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Research Article
FT-IR and FT-Raman Spectroscopic Analyzes of Indeno Quinoxaline Derivative Crystal

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Abstract

Background and Objective: The single crystal of ethyl 6'-cyano-7'-phenyl-1',6',7',7a' tetrahydro-3'H-spiro[indeno[1,2-b] quinoxaline-11,5'-pyrrolo [1,2-c] thiazole-6'-carboxylate (ECPTSIPTC) was crystallized by slow evaporation method after synthesis of compound. The main objective of the present study was to analyze complete vibration spectra of ECPTSIPTC compound through the FT-IR and FT-Raman techniques. **Materials and Methods:** Indeno quinoxaline, thioproline, ethyl cyano acetate, benzaldehyde, ethyl acetate and chloroform were used to grow the single crystal of title compound which were purchased from Sigma Aldrich company through local scientific companies in Tamil Nadu, India. The slow evaporation technique was employed to grow needle shaped ECPTSIPTC crystal using the chloroform as a solvent. **Results:** The vibrational spectra were recorded at room temperature using the FT-IR and FT-Raman spectrometers in the wavelength range 4000-400 cm^{-1}. The optical property was performed by double beam spectrophotometer in the wavelength range 200-1100 nm. **Conclusion:** The FT-IR, FT-Raman vibrational spectral studies confirmed the various functional groups present in the title compound. The optical property of the title compound shows that the grown crystal has high transparency in the entire visible region and the energy gap was found to as 4.8 eV. Due to the wide applications of title compound in biological and pharmaceutical fields, it was considered for study in this present work.

Key words: Heterocyclic compound, FT-IR, FT-raman, UV-visible spectroscopy

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

INTRODUCTION

Spiro and its heterocyclic compounds have more interest due to their biological properties[1-3]. In addition, the nitrogen containing heterocyclic compound of quinoxaline have wide range of applications in biological and pharmaceutical fields[4,5]. It is used as a dye, DNA cleaving agent, organic semiconductors, efficient electroluminescent, cavitands and dihydroannunulenes[6]. The fusion of various compounds into the quinoxaline moiety modify its structure which provide the development of biological diversities, therapeutic targets, drug design and future drug discovery[7-9]. The quinoxaline derivatives possess anti-protozoal, anti-cancer, anti-malarial, anti-microbial anti-viral, anti-inflammatory, antidiabetic, anti-tubercular, anti-nociceptive, anthelmintic and as a kinase inhibitor[10-12]. Also the thiazole and its derivatives exhibit the herbicidal, anti-bacterial, anti-fungal and anti-inflammatory activities[13-16]. In view of the important biological activities of indeno quinoxaline pyrolothiazole derivatives, an attempt was made to synthesis the quinoxaline fused ring derivatives led us to the title compound. The crystal structure of ECPTSIPTC compound was recently reported by Muthuselvi *et al.*[17]. The chemical diagram of ECPTSIPTC crystal is depicted in Fig. 1 which was taken from the recently published X-ray paper of Muthuselvi *et al.*[17]. In the present work, the vibrational analyzes of the title compound was performed in order to establish its conformation through FT-IR, FT-Raman and UV-Visible spectroscopy techniques. The motivation of this study is that it will help the researchers to synthesis the new hetero cyclic compound with medicinal and biological activity for research in organic and medicinal chemistry.

MATERIALS AND METHODS

The raw materials used for this crystallization were indeno quinoxaline, thioproline, ethyl cyano acetate, benzaldehyde, ethyl acetate and chloroform which were purchased from Sigma Aldrich Company. Primarily, an equimolar amount of indeno quinoxaline and thiazolidine-4-carboxylic acid was dissolved in a round bottom flask containing 20 mL of
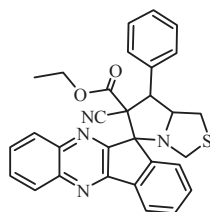

Fig. 1: Molecular structure of ECPTSIPTC Crystal

methanol and refluxed under water bath for 2 min. Then equimolar amount of propyl (E)-2-cyano acrylate added to the reaction mixture and continued for refluxing until completion of the reaction. The reaction progress was monitored intermittently using thin-layer chromatography (TLC). As evident from the TLC the reaction attained completion after 4 h of continuous refluxing. The precipitated solid was fitered and washed with methanol to obtain the compound in good yields (94-98%). The colourless needle shaped crystals were so obtained by the slow evaporation of chloroform solution. For the grown crystal, the FT-IR vibrational spectrum was recorded by using SHIMADZU FT-IR spectrometer in the range 4000-400 cm^{-1}. Also, the FT-Raman spectrum was recorded by using the BRUKER: RFS 27 Raman spectrometer in the wave number range 4000-400 cm^{-1}. These vibrational spectral data was recorded at SAIF, IIT Madras, Chennai. The optical absorption spectrum of title compound has been recorded at Research Department of Chemistry, V. H. N. S. N. College, Virudhunagar with SHIMADZU-UV1800 double beam spectrometer in the wavelength range 200-1100 nm insteps of 1 nm. The present work reported in this article was done by us at Research Department of Physics, Devanga Arts College, Aruppukottai, Tamil Nadu, India, during the year 2018 and completed within two months duration.

RESULTS AND DISCUSSION

Spectroscopic analyses: The spectroscopic method is a powerful tool for understanding the fundamental vibrational properties of compound. Regarding to this, the vibrational spectra of ECPTSIPTC crystal was analyzed by using the FT-IR and FT-Raman spectroscopy techniques. The title compound has C-H, CH$_2$, CH$_3$, C=O, C-O, C-N, C=N, C$\equiv$N, C-S, C-C functional groups. The FT-IR and FT-Raman spectra of title compound are depicted in Fig. 2 and 3, respectively. The detailed wave number assignments for this compound are shown in Table 1.

Indeno quinoxaline vibrations: Indeno quinoxaline fused rings have C-H stretching, C-H in-plane bending, C-H out-of-plane bending, C-C, C=C, C-N and C=N stretching vibrations. The C-H stretching vibrations show the characteristic bands in the region of 3100-3000 cm^{-1} for hetro aromatic ring which were not affected appreciably by the nature of the substituent[18-20]. Subramanian *et al.*[21] reported the C-H stretching vibrations of quinoline ring in B3LYP method at 3062, 3052, 3038, 3029 and 3026 cm^{-1}. In the present work, the C-H stretching vibration for indeno quinoxaline ring is observed at 3063 and 3038 cm^{-1} in FT-IR and at 3064 and 3037cm^{-1} in FT-Raman spectra for C-H vibrations, respectively. The in-plane and out-of-plane aromatic C-H deformation
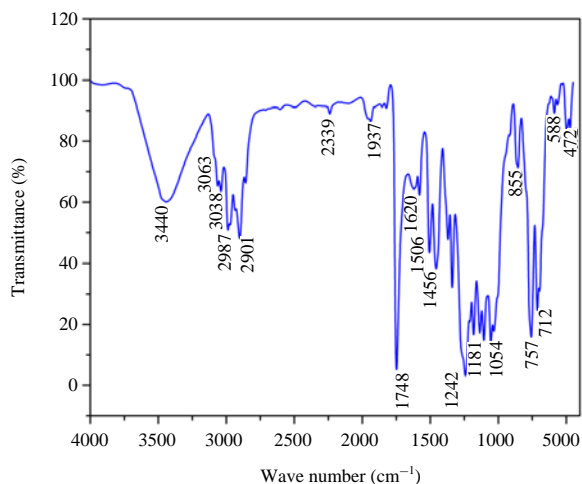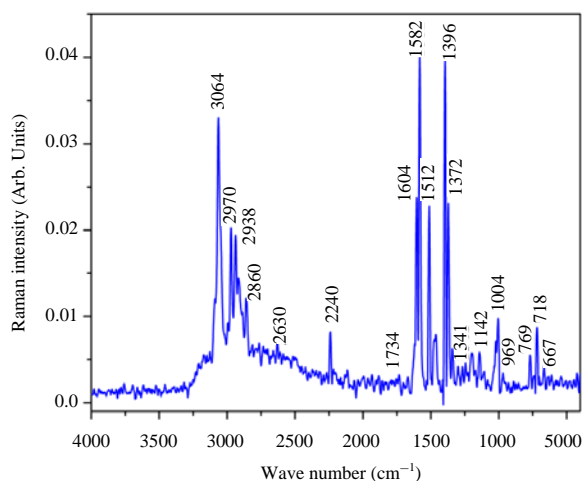
Fig. 2: FT-IR spectrum for ECPTSIPTC crystal

Fig. 3: FT-Raman spectrum for ECPTSIPTC crystal

vibrations occur in the region[19] 1300-1000 cm⁻¹. Babu *et al.*[22] have predicted C-H in-plane bending vibrations by B3LYP at 1406, 1394, 1344,1308, 1293, 1278, 1259, 1231, 1164, 1128 and 1117 cm⁻¹. For the title compound, β(C-H) mode is identified by the strong bands at 1242, 1209, 1181, 1135, 1105, 1054 and 1032 cm⁻¹ in IR and weak bands at 1245, 1200, 1193 and 1142 cm⁻¹ in Raman spectra respectively. The out-of-plane bending mode of C-H group appears in the region[20] 900-667 cm⁻¹. Li *et al.*[23] observed the out-of-plane bending mode of C-H group at 816 cm⁻¹ and also its calculated wave numbers fall at 960, 934 and 835 cm⁻¹ and 803 cm⁻¹ in DFT/B3LYP method. The wave numbers due to γ (C-H) of indeno quinoxaline are assigned due to strong bands at 855, 757, 712 cm⁻¹ and 696 cm⁻¹ in IR spectrum. In Raman spectrum this mode is observed as medium bands at

769,718 and 667 cm⁻¹. The ring carbon-carbon stretching vibrations occur in the region[20] 1625-1430 cm⁻¹. By Rofouei *et al.*[24] the C-C stretching modes have been observed at 1589 and 1516 cm⁻¹ in FT-IR and at 1596 and 1541 cm⁻¹ in FT-Raman spectra. For the title compound the wave numbers observed in IR spectrum at 1579 and 1506 cm⁻¹ and at 1582 and 1512 cm⁻¹ in Raman spectrum is assigned to this C-C stretching modes. The C=C stretching vibrations appear in the range[20] 1674-1504 cm⁻¹. In the present study, it is observed as medium bands at 1620 cm⁻¹ in IR and at 1604 cm⁻¹ in Raman spectra, respectively for title compound. The appearance of strong absorption band in the region 1630-1600 cm⁻¹ corresponds to υ (C=N) stretching frequency. The band present in the range 1150-1130 cm⁻¹ was assigned due to ν (C-N) vibration[25,26]. Al Jibouri *et al.*[27] reported the (C=N) mode at 1610 cm⁻¹ for amide pyrazine compound. Gulluoglu *et al.*[25] reported the C-N stretching mode at 1135 cm⁻¹ for piperidine molecule. Based on the literature data, the C-N and C=N stretching modes of indeno quinoxaline ring are attributed at 1135 and 1620 cm⁻¹ in IR and at1142, 1604 cm⁻¹ in Raman spectra, respectively. Generally, it has been observed that the strong band in the region nearly around 500 cm⁻¹ is due to C-C-N group deformation mode[28]. Gunasekaren *et al.*[29] reported the deformation mode for C-C-N group 669, 612 and 601 cm⁻¹ and 565 cm⁻¹ for piperazine compound. In the present investigation, the medium IR bands observed at 696, 588 and 564 cm⁻¹ and Raman bands at 667, 621, 568 and 536 cm⁻¹ are attributed to C-C-N deformation mode.

Pyrrolothiazole ring vibrations: The pyrrolothiazole ring modes are discussed on the basis of the vibrations of substituted cyclopentane five membered ring (CH₂, C-C and C-H), C-N and C-S modes. The CH₂ anti-symmetric stretching vibrations are generally observed in the region 3000-2900 cm⁻¹, while the CH₂ symmetric stretch will appear between[30,31] 2900 and 2800 cm⁻¹. Babu *et al.*[22] observed the CH₂ anti-symmetric stretching vibration at 2943 cm⁻¹ in FT-IR spectrum for Irinotecan molecule. The calculated anti-symmetric and symmetric CH₂ stretching vibrations of the Irinotecan molecule are in the range 3008-2951 and 2948-2903 cm⁻¹, respectively. In the present work, anti-symmetric stretching mode of CH₂ is identified at 2934 and 2938 cm⁻¹ in IR and Raman spectra, respectively. Also, the symmetric stretching mode of the CH₂ group of five membered ring is assigned at 2857 cm⁻¹ in IR and at 2860 cm⁻¹ in Raman spectra, respectively for the title compound. The general wave number assignment order for the CH₂ bending modes are as follows[22]: CH₂scis>CH₂wag>CH₂twist>CH₂rock. Babu *et al.*[22] reported

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

FT-IR ($\bar{\upsilon}$/cm^{-1})	FT-Raman ($\bar{\upsilon}$/cm^{-1})	Assignment
-	3153 (w)	υ (C-H)$_{Pyrrolo\ thiazole}$; υ(C-H)$_{Phenyl}$
-	3116 (w)	υ (C-H)$_{Phenyl}$
3063 (m)	3064 (s)	υ (C-H)$_{Indeno\ quinoxaline}$
3038 (m)	3037 (w)	υ (C-H)$_{Indeno\ quinoxaline}$
2987 (m)	-	υ_{as} (CH$_3$)$_{Ethyl\ cyano\ acetate}$
2971 (m)	2971 (w)	υ_{as} (CH$_3$)$_{Ethyl\ cyano\ acetate}$
2934(m)	2938 (m)	υ_{as} (CH$_2$)$_{Ethyl\ cyano\ acetate}$; υ_{as}(CH$_2$)$_{Pyrrolo\ thiazole}$
2901 (m)	-	υ_{s} (CH$_3$)$_{Ethyl\ cyano\ acetate}$
2857 (w)	2860 (m)	υ_{s} (CH$_2$)$_{Ethyl\ cyano\ acetate}$; υ_{s}(CH$_2$)$_{Pyrrolo\ thiazole}$
2239 (w)	2240 (w)	υ (C$\equiv$N)$_{Ethyl\ cyano\ acetate}$
1748 (s)	1734 (w)	υ (C=O)$_{Ethyl\ cyano\ acetate}$
1620 (m)	1604 (w)	υ (C=O)$_{Ethyl\ cyano\ acetate}$ υ(C=C)$_{Phenyl}$; υ(C=N)$_{Indeno\ quinoxaline}$; υ (C=C)$_{Indeno\ quinoxaline}$
1579 (m)	1582 (s)	υ (C-C)$_{Pyrrolo\ thiazole}$; υ(C=C)$_{Phenyl}$; υ(C-C)$_{Indeno\ quinoxaline}$
1506 (m)	1512 (s)	υ (C-C)$_{Indeno\ quinoxaline}$; υ(C-C)$_{Pyrrolo\ thiazole}$
1456 (m)	1463 (m)	υ (C-N)$_{Pyrrolothiazole}$; δ_{as}(CH$_3$)$_{Ethyl\ cyano\ acetate}$; ρ(CH$_2$)$_{Ethyl\ cyano\ acetate}$; υ(C-C)$_{Pyrrolo\ thiazole}$; ρ(CH$_2$)$_{Pyrrolo\ thiazole}$
-	1396 (w)	υ (C-C)$_{Pyrrolo\ thiazole}$; υ(C-C)$_{Phenyl}$; δ_{s}(CH$_3$)$_{Ethyl\ cyano\ acetate}$
1369 (m)	1371 (m)	υ (C-C)$_{Phenyl}$; ω (CH$_2$)$_{Pyrrolo\ thiazole}$; ω (CH$_2$)$_{Ethyl\ cyano\ acetate}$; υ(C-C)$_{Pyrrolo\ thiazole}$
1338 (s)	1341 (w)	υ (C-C)$_{Phenyl}$; ω (CH$_2$)$_{Pyrrolo\ thiazole}$; ω (CH$_2$)$_{Ethyl\ cyano\ acetate}$
1242 (s)	1245 (w)	β (C-H)$_{Indeno\ quinoxaline}$; t (CH$_2$)$_{Pyrrolo\ thiazole}$; β (C-H)$_{Pyrrolo\ thiazole}$; t (CH$_2$)$_{Ethyl\ cyano\ acetate}$; υ(C-O)$_{Ethyl\ cyano\ acetate}$
1209 (w)	1200 (w)	β (C-H)$_{Indeno\ quinoxaline}$; t (CH$_2$)$_{Pyrrolo\ thiazole}$; β (C-H)$_{Pyrrolo\ thiazole}$; t (CH$_2$)$_{Ethyl\ cyano\ acetate}$
1181 (s)	1193 (m)	β (C-H)$_{Indeno\ quinoxaline}$; β (C-H)$_{Phenyl}$; β (C-H)$_{Pyrrolo\ thiazole}$
1135 (s)	1142 (w)	β (C-H)$_{Indeno\ quinoxaline}$; υ(C-N)$_{Indeno\ quinoxaline}$; β (C-H)$_{Pyrrolo\ thiazole}$; υ_{as}(C-O-C); β (C-H)$_{Phenyl}$
1105 (s)	-	β (C-H)$_{Indeno\ quinoxaline}$; β (C-H)$_{Pyrrolo\ thiazole}$; β (C-H)$_{Phenyl}$
1054 (s)	-	β (C-H)$_{Indeno\ quinoxaline}$; υ_{as}(C-O-C)$_{Ethyl\ cyano\ acetate}$; τ (CH$_3$)$_{Ethyl\ cyano\ acetate}$; β (C-H)$_{Phenyl}$; β (C-H)$_{Pyrrolo\ thiazole}$
1032 (s)	-	β (C-H)$_{Indeno\ quinoxaline}$; τ (CH$_3$)$_{Ethyl\ cyano\ acetate}$; β (C-H)$_{Pyrrolo\ thiazole}$; β (C-H)$_{Phenyl}$
-	1021 (m)	Mono substituted benzene ring breathing mode
-	969 (w)	γ (C-H)$_{Pyrrolo\ thiazole}$; υ_{s}(C-O-C)$_{Ethyl\ cyano\ acetate}$; τ (CH$_2$)$_{Ethyl\ cyano\ acetate}$; γ(C-H)$_{Phenyl}$
-	923 (w)	τ (CH$_2$)$_{Ethyl\ cyano\ acetate}$; γ(C-H)$_{Phenyl}$
-	900(w)	γ (C-H)$_{Phenyl}$; Five membered ring breathing mode
-	869(w)	γ (C-H)$_{Phenyl}$
855 (m)	-	γ (C-H)$_{Phenyl}$; γ(C-H)$_{Indeno\ quinoxaline}$; υ(C-S)$_{Pyrrolo\ thiazole}$; γ(C-H)$_{Pyrrolo\ thiazole}$
-	812(w)	γ (C-H)$_{Phenyl}$
757 (s)	769 (m)	γ (C-H)$_{Indeno\ quinoxaline}$; γ(C-H)$_{Phenyl}$
-	741(w)	τ (CH$_2$)$_{Pyrrolo\ thiazole}$
712 (s)	718(w)	γ (C-H)$_{Indeno\ quinoxaline}$; υ(C-S)$_{Pyrrolo\ thiazole}$; τ (CH$_2$)$_{Pyrrolo\ thiazole}$
696 (w)	667 (m)	γ (C-H)$_{Indeno\ quinoxaline}$; δ(C-C-N)$_{Indeno\ quinoxaline}$; β(C=O)$_{Ethyl\ cyano\ acetate}$
-	621 (m)	δ (C-C-N)$_{Indeno\ quinoxaline}$; β(C-C-C)$_{Phenyl}$
588 (w)	-	δ (C-C-N)$_{Indeno\ quinoxaline}$; γ(C=O)$_{Ethyl\ cyano\ acetate}$; γ(C-C-C)$_{Phenyl}$
564 (w)	568 (m)	δ (C-C-N)$_{Indeno\ quinoxaline}$
-	536 (w)	δ (C-C-N)$_{Indeno\ quinoxaline}$
497 (w)	-	γ (C-C-C)$_{Phenyl}$

s: Strong, w: Weak, m: Medium, υ: Stretching, υ_{s}: Sym.stretching; υ_{as}: Anti sym.stretching, δ_{s}: Sym. bending, δ_{as}: Anti sym. bending, γ: Out-of-plane bending, β: In-plane bending, τ: Rocking, ω: Wagging, ρ: Scissoring, t: Twisting

theoretically the computed values of CH$_2$ scissoring modes fall in the range 1482-1437 cm^{-1} and also observed FT-IR and FT-Raman bands at 1435 and 1449 cm^{-1}, respectively for Irinotecan molecule. It is attributed as medium bands at 1456 and 1463 cm^{-1} in both spectra. The CH$_2$ twisting and wagging vibrations were observed in the region[20] 1180-1390 cm^{-1}. The CH$_2$ wagging and twisting modes were assigned by Babu *et al.*[22] at 1373, 1323, 1233 and 1222 cm^{-1} (B3LYP), 1373, 1329 cm^{-1}(IR), 1376, 1236 and 1223 cm^{-1} (Raman), respectively. The absorption bands at 1369, 1338, 1242 and 1209 cm^{-1} (IR) and at 1371, 1341, 1245 and 1200 cm^{-1} (Raman) on pyrrolo thiazole ring of title compound has been interpreted as due to CH$_2$ wagging and twisting vibrations, respectively. The rocking vibration of cyclopentane group appears at 730 and 720 cm^{-1}. This splitting is caused by crystallinity[20]. In this present work, the bands present in Raman spectrum at 741, 718 and at 712 cm^{-1} in IR spectrum are assigned to the rocking modes of CH$_2$ group of pyrrolo thiazole ring of title compound. The ring breathing mode for pyrrolidine five membered ring appears[20] at 902 cm^{-1}. This mode is identified at 900 cm^{-1} in Raman spectrum.

The appearance of bands in the region 3100-3000 cm^{-1} was due to C-H stretching mode for hetero aromatic compound such as furans, pyrroles and thiophenes[32]. Magdaline *et al.*[33] computed the C-H stretch for 2-thiophene carboxylic acid compound in the range 3117-3080 cm^{-1} by B3LYP method. In the present work C-H stretch for pyrrole ring is assigned as a weak band at 3153 cm^{-1} in Raman spectrum

only. The C-H in-plane bending wave numbers appear in the range 1300-1000 cm^{-1} and C-H out-of plane bending in the range[34] 1000-750 cm^{-1}. Also Magdaline *et al.*[33] reported bands at 1283, 1105 and 1041 cm^{-1} in FT-IR and at 1114 cm^{-1} in FT-Raman are described to C-H in plane bending modes. The C-H out-of-plane bending vibrations were assigned to the medium bands observed at 910 and 858 cm^{-1} in FTIR and to a weak band at 862 cm^{-1} in FT-Raman for the 2-thiophene carboxylic acid[34]. Based on the literature data, the β(C-H) mode is attributed at 1242, 1209, 1181, 1135, 1105, 1054 and 1032 cm^{-1} in IR and at 1245, 1200, 1193 and 1142 cm^{-1} in Raman spectra, respectively for the title compound. The γ(C-H) mode is assigned due to bands at 855 and 969 cm^{-1} in IR and Raman spectra, respectively.

The observed band at 1425 cm^{-1} can be assigned to the C-N stretching vibration of 1,2,4 triazole ring by Rao[32] and the calculated value of this mode was found at 1440 cm^{-1}. In the present study, observed medium bands at 1456 and 1463 cm^{-1} in both spectra are assigned to C-N stretching modes of thiazole ring of present compound respectively. The C-C stretching vibrations occur generally in the region 1600-1350 cm^{-1}. But for the five membered heterocyclic rings, position and intensity of the bands are more sensitive than the corresponding bands of benzene due to changes in the substituent. So that wide wave number variation can occur. For 2-substituted thiophenes four bands were observed in the ranges[32] 1532-1514, 1454-1430 and 1367-1347 cm^{-1}. Rao[32] observed IR bands at 1528 and 1352 cm^{-1} which were assigned to C-C stretching vibrations. Magdaline *et al.*[33] theoretically predicted the C-C stretching vibrations at 1526, 1410 and 1356 cm^{-1} by DET/B3LYP method. In the present work, the stretching of the C-C bonds in the thiazole ring are identified at 1579, 1506, 1456, 1369 cm^{-1} in IR and at 1582, 1512, 1463, 1396 and 1371 cm^{-1} in Raman spectra, respectively which shows good agreement with the reported spectral data[32-34]. Coats[35] observed C-S stretching modes between 710 and 687 cm^{-1} and Nogueira *et al.*[36] reported C-S stretching vibration at 839 and 608 cm^{-1}. Magdaline *et al.*[33] observed theoretically the stretching of the C-S bond in the thiophene ring at 852 and 649 cm^{-1} but only one peak is observed at 647/637 cm^{-1} in the experimental FT-IR/FT-Raman spectra. For the title compound, strong bands occur at 855 and 712 cm^{-1} in IR and 718 cm^{-1} in Raman are assigned to C-S stretching mode of thiazole ring. The small wave number changes for this mode resulting from the mixing of two rings and substituent group.

Ethyl cyano acetate vibrations: Normally, the C≡N stretching mode was observed as sharp intense band in the region[37]

2270-2210 cm^{-1}. For 3, 5-bis (3, 4-dicyanophenoxy) aniline molecule, this mode has been assigned by Zeng *et al.*[38] at 2233 cm^{-1}. In this study, this mode is observed at 2239 cm^{-1} in IR and at 2240 cm^{-1} in Raman spectra, respectively. The C=O stretching vibration was observed in the range[39,40] of 1850-1550 cm^{-1}. Inkaya *et al.*[40] theoretically reported at 1851 cm^{-1} and at 1745 cm^{-1} by HF and B3LYP methods respectively for this mode. Also, C=O stretching mode was experimentally assigned at 1730 cm^{-1} in FT-IR spectrum[40]. The carbonyl group gives rise to bands at 1748 and 1620 cm^{-1} in IR and at 1734 and 1604 cm^{-1} in Raman spectra is due to the C=O stretching vibration for ethyl cyano acetate group of title compound. The in-plane and out-of-plane deformation vibration of C=O group was appear in the regions 680-630 and 580-570 cm^{-1}, respectively[40,41]. In our case, weak bands observed at 696 and 588 cm^{-1} in IR are assigned to β(C=O) and γ(C=O) modes, respectively. The C-O stretching mode of carboxyl group have strong band in the region[20] 1395-1200 cm^{-1}. Sert *et al.*[37] reported C-O stretching mode for ethyl (2E)-2-cyano-3-(4-methoxyphenyl)-acrylate molecule by B3LYP method at 1267 cm^{-1} and experimentally at 1259 cm^{-1} in IR spectrum. For the title compound, C-O stretching mode is attributed as strong band at 1242 cm^{-1} in FT-IR and as a weak band at 1245 cm^{-1} in Raman spectra, respectively. The C-O-C antisymmetric and symmetric stretching vibrations were identified by Inkaya *et al.*[40] at 1083 and 945 cm^{-1}, respectively. Bhagyasree *et al.*[42] reported C-O-C stretching modes at 1144 and 1063 cm^{-1} (IR), 1146 cm^{-1}, 1066 cm^{-1} (Raman) and at 1153 cm^{-1} theoretically. For the title compound, as expected the antisymmetric C-O-C stretching vibration is assigned at 1135 and 1054 cm^{-1} (IR), 1142 cm^{-1} (Raman) and the symmetric stretching mode at 969 cm^{-1} in Raman spectrum only.

The antisymmetric stretch, symmetric stretch and scissoring vibrations of CH$_2$ group appear in the region 2925±10, 2855±10 and 1463±10 cm^{-1}, respectively[20]. Joseph *et al.*[43] predicted the mode for ν$_{as}$(CH$_2$) at 3029 and 2974 cm^{-1} and ν$_s$(CH$_2$) at 2950 and 2884 cm^{-1}, respectively by B3LYP method. The bands observed at 3035 and 2868 cm^{-1} (IR) and 2945 and 2882 cm^{-1} (Raman) were assigned to these CH$_2$ stretching modes[43]. In the present study, ν$_{as}$(CH$_2$) mode is assigned at 2934 cm^{-1} in IR and at 2938 cm^{-1} in Raman spectra, respectively for the title compound. Also, the ν$_s$(CH$_2$) mode is assigned at 2857 cm^{-1} (IR), 2860 cm^{-1} (Raman) for the title compound. The scissoring vibration of CH$_2$ group is identified as medium bands at 1456 and 1463 cm^{-1} in both spectra in the present study. The wagging and twisting vibrations of CH$_2$ group were observed in the region[40,20] 1390-1180 cm^{-1}. Inkaya *et al.*[40] reported the

CH_2 wagging and twisting modes of ethyl cyano acetate group at 1373, 1323, 1233 and 1222 cm^{-1} (B3LYP), 1373 and 1329 cm^{-1} (IR), 1376, 1236 and 1223 cm^{-1}, (Raman), respectively. The bands observed at 1369, 1338, 1242 and 1209 cm^{-1} in IR and at 1371, 1341, 1245 and 1200 cm^{-1} in Raman spectra are assigned to the wagging and twisting modes of CH_2 group for the title compound. Also, the bands calculated at 968 and 914 cm^{-1} were assigned as the rocking modes of CH_2[40]. In the present study this mode is identified as weak bands at 969 and 923 cm^{-1} in Raman spectrum only. The stretching vibrations of the CH_3 group were expected in the range[44,20] of 3050-2900 cm^{-1}. Sebastian *et al.*[44] calculated the antisymmetric stretching modes of the methyl group at 3023 and 3011 cm^{-1}, 2976 and 2971 cm^{-1} and the symmetric stretching modes of methyl group at 2927 cm^{-1} by B3LYP method, respectively. The bands observed at 2977 and 2925 cm^{-1} in the Infrared spectrum and at 3005, 2980, 2966 and 2920 cm^{-1} in the Raman spectrum have been assigned as stretching modes of the CH_3 group[44]. In the present case, the antisymmetric and symmetric stretching modes of the CH_3 group are attributed at 2987 and 2971 cm^{-1} (IR), 2971 cm^{-1} (Raman) and at 2901 cm^{-1} (IR), respectively. The anti-symmetric and symmetric bending vibrations of the methyl group normally appear in the region[42,43] of 1485-1400 and 1420-1380 cm^{-1}. Bhagyasree *et al.*[42] observed the bands at 1455 cm^{-1} in the IR spectrum and at 1464 cm^{-1} in the Raman spectrum were assigned as CH_3 bending modes. The anti-symmetric bending mode of CH_3 group is assigned as a medium band at 1456 cm^{-1} in the IR spectrum and at 1463 cm^{-1} in the Raman spectrum respectively for the title compound. Also, the symmetric bending mode of CH_3 group of title compound was identified at 1396 cm^{-1} in Raman spectrum. Joseph *et al.*[43] calculated the rocking modes of methyl group by B3LYP method to be at 1045, 1037, 1024 and 992 cm^{-1} and were observed at 1048 cm^{-1} in the IR spectrum and at 1027 cm^{-1} in the Raman spectrum. This mode is appeared at 1054 and 1032 cm^{-1} in IR spectrum for the title compound.

Mono-substituted benzene ring vibrations: Normally the phenyl C-H stretching modes were expected above[45] 3100 cm^{-1}. Renjith *et al.*[46] observed bands at 3146 and 3109 cm^{-1} in the Raman spectrum which is assigned as C-H stretching modes of the phenyl ring for 1-phenylpyrrole. In the present work, the C-H stretching mode for mono-substituted benzene ring is observed as weak bands at 3153 and 3116 cm^{-1} in Raman spectrum only. The C-H in-plane bending

modes of the benzene ring were observed at 1261, 1188, 1133 and 1022 cm^{-1} in the IR spectrum, 1195, 1060 and 1030 cm^{-1} in the Raman spectrum and at 1290, 1188, 1176, 1067 and 1026 cm^{-1} theoretically (DFT) by Varsanyi *et al.*[18]. For the title compound, this mode was assigned at 1181, 1135, 1105, 1054 and 1032 cm^{-1} in the IR spectrum and at 1193 and 1142 cm^{-1} in Raman spectrum, respectively. The out-of-plane C-H deformation bands of the phenyl ring were assigned at 988, 960, 911, 828 and 726 cm^{-1} theoretically[18]. The absorption peaks at 855, 757 cm^{-1} in IR and at 969, 923, 900, 869, 812 and 769 cm^{-1} in Raman spectra are attributed to C-H out-of-plane bending mode for the title compound. Generally the C=C stretching vibrations in aromatic compounds form the band in the region of 1650-1430 cm^{-1} and the C-C stretching vibrations occurs in the range[45,46] 1400-1300 cm^{-1}. Varsanyi[18] observed the in-plane and out-of plane C-C-C bending vibrations at 610 and 590, 500 and 350 cm^{-1} in FT-IR, respectively. Based on the literature data, C=C stretching mode is attributed due to medium bands at 1620, 1579 cm^{-1} (IR), 1604 and 1582 cm^{-1} (Raman) . Also the C-C stretching mode is identified at 1369 and 1338 cm^{-1} in IR and at 1371 and 1341cm^{-1} in Raman spectra respectively. The in-plane and out-of plane C-C-C bending vibrations are assigned at 621 cm^{-1} (Raman) and 588 and 497 cm^{-1} (IR), respectively. The ring-breathing mode of mono-substituted benzenes appears near 1000 cm^{-1} and Varsanyi[18] assigned theoretically at 1011 cm^{-1} for the ring-breathing mode. In Raman spectrum of title compound, this mode is identified as a medium intensity band at 1021 cm^{-1} in the present study.

Hydrogen bonding: The crystalline assembly of ECPTSIPTC crystal was stabilized through weak hydrogen bonds by C-H···N and C-H···O interactions[17]. The presence of these weak hydrogen bonds plays an important role to stabilize the crystal structure of biological macromolecule. They do not shifting wave number of related functional group of stretching and bending modes frequencies.

Optical analysis: The UV-Visible spectrum of ECPTSIPTC crystal was recorded using SHIMADZU-UV1800 double beam spectrometer in the wavelength range 200-1100 nm. The absorbance spectrum of title compound is shown in Fig. 4. It shows that the crystal has the maximum absorbance peaks at 268 and 351 nm. The lower cut-off wavelength is found to be at 312 and 397 nm. The title crystal has 100% transmittance in the entire visible region which makes the crystal usefulness of material for optical application. The Tauc's relation $(\alpha h\nu)^2 = A (h\nu - E_g)$ is used to determine the energy gap value E_g of title
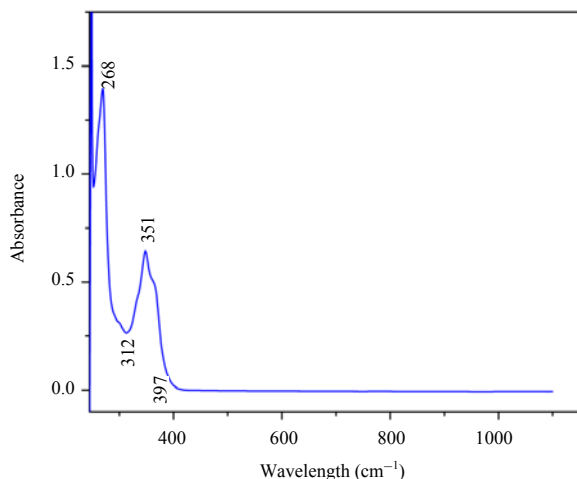
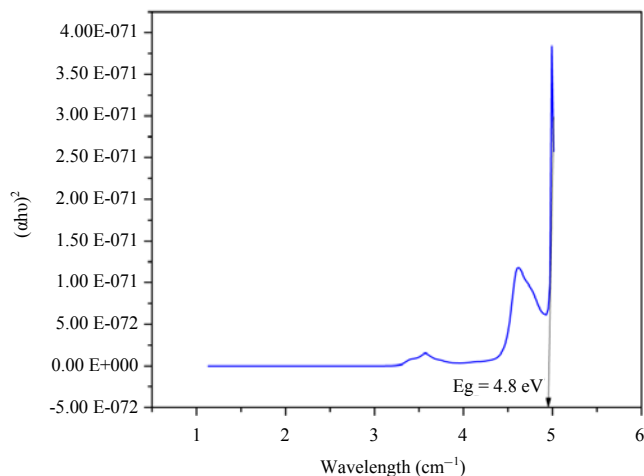Fig. 4: Absorbance spectrum for ECPTSIPTC crystal

Fig. 5: Optical band gap for ECPTSIPTC crystal

crystal by plotting $(\alpha h\nu)^2$ Vs photon energy. The linear portion of $(\alpha h\nu)^2$ is extrapolated to the photon energy axis to determine the energy gap value of title crystal. From the Fig. 5, the energy gap value was determined as 4.8 eV for ECPTSIPTC crystal.

CONCLUSION

The ECPTSIPTC crystal has been synthesized by slow evaporation method. The complete vibrational FT-IR and FT-Raman spectra of title compound in solid phase have been recorded at room temperature. All the fundamental frequencies of the molecule were assigned which has been seen to be in good agreement with the corresponding results in the literature. Using UV-Visible spectroscopy analyzes the

optical band gap was determined as 4.8 eV. This large band gap shows that the grown crystal is a typical of dielectric material.

SIGNIFICANCE STATEMENT

This study discovers the new indeno quinoxaline derivative compound that can be play considerable roles in the biological and pharmaceutical fields. Also, the fusions of various compounds into the quinoxaline moiety modify their structures which provide the development of biological diversities and future drug discovery. This study will help the researcher to develop and synthesis of new heterocycles with medicinal and biological activity for research in organic and medicinal chemistry. Thus a new attempt was made on the growth of indeno quinoxaline derivative crystal by substitution of ethyl cyano acetate and analyzed by spectroscopic approach may be arrived at.

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