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Ultra-Violet and FTIR Spectroscopic Studies of Thiourea Single Crystals

Minal N. Vansia[1], Kishor C. Poria[2]
[1]Assistant Proffesor,Shree Ramkrishna Institute of Computer Education and Applied Science, Surat, Gujarat,India.
[2]Vice-Chancellor, Hemchandracharya North Gujarat University, Patan, *Gujarat* India.
[1] minalvansia@gmail.com

Abstract : Thiourea (NH_2CSNH_2) single crystals have attracted significant attention due to their nonlinear optical (NLO) properties, wide optical transparency, and structural flexibility for forming molecular complexes. In this study, high-quality thiourea single crystals were grown by the slow evaporation solution growth technique and subjected to ultraviolet–visible (UV–Vis) and Fourier transform infrared (FTIR) spectroscopic analyses. The optical transmission spectrum reveals excellent transparency in the visible region with a sharp absorption edge, enabling the estimation of the optical band gap. FTIR spectral analysis confirms the presence of characteristic functional groups such as N–H, C–N, and C=S vibrations, validating the structural purity of the grown crystal. The combined results highlight the potential of thiourea single crystals for photonic and optoelectronic device applications.

Index Terms **: Thiourea single crystal, UV–Vis spectroscopy, FTIR spectroscopy, Optical band gap, Nonlinear optics**

I. INTRODUCTION

Thiourea is an organic compound of significant importance in nonlinear optics, crystal engineering, and material science. Its strong dipole moment and ability to form hydrogen bonds make it a versatile candidate for second harmonic generation (SHG) and other optical applications. Optical spectroscopy provides a direct method to evaluate the suitability of thiourea crystals for such applications. In this work, UV–Vis and FTIR techniques are employed to investigate the optical properties and vibrational characteristics of pure thiourea single crystals.

II.EXPERIMENT

Thiourea single crystals were grown by the **slow evaporation solution growth technique** using analytical reagent grade thiourea dissolved in deionized water. Transparent crystals were harvested after several days of controlled growth.

- **UV–Vis spectroscopy:** Optical transmission studies were carried out in the range 200–800 nm.
- **FTIR spectroscopy:** Recorded in the range 400–4000 cm^{-1} to identify functional groups.

III. UV-VIS Absorption Spectra of Thiourea Crystal

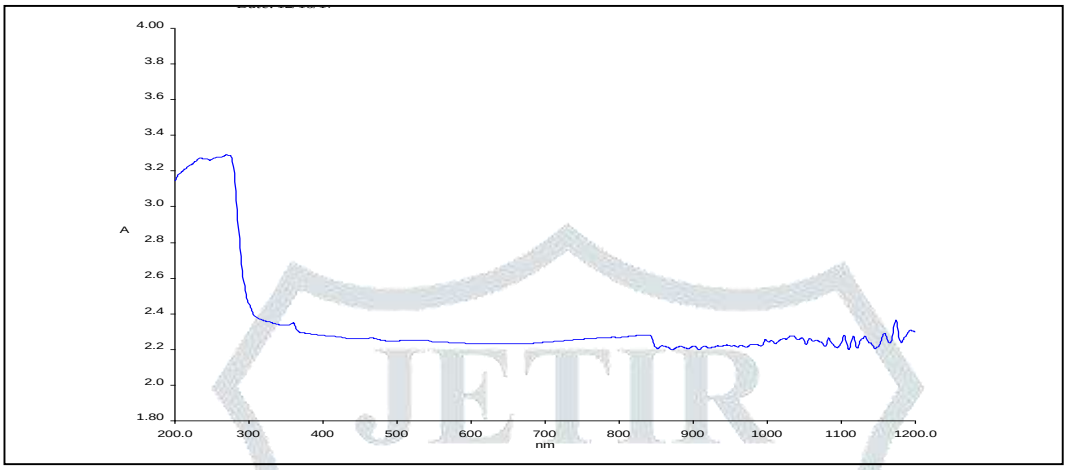

Figure:1: UV-VIS Absorption Spectra of Thiourea Crystal

Table:1: Analysis of UV-VIS Absorption Spectra

Abscissa : Wavelength nm	Ordinate: Absorption A	Abscissa : Wavelength nm	Ordinate: Absorption A
250.00	3.2663	263.00	3.2787
251.00	3.2690	264.00	3.2800
252.00	3.2713	265.00	3.2820
253.00	3.2729	266.00	3.2844
254.00	3.2741	267.00	3.2869
255.00	3.2754	268.00	3.2888
256.00	3.2768	269.00	3.2900
257.00	3.2779	270.00	3.2903
258.00	3.2786	271.00	3.2899
259.00	3.2789	272.00	3.2895
260.00	3.2786	273.00	3.2895
261.00	3.2782	274.00	3.2894
262.00	3.2781	275.00	3.2879

3.1. Calculations of Energy Band Gap (E)

Energy Band Gap (E) = h*C/λ

h = Planks constant = 6.626 x 10^{-34} Joules sec
C = Speed of light = 3.0 x 10^{8} meter/sec
λ= Cut off wavelength = 270.00 x 10^{-9} meters

h in J.s	C in ms^{-1}	λ in m	E in J	E in eV
6.626 x10^{-34}	3.0 x10^{8}	270.00 x10^{-9}	1.6 x 10^{-19}	4.601

3.1.2 Results of UV–Visible Spectral Analysis

The spectrum indicates that thiourea crystals exhibit high optical transparency above ~250 nm, with minimal absorption in the visible region. The optical energy band gap (Eg) was calculated and found to be approximately 4.601 eV, confirming the wide band gap nature of thiourea.

IV. FTIR Spectra of Thiourea Crystal

FTIR spectroscopy was carried out with Model Spectrum GX, Make:Perkin Elmer, U.S.A., having optical resolution of 0.04 cm^{-1} in the range from 4000 cm^{-1} to 400 cm^{-1} in KBr palate medium..Spectra is shown in figure:2 for the grown Thiourea crystals. The analysis of the spectra is summarized in Table:3.5.

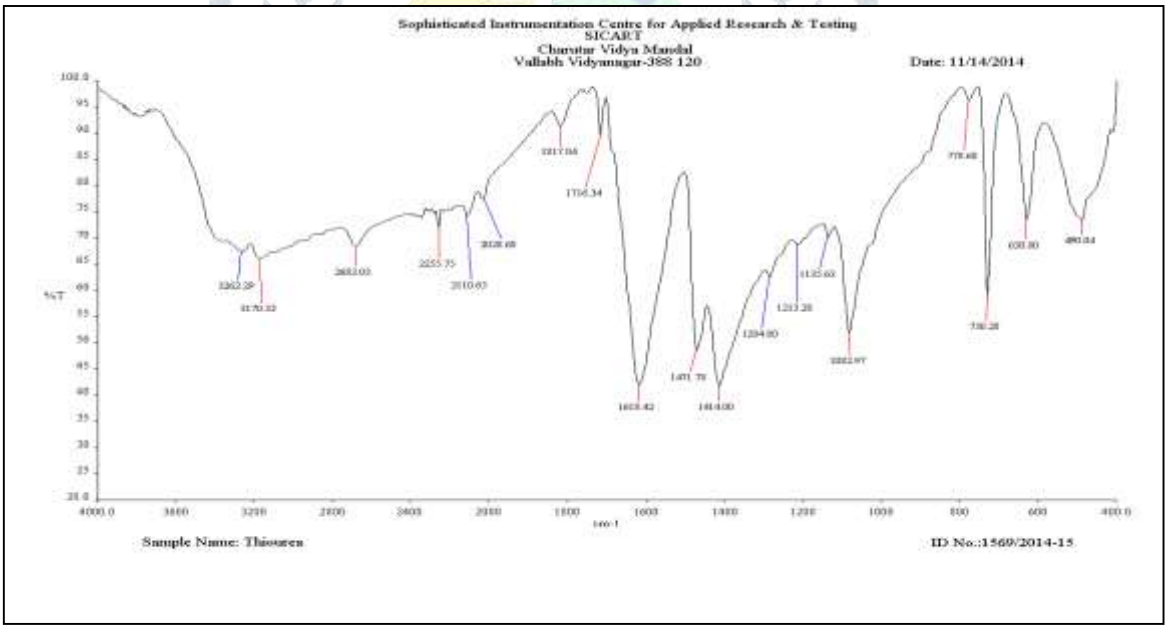

Figure:2: FTIR Spectra for Thiourea

Table:2: Analysis of FTIR spectra for Thiourea crystal

wave number cm^{-1}	Assignment	wave number cm^{-1}	Assignment
3262.29	Asymmetric NH_2 Stretching	1082.97	Asymmetric N – C – N stretching
3170.33	Symmetric NH_2 stretching	730.28	Symmetric C = N stretching
1618.42	NH2 bending	630.80	C – Br stretching
1414.00	Asymmetric C = S stretching	490.04	S – C – N stretching

4.2. Results of FTIR Spectral Analysis

The C = S group is less polar then the C =O group and has considerably weaker bond and also the bond is not intense and it falls at lower frequencies where it is much more susceptible to coupling effects. Thiourea can make non linear optical derivatives easily and forms more noncentro symmetry. It also shows absorption in 3380 – 450 cm^{-1} region. The absorption occurs in region 730 cm^{-1} as C = N stretching. It also shows absorption for asymmetric stretching bond for N-C-N in the region 1414 cm^{-1}. The other bond symmetric and asymmetric NH_2 stretching in the bond region of 3380 - 3170 cm^{-1} , NH_2 bending shows at 1618 cm^{-1}, and Asymmetric N-C-N and S- C-N stretching observed at 1082 cm^{-1} and 490 cm^{-1} respectively, it also attributed to vibrations involving interaction between C = S stretching and C – N stretching.

V.CONCLUSION

UV–Vis and FTIR studies of thiourea single crystals confirm their excellent optical transparency, wide band gap, and structural purity. The wide transparency window and stable vibrational structure make thiourea an excellent candidate for nonlinear optical devices, photonic applications, and optoelectronic components.

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