hydrogen bonding:** The crystalline assembly of BPNTSIPT crystal was stabilized through weak intermolecular C-H...Br, C-H...S, C-H...N and C-H...O interactions<sup>11</sup>. But the presence of these hydrogen bonds was weak in title crystal. They play an important role to stabilize the crystal structure of biological macromolecule. However, in the spectroscopic features, they do not involved wavenumber shifting of related functional group stretching and bending mode frequencies.

**Optical analysis:** The UV-Visible absorbance spectrum of BPNTSIPT crystal was recorded and shown in Fig. 4. The crystal has the maximum absorbance peaks at 267, 347 and 369 nm. The lower cut-off wavelength was found to be at 314 and 364 nm. The title crystal has 100% transmittance in the entire visible region. The Tauc's relation  $(\alpha h\nu)^2 = A(h\nu - E_g)$  was used to determine the energy gap value  $E_g$  of title crystal by plotting  $(\alpha h\nu)^2$  Vs photon energy. The linear portion of  $(\alpha h\nu)^2$  is extrapolate to the photon energy axis gives the energy gap values of title crystal. From the Fig. 5, the energy gap value

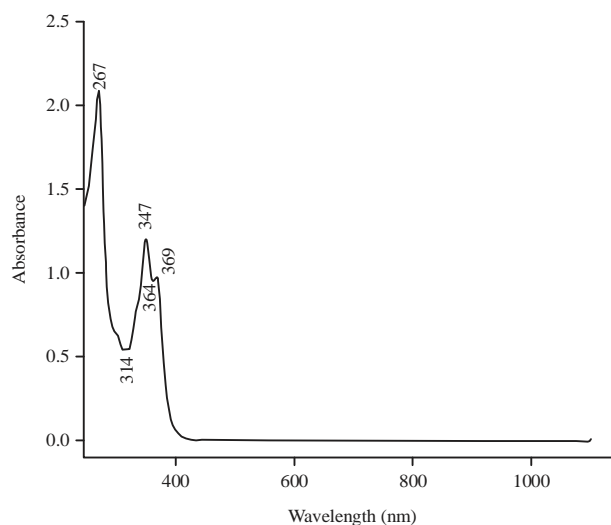


Fig. 4: Absorbance spectrum for BPNTSIPT crystal



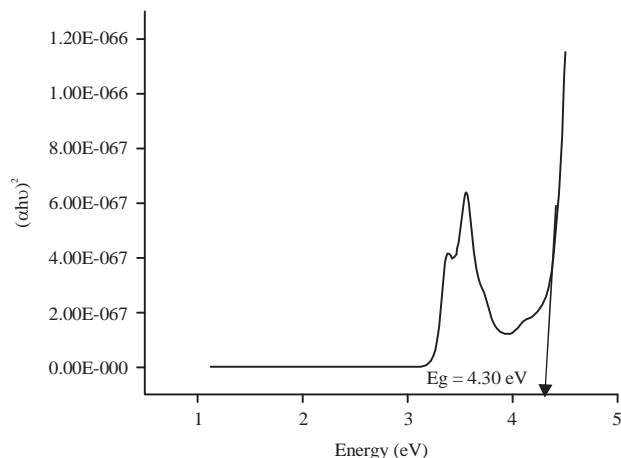


Fig. 5: Optical band gap for BPNTSIPT crystal

was determined as 4.3 eV for 6'-(3-bromo phenyl)-7'-nitro-1', 6', 7', 7a'-tetrahydro-3'H-spiro[indeno[1,2-b]quinoxaline-11, 5'-pyrrolo[1,2-c]thiazole]. This large band gap showed that the grown crystal is a predictable dielectric material.

### CONCLUSION

A halogen substituted indeno quinoxaline derivative crystal was successfully synthesized and crystallized by slow evaporation method. The complete vibrational FT-IR and FT-Raman spectra were interpreted in terms of functional group wavenumbers and their assignments which have been seen to be in good agreement with the corresponding results in the literature. The presence of weak hydrogen bonds does not involve in wavenumber shifting to up or down. The crystal has the maximum absorbance peaks at 267, 347 and 369 nm. The optical band gap was found to be as 4.3 eV which showed that the grown crystal is a predictable dielectric material.

### SIGNIFICANCE STATEMENT

This study discovers the new heterocyclic compound of halogen substituted indeno quinoxaline derivative crystal that can be beneficial for human beings in pharmaceutical field. This study will help the researcher to uncover the critical areas of crystal growth in halogen substituted indeno quinoxaline derivatives that many researchers were not able to explore. Thus a new attempt is made on the growth of indeno quinoxaline derivative crystal by bromine substitution and analyzed by spectroscopic approach may be arrived at.

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