iJRASET
International Journal For Research in Applied Science and Engineering Technology



INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 5 **Issue:** XI **Month of publication:** November 2017

DOI: http://doi.org/10.22214/ijraset.2017.11067

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International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor:6.887
Volume 5 Issue XI November 2017- Available at www.ijraset.com

Growth, X-Rays Diffraction (XRD), Ultra-Violet and FTIR Spectroscopic Studies of Thoreau Single Crystals.

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Abstract: ***Single crystals of pure Thiourea(NH_2CSNH_2) were grown by slow evaporation technique. Thiourea is an organic nonlinear optical (NLO) material. Main feature of these crystals are their simple and inexpensive growth technique and wide possibilities for their attractive optical and mechanical properties. Single crystal structure was determined by X-Rays diffraction data and it reveals that the crystals belong to hexagonal and tetragonal crystal system with the space group of P_{nma}. Vibrational spectroscopy reveals the symmetries of molecular vibrations and the functional group of the grown crystals was found by FTIR analysis. The spectral bands have been comparing with similar Thiourea compound using FTIR spectrum in the range 400-4000cm^{-1}. The UV-VIS was performed to know the optical behavior of the grown crystals. The results are summarized in this paper.***

Keywords: Thiourea crystals, XRD, UV-VIS, FTIR

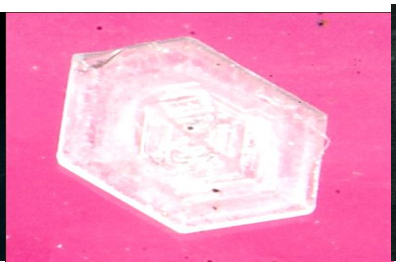
I. INTRODUCTION

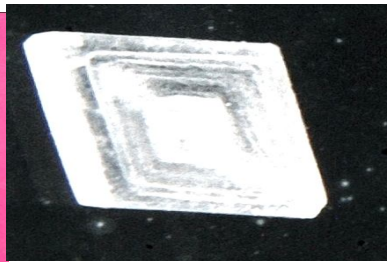
Crystals are unacknowledged pillar of modern technology. Without crystals there would be no electronic industry, no photonic industry and no fiber optic communications. Single crystals of Thiourea(NH_2CSNH_2) are being used broadly in electro-optic industry as polarization filters, electronic light shutter,electronic modulator,optical voltmeter and as elements of electro-optic and electro-acoustic devices. Thiourea crystals exhibit piezoelectric effect, which is utilized in infrared (IR) and ultraviolet (UV) and Scanning Electron Microscopy (SEM) detectors and infrared imaging. In this paper, the method of crystal growth with emphasis on low temperature, solution growth technique was described. The solvent to be chosen to grow good quality crystals from solution is also discussed. Grown crystals are characterized through XRD, UV-VIS and FTIR spectroscopy. The results are summarized in this paper.

A. Experimental

Thiourea is an organic material. Its molecular weight is 76.12gm/mol. An analytical grade Thiourea powder was dissolved into double distilled water, the solution is stirred for an hour using magnetic stirrer to ensure homogenous temperature and concentration throughout the volume of the solution. After attaining the saturation, the equilibrium concentration of the solute was analyzed gravimetrically. The experiment was carried out for various temperature ranges as 30,35,40,45 and 50°C. For crystal growth the super saturated solution is poured into neat and clean Petri dish, which is kept in undisturbed condition. After 3 to 4 days good hexagonal and tetragonal shaped crystals were seen. The size of crystals was varied in 40mm×28mm×1mm to 1.5mm×1.5mm×0.5mm. Thetransparency of crystals was also varied from fairly transparent to opaque. The grown crystals were shown in Figure-1(a),1(b),1(c).


Figure:1(a)


Figure:1(b)


Figure:1(c)

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B. X-Rays Diffraction:

The powder XRD pattern of the grown crystal were recorded using Cu K α radiation (λ= 1.5418Å). This analysis confirms the crystalline nature and also to identify the unit cell parameters using model: Xpert MPD,Make: Phillips, Holland.It is observed that Thiourea single crystals crystallize in the orthorhombic system with lattice primitive and space group parameters. The X-Rays diffraction spectra for grown Thiourea crystal are shown in Figure-2. The position of the peaks are found to be in good harmony with the data available in JCPDS files and tabulated in Table-1.

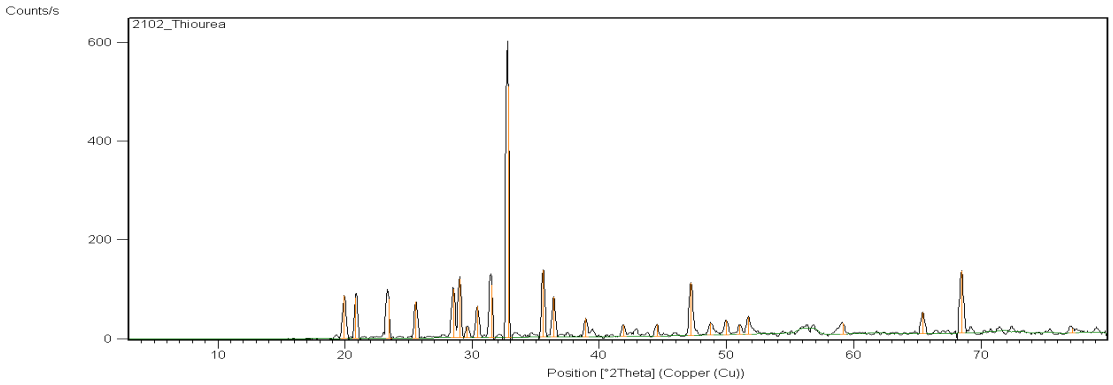


Figure:2: The X-Rays diffraction spectra for grown Thiourea crystal

Crystal	System	2Θ	h k l	Lattice parameters	Reference
Thiourea	Orthorhombic	23.25	2 0 0	a= 7.481	7.644
		20.81	0 2 0	b= 8.535	8.559
		32.57	0 0 2	c= 5.472	5.492
					α=β=ɤ=90°

Table:1

C. UV-VISSpectroscopy

UV-VIS spectrum analysis has been carried out using model-LAMBDA19 in the wavelength range of 1.0000nm shown in Figure:3Transmission spectra are very important for any NLO material because a NLO material can be of practical use only if it has wide transparency window [2]. The optical transmission spectra for Thiourea crystals are recorded and It is observed that Thiourea has high transmittance in the entire visible and IR region. This is important for material possessing NLO properties. The UV cut off wave lengthfor the pure Thiourea crystals are found to be 224nm.[3] The large transmission range and short cut off wavelength enables it to be a potential material for second and third harmonicgeneration[4].

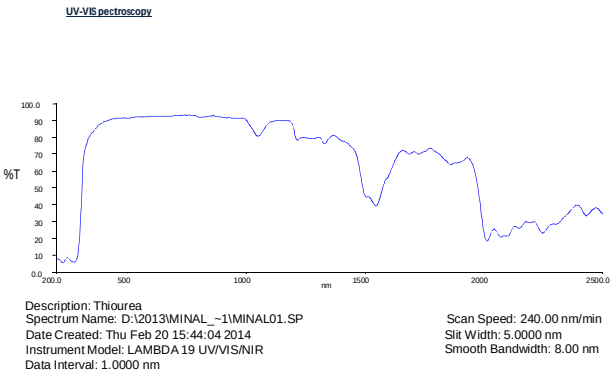


Figure:3: UV-VIS spectrum

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D. FTIRSpectroscopy

Infrared spectroscopy studied were carried out on the grown crystals to understand the structure and bonding in them. The FTIR spectra were recorded on a Model:Spectrum GX, Make: Perkin Elmer, U.S.A. and it is shown in Figure:4. The analysis of the spectra is summarized in Table-2. These investigations were well compared with earlier reports [5,6].

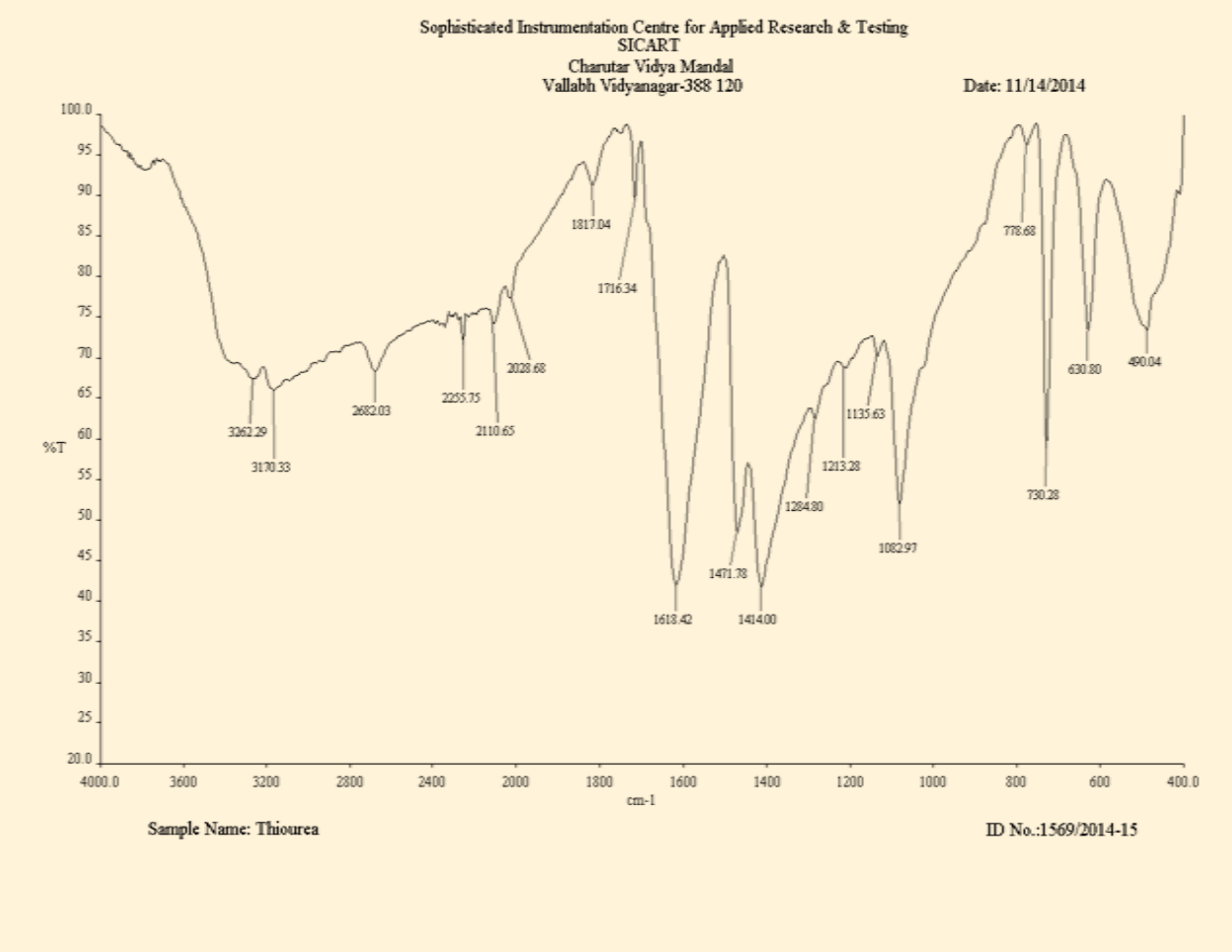


Figure:4: FTIR spectra

Wave number cm^{-1}	Assignment	Wave number cm^{-1}	Assignment
3262.99	NH bending	1082.97	COH stretching
2682.03	C-H bending	1414.00	N-C-Nasymmetric stretching
1716.34	-C=C-alkene stretch	730.28	C=S stretching and N-C-N stretching
1618.42	NH_2 bending	490.04	N-C-N deformation

Table-2

II. CONCLUSIONS

Thiourea single crystals were grown by slow evaporation technique. The grown crystals were characterized using crystal X-rays diffraction analysis, which shows that Thiourea belongs to orthorhombic system. The presence of functional groups and bond interaction has been confirmed by FTIR analysis. UV-VIS optical transmittance studies, the values of band gap energy were

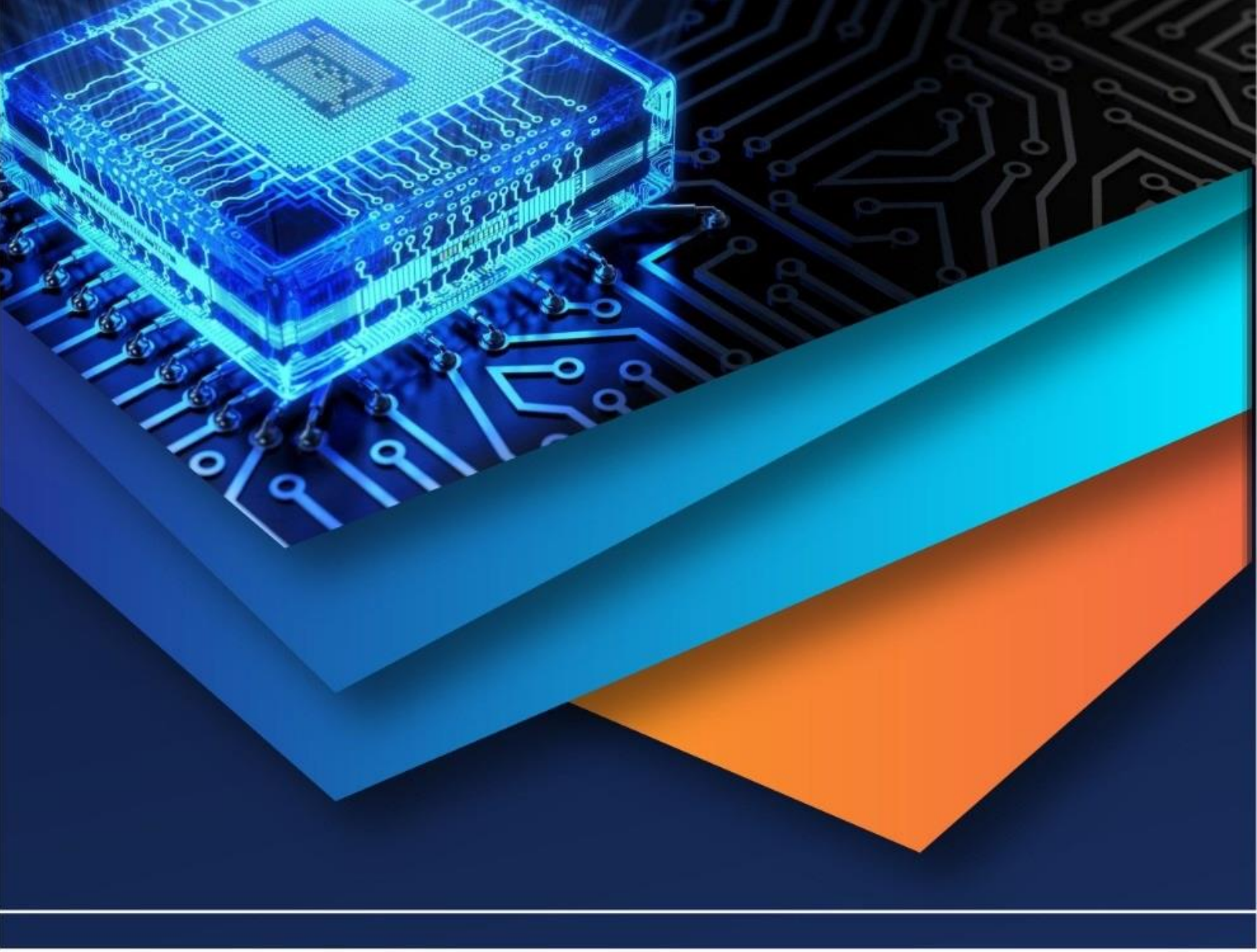
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determined to be 4.45eV.Opens up new possibilities for improved performance and suggest its suitability for the fabrication of various optoelectronic devices.

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