

Vehicle Sharing and Use of Bicycle for Travelling: An Effective Panacea to deal with Automobile Pollution

Santhosh Kumar, R., Lalithambika, R., Noor, S. Kumar and Ravendran, P.B.

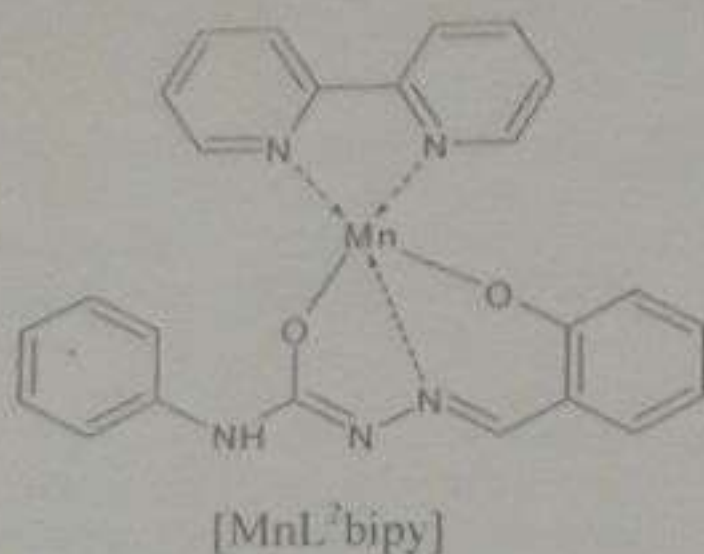
Post Graduate Department and Research Centre of Botany, Mahatma Gandhi College, Thiruvananthapuram,
Post Graduate Department of Economics, Mahatma Gandhi College, Thiruvananthapuram, Kerala.

Abstract

Pollution is generally defined as the negative or undesirable alteration in the environment, usually the accumulation of something harmful or detrimental. Different developmental activities such as construction, transportation and manufacturing not only deplete the natural resources but also produce large amount of wastes that leads to various pollution to the environment. Pollution is thus direct or indirect changes in any component of the biosphere that is harmful to the biotic component in the ecosystem and in particular detrimental for human beings, affecting adversely the industrial level progress, cultural and natural assets or environment at local and global level. Transportation is one of the main causes for air pollution. In current situation a number peoples depends various vehicles or their travel or other transportation. In that situation a lot of unwanted carbon pollution is formed and transfer to the environment. In this present article, discussing a chance to introduce new methods to overcome the automobile pollution, including sharing of vehicles, use of cycle for short distance travelling. Cycling is not only help in travelling but also it is a good exercise as compared to other heavy exercise such running or reselling. New government policies are needed and to be implemented for the smooth functioning of such practices.

Introduction

Pollution is generally defined as the negative or undesirable alteration in the environment, usually the accumulation of something harmful or detrimental. Different developmental activities such as construction, transportation and manufacturing not only deplete the natural resources but also produce large amount of wastes that leads to various pollution to the environment. Pollution is thus direct or indirect changes in any component of the biosphere that is harmful to the biotic component in the ecosystem and in particular detrimental for human beings, affecting adversely the industrial level progress, cultural and natural assets or environment at local and global level.



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CRYSTAL STRUCTURE, SPECTRAL, THERMAL AND DIELECTRIC STUDIES OF A POLYMER OF SODIUM COMPLEX OF MALEIC ACID

Bijini B.R.¹, Lekshmi P Nair¹, Prasanna S.¹, Deepa M.², C.M.K. Nair¹ and Rajendra Babu K.^{1*}

¹Postgraduate Dept. of Physics, M.G.College, Thiruvananthapuram-695004, India

²Department of Physics, All Saints' College, Thiruvananthapuram-695037, India

*Corres.author: bijiniyothis@gmail.com,

PP-29

Abstract

Single crystals of sodium complex of maleic acid was grown in gel medium for the first time. Single crystal X-ray diffractometry reveals that the crystal lattice of the complex is triclinic (P-1) and the complex is in an 1D polymeric form. FT-IR spectral studies were used to identify the functional groups and the bonding sites of the ligand with the metal atoms.

Key words: Maleic acid, Sodium metasilicate gel, Crystal growth.

Introduction

Metal-organic frameworks (MOFs) constitute an emerging class of materials useful in gas storage, gas purification, separation applications and research on biomedical applications of MOFs is gaining momentum and this emerging new class of porous materials is likely to replace the traditional nanoporous materials in drug delivery and storage in the future¹. Maleic acid is widely used in medicine, in the preparation of drugs, in agriculture as the plant growth regulators, in food industry etc. Maleic acid is used extensively in the pharmaceutical industry for making maleate salts of drugs. Sodium is one of the four important biologically active cations.

Among many methods available for crystal growth, gel technique is commonly adopted due to its

simplicity and ability to suppress nucleation centers. Slow diffusion of reactants in the gel medium can be considered to mimic the growth of crystals in a human body². The principal aim of the present study mainly focuses on the growth of Sodium complex of maleic acid on sodium metasilicate gel.

Experimental procedure

Crystallization method

The apparatus used for crystallization of single crystals by gel technique consists of borosilicate glass tubes of length 20cm and diameter 2.5cm. Silica gel was prepared by adding a solution of sodium metasilicate to 20% maleic acid slowly with continuous stirring. The specific gravity of sodium metasilicate was varied between 1.04 g/cc and 1.05g/cc and pH was adjusted in the range 3 – 6. About 20ml of gel solution with the desired value of pH was then transferred to several test tubes and 5ml of acetone was added to each test tube to reduce solubility. Over the set gel, acetone was added.

Results and discussion

Crystal growth

Tiny crystals were observed at the gel solution interface in the third week after incorporation of the top solution. The optimum

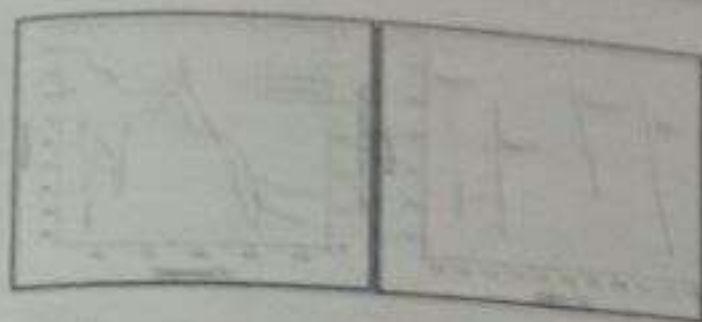


Fig 2: TGA/DTA curves plots

Fig 3: Coats and Redfern plots

The compound is thermally stable upto 100°C. The TGA curve shows a mass loss of 18.94 % within the temperature range 40-240°C, which corresponds to the loss of water molecules (calc-19.22%). Thus the two endothermic peaks upto 238.27°C indicates the loss of two water molecules. The anhydrous calcium maleate gets decomposed into calcium oxalate with the elimination of acetylene molecule, confirmed by the exothermic peak at 505°C in the DTA curve. Further heating results in the conversion of calcium oxalate to CaO with the evolution of CO and CO₂. The observed and calculated percent of weight loss in the temperature range 490°C - 790°C during the above said decomposition process is 49.5 and 50.75.

Kinetic parameters				Thermodynamic parameters		
Stage	n	E(KJ/mol)	logA(S ⁻¹)	ΔS(J/Kmol)	ΔH(KJ/mol)	ΔG(KJ/mol)
I	0.9	162.87	18.23	105	156.63	101.72
II	0.9	124.10	9.94	-58.49	115.74	145.15
III	0.9	516.54	31.60	352.78	503.58	228.69
IV	1.1	489.00	21.68	160.81	473.00	318.3

respectively. Coats and Redfern plots for the thermal decomposition stages are depicted in figure 3. Table 1 provides the kinetic and thermodynamic parameters of the compound.

Conclusion:

Calcium complex of maleic acid have been successfully grown by gel method. Sodium metasilicate of gel density 1.04g/cc and pH6.5 produced good quality crystals. Elemental analysis gives the formula of the compound as CaC₄H₂O₄·2H₂O. Thermal decomposition of the complex was studied by TGA/DTA.

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Screening of enzymatic activity in different bacterial isolates treated with phenol

Dr. J. K. Reshma¹, Anu Mathew^{1*}, Dr. V. Salom Gnana Thanga²

¹Post Graduate Department of Environmental Sciences, All Saints' College, Thiruvananthapuram, Kerala ²Department of Environmental Sciences, Kariavattom campus, Thiruvananthapuram, Kerala

*Corresponding Author: anumathew85@yahoo.co.in

PP-19

Abstract

Coir-retting environment harbours a variety of potential microbes which can degrade phenols. Microorganisms capable of degrading phenol do so with the action of a variety of enzymes. So, a study

was carried out to analyse the enzymes present in Kadinamkulam retting area to highlight the importance of enzymes in degradation of phenol compounds. In this study phenol oxidase activity and cellulose enzyme complex (Cellulase, β-1,

PP-032

Novel Calix[4]pyrrole receptor: Colorimetric sensing of Fluoride Ions

Keyur D. Bhatt^{1*}, Pooja Y. Raval¹, Sanjay D. Gupta¹, Bharat A. Makwana², Savan M. Darjee²

¹Department of Chemistry, B.V. Shah College of Science, C. U. Shah University, Wadhwan-city, Gujarat, India
²Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India
 *dkbhatt@outlook.com

A new calix[4]pyrrole receptor (meso-tetra(methyl) meso-tetra(4-hydroxy-3-methoxy-phenyl)-calix[4]pyrrole) HMCP, has been synthesized via conventional as well as microwave assisted methods. HMCP was characterized by ¹H-NMR, ¹³C-NMR, FTIR and by ESI-MS. The ion binding properties of calix[4]pyrrole with various anions were investigated using UV-Visible spectrophotometry. The red-shift in absorption band of HMCP was observed only in presence of fluoride ions. The results obtained from absorption spectra indicate that HMCP is linked with fluoride ions through hydrogen bonding. Among all the investigated anions, only fluoride ions showed sharp colour change from yellow to dark red, which was easily detectable by naked-eye even at very low concentration level of 1 µM.

PP-033

Crystal structure and dielectric study of Glycinium Maleate

B. R. Bijini^{1*}, K. Rajendra Babu²

¹Department of Physics, HHMSPB NSS College for women, Thiruvananthapuram, Kerala, India
²Post Graduate Department of Physics, M.G. College, Thiruvananthapuram, Kerala, India
 *bijiniyothis@gmail.com

Amino acids are vital components of a variety of biological, industrial and environmental samples. Glycine, the simplest amino acid is an important constituent of proteins, enzymes and a major inhibitory neurotransmitter in spinal cord and brainstem of vertebrate nervous system. In a strongly acidic medium Glycine exists in its protonated form (monocation) i.e. NH₃⁺CH₂COOH. Maleic acid, a dibasic unsaturated carboxylic acid is widely used in medicine. Glycinium maleate single crystals were grown by solution method. Good quality crystals were formed in solution of glycine and Maleic acid in the 1:1 molar ratio. The single crystal X-ray diffraction studies gave new insight into the crystal structure of the title compound. The study shows that the grown crystals belong to monoclinic system (C/c) with unit cell parameters a=17.9137(12) Å, b=5.6869(3) Å, c=17.4483(11) Å, β=112.710(5). Crystal structure reveals that the glycine molecule exists as a positively charged ion with protonated amino group. The anion is the singly negatively charged maleic acid in which one of the two carboxyl functional groups of maleic acid has been deprotonated. The Maleic acid is interconnected to glycine molecule through Hydrogen bonds. The crystal structure is stabilized by these hydrogen bonds between Glycine cation and Maleate anion. Fermi gap, Penn gap and Plasma energy of the grown crystals were calculated from unit cell parameters and dielectric studies.

PP-034

FT-IR and Raman spectroscopic studies of Thiosemicarbazide potassium chloride

Bincy Annie Philip¹, Anju Mary John¹, Shyamal Sreedhar¹, C. Ravikumar^{1*}

¹Department of Physics, CMS College, Kottayam-686 001, Kerala, India
 *rkz.ravi@gmail.com

The nonlinear optical (NLO) compound of interest Thiosemicarbazide potassium chloride crystal (TSPC) was grown by slow evaporation method. The molecular structure generated with the aid of density functional theory (DFT). Raman and IR spectra were recorded and analyzed. The harmonic wavenumbers and IR and Raman intensities were computed with the B3LYP method. The observed vibrational wavenumbers were compared with the theoretical values.

oxidation, increases interlayer distance between graphitic layers, and reduces the crystalline size of GO.¹

We are also exploring the possibility of utilizing Metal Organic Frameworks (MOFs) for supercapacitor application. We have synthesised a cobalt based metal-organic-frameworks [CoNIm(RHO)] and the material was tested for supercapacitor application using electrochemical techniques such as cyclic voltammtery (CV), AC impedance, and chronopotentiometry. The MOF showed a specific capacitance value of 263 F/gm in KOH electrolyte.

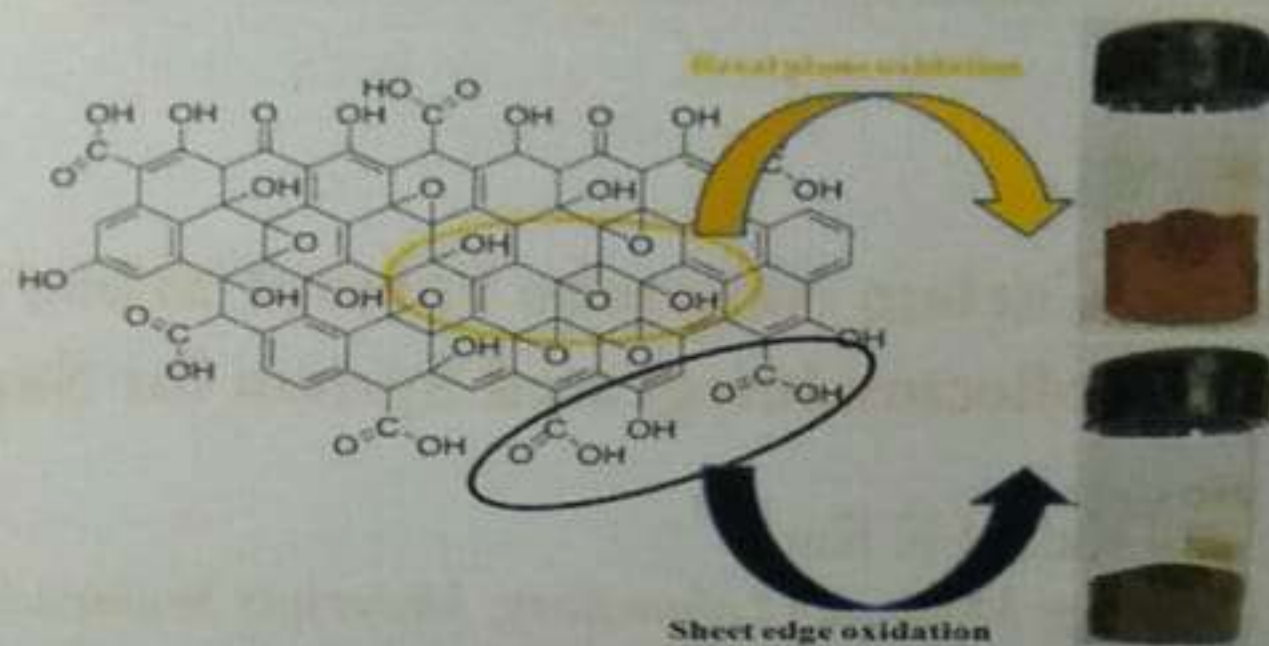


Figure 1. Graphite oxidation

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P 004 Influence of Al Co-Dopants on the Thermoluminescence Spectra of SrSO₄: Eu Phosphor Matrix

Jayasudha. S^{*1}, Resmi G Nair¹, Dr. K. Madhukumar¹, Dr.V.N. Praveen¹ and T.S. Elias²

¹Dept. of Physics, Mahatma Gandhi College, Thiruvananthapuram-695004.

²Regional Cancer Centre Thiruvananthapuram

Email: jsnair.india@gmail.com

Thermoluminescence Dosimetry is a powerful technique used for the estimation of both high and low ionising radiations. Various models of TL suggests that the impurities added can introduce high luminescence efficiency and to control the glow peak temperature. In the present work, the effect of codoping with Al in the SrSO₄ lattice is studied in detail. SrSO₄: Eu, Al phosphor have been irradiated using gamma-rays of Co⁶⁰ and the TL glow

conditions to grow the best quality single crystals were at pH 5 and gel density, 1.04 g/cc.

Single crystal X-ray diffraction studies

The crystallographic data reveals that the crystal lattice of the complex is triclinic (P-1) with unit cell parameters $a=5.9512(3)\text{\AA}$, $b=6.3891(4)\text{\AA}$, $c=11.2178(7)\text{\AA}$, $\alpha=104.219(2)^\circ$, $\beta=91.490(2)^\circ$, $\gamma=100.165(2)^\circ$. Coordination environment of the complex with atom numbering scheme is shown in fig.1. The central Na atom is surrounded by six oxygen atoms and forms an octahedral environment. It means that the Na(I) is bonded to one maleate ligand with O(4)-Na(1) distance 2.373\AA and to five aqua oxygen atoms to form an octahedral environment. The bridging bond Na(1)-O(5) builds one dimensional polymeric structure.

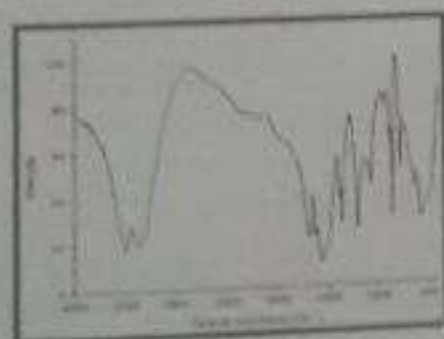
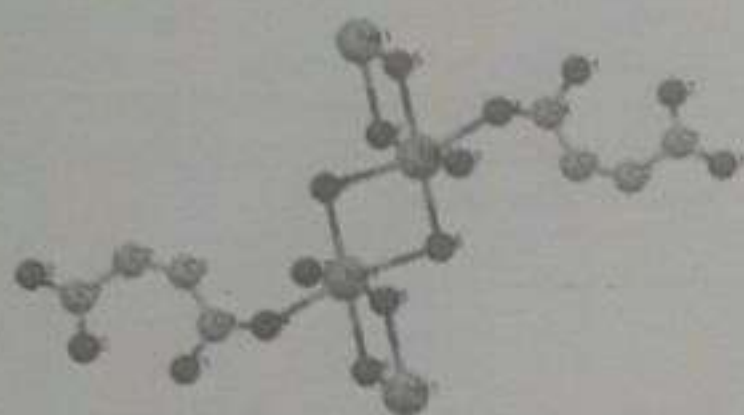


Fig.1 Molecular structure of $C_4H_4NaO_7$

Fig.2 FT- IR spectrum of the grown crystals

Fourier transform infrared (FTIR) spectra

The FT-IR spectrum of the grown crystal is as shown in fig. 2. The spectrum contains two sets of strong bands due to $\nu_{as}(\text{COO})$ at 1694, 1621 cm^{-1} and $\nu_s(\text{COO})$ at 1397, 1364 cm^{-1} of maleate ligand. For one of the carboxylate groups, the separation between $\nu_{as}(\text{COO})$ and $\nu_s(\text{COO})$ of 297 cm^{-1} is significantly larger than the value of 248 cm^{-1} for free maleic acid, indicating that one of the carboxylate groups coordinated to the central sodium ion in monodentate fashion. The band at 1214 cm^{-1} corresponds to C-O stretching which is shifted to lower frequency region with respect to the ligand (1261 cm^{-1}) due to the coordination with the central sodium atom.

Conclusions

Single crystals of Sodium complex of Maleic Acid have been successfully grown by gel diffusion method. Sodium metasilicate of gel density 1.04g/cc and pH 5 produced good quality crystals. X-ray diffraction study confirms that the grown crystals belong to triclinic system with unit cell parameters $a=5.951(3)\text{\AA}$, $b=6.389(4)\text{\AA}$, $c=11.217(7)\text{\AA}$, $\alpha=104.21(2)^\circ$, $\beta=91.49(2)^\circ$, $\gamma=100.16(2)^\circ$ and the molecules are built in a manner to form a polymerized infinite chain.

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STUDIES ON NEW COPPER (II) COMPLEXES OF N²-PHENYL-N⁴,N⁶-DI(THIAZOL-2-YL)-1,3,5-TRIAZINE-2,4,6-TRIAMINE

M.Vathananaruba^{*}, P.Tharmaraj^{*}, C.D.Sheela[#]

^{*} PG & Research Department of Chemistry, Thiagarajar College, Madurai-9

[#] PG & Research Department of Chemistry, The American College, Madurai-2

Email: ptharmaraj@rediffmail.com

PP-30

Abstract

A new series of copper(II) complexes of 1,3,5-triazine based NNN donor ligand, N²-phenyl-N⁴,N⁶-di(thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine have

been synthesized. The structural feature of the ligand and complexes has been arrived by elemental analysis, magnetic susceptibility measurements, molar conductance, spectral techniques. The free ligand and their metal complexes have been screened

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- 2) Meng, C.; Lui, C.; Fan, S. *Electrochem. Commun*, 11, 186- 189

P 007 Study on the Dielectric Properties of Barium tetrakis (Maleate) Dihydrate

Lekshmi P. Nair^a, Dr. Bijini B. R.^a and Dr. Deepa M.^b

^aPost Graduate Department of Physics, M.G. College, Thiruvananthapuram.

^bDepartment of Physics, All Saints' College, Thiruvananthapuram.

E-mail: lekshmipadma@gmail.com

Metal co-ordination compounds of dicarboxylic acids are technologically very important as they have immense technological application. Maleic acid, a dicarboxylic acid, is biologically important and its interaction with different metal ions opens new potentialities with targeted properties. Barium complex of maleic acid (BM) is grown by gel method. Dielectric properties relate to the ability of a material to polarise under the influence of an external electromagnetic field. The study of dielectric property is concerned with the storage and dissipation of electric and magnetic energy in materials. The frequency dependent dielectric property of gel grown BM was studied at room temperature using a Hioki 3532 LCR Hitester meter. The variation of dielectric constant, dielectric loss, and ac conductivity with log frequency is plotted. From the spectrum it is observed that the dielectric loss and dielectric constant decreases with increase in frequency. The high value of dielectric constant at low frequency is attributed to the dipole and space charge polarisation. Using the results of Single crystal XRD, UV-Visible spectrum and the value of dielectric constant at higher frequencies, the Plasma energy, Penn Gap, Fermi energy and polarisability of the grown crystals are calculated and tabulated.

References

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^aPost Graduate Department of Physics, M.G. College, Thiruvananthapuram.

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Thermally stimulated luminescence of SrSO₄:Eu,Mn phosphor under gamma excitation for TLD applications

Jayasudha S^{1*}, Dr. K. Madhukumar¹, Resmi G. Nair¹ & T.S. Elias²

¹*Department of Physics, Mahatma Gandhi College, Pattom P.O.,
Thiruvananthapuram-695004, India*

²*Regional Cancer Centre, Medical College P.O., Thiruvananthapuram-695011, India*

**jsnair.india@gmail.com*

Abstract - The thermoluminescence (TL) properties under gamma excitations of SrSO₄:Eu,Mn phosphor prepared via chemical precipitation technique is investigated. XRD pattern proved the orthorhombic structure and single phase of the host lattice. The line broadening of the peaks showed that the crystallites are nano in size. Uniformly distributed particles with different morphologies were observed in the SEM micrographs. The dopant compositions in the host matrix observed from the Energy Dispersive Spectra were 0.18 at% Eu and 0.3 at% Mn. The thermoluminescence studies of SrSO₄:Eu,Mn phosphor shows an emission at 306p C with a fairly high intensity, when the phosphor is subjected to gamma irradiation of 1Gy dose at room temperature from Co⁶⁰ buildup. This study is novel as the reported TL emission temperature of the widely used standard CaSO₄:Dy TLD is only 240p C. The high temperature emission of SrSO₄:Eu,Mn phosphor indicates its ability of long storage of trapped charge carriers at room temperature. The TL spectrum also shows the simple trap distribution of the lattice, which is desirable for dosimetric applications. The stability of the phosphor against gamma storage days were also investigated. An attempt is also made to calculate the activation energy of the traps by analyzing the kinetics of TL emission.

Keywords—Thermoluminescence, Radiation dosimetry.

President of INCA, K. S. V. Subramanian, in his speech, said, "The INCA is a very young organization and it is in the process of growing and expanding its activities. It is a very young organization and it is in the process of growing and expanding its activities."

Pollutants are the substances which causes pollution. It may thus include any chemical or biochemical such as dust particle, sediment or gas. These component in its product, or physical factors such as heat are released intentionally by man into the environment in such a concentration that may have adverse or harmful or unpleasant effects.

A chance to Introducing a new policy to control Air pollution

Importance of Cycling

Cycling is a good practice for short distance travelling as well as it is a good exercise for human beings. So it will help for improving human health and saving money which can be used for other mode of travelling. Other importance of Bicycle and cycling including low cost of production, petroleum product and or any other energy source is not utilized while travelling, complete protection from the formation of pollutants etc.

Case study

Cycle Village, a new concept was formed at Edakulangara, it is a village situated in Kariyapattanam Taluk, Kollam District, Kerala. The concept of cycle village was formulated by a few people and then it was discussed with others, they are engaged in different field, including retired government officials, politicians, architects, common people etc. After the formation of cycle village, they conducted different activities in connection with the importance of bicycle and cycling in daily life. At present, more people in the area, using bicycle for short distance travelling and cycling is also using as the purpose of exercise instead of other exercise like walking and running.

Importance of sharing the vehicles

Sharing of vehicle is not a new idea; it was successfully working in selected areas of major cities in the World. At present situation large sized and more energy consuming vehicles are purchased by people as a part of the society. Most vehicles running with single individuals while travelling. The result of such type of one vehicle - one man travelling creates more traffic nuisance in congested areas of major towns or cities. For overcome the above problem Government must introduce a new policy to ban one vehicle - one man travelling and



encourage more people in a vehicle as expenditure sharing basis while travelling. This type of government policies is help to overcome the traffic problem in cities as well as promote sustainable use of petroleum products. And also it will help to reduce the atmospheric air pollution and sound pollution.

Case study

A number of cities successfully practiced the vehicle sharing method in the World. The sharing of Auto Rickshaws for travelling was successfully practiced in a number of cities in North India. It will help to not only reduce the air pollution but also it may help to save the money of peoples in the society.

Conclusion

The decisions at Government level is only the way to introduce the sharing of vehicles and popularization of cycling in the state. And also give more advertisement may help to promote the method in the society.

Acknowledgement

We are thankful to Dr. Sumitha, V.R., Assistant Professor, Department of Botany, Mahatma Gandhi College, Thiruvananthapuram, Kerala, for encouragement during the study.

Pesticide Slow

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High temperature thermoluminescence emissions of SrSO₄ nano phosphors doped with Eu and Mn

Jayavelan S¹*, K. Madhukumar¹, C.M.K. Nair¹,
Ramesh G. Nair², V.M. Arunakumar²

¹Department of Physics,
Vidyalaya College,
Thiruvananthapuram-695004, India
* jayvelan_india@yahoo.com

T.S. Eban²

²Regional Cancer Centre
Thiruvananthapuram-695011, India

Abstract— High temperature Thermoluminescence (TL) emissions of SrSO₄:Eu,Mn phosphor at 340°C is reported here for the first time. The nanocrystalline phosphors were prepared by wet chemical precipitation method. The glow curve shows an intense peak at 340°C, when the phosphor is subjected to X-irradiation. Co-doping with Mn enhances the trap depth and hence the TL emission temperature. Even though the luminescence intensity is found to be low, the phosphor becomes significant owing to its high temperature afterglow, which is one of the stringent requirements of a commercial thermoluminescent dosimeter (TLD). This phosphor appears to be fairly stable for TL measurements. Preliminary crystallographic and morphological studies of the phosphors were done using Powder X-ray Diffraction and Scanning Electron Microscopy (SEM). The phosphor has a single phase orthorhombic structure and the crystallites are sized in nano range. The dopant composition in the host matrix observed from the Energy Dispersive Spectra (EDS) were 8.18 atom% Eu and 8.15 atom% Mn. The single and well defined high temperature glow curve makes the phosphor suitable for high temperature radiation dosimetry applications.

Keywords— Thermoluminescence, Radiation dosimetry.

1. INTRODUCTION

Thermoluminescent (TL) phosphors were proved to be highly sensitive radiation detectors and are widely used for radiation dosimetry applications. Thermal ejection of relatively stable electrons trapped by means of ionizing radiation with X-ray, gamma ray, alpha, β -beam or other fast particles leads to TL. Studies are on in the search of suitable host-dopant combinations due to the constant need for high sensitivity TL dosimetry phosphors for different applications [1]. Recently, nanostructured materials are in focus, because of their potential impact in many areas such as electronics, photonics, catalysis and sensing [2-4]. Among the various phosphors alkaline earth sulphates are of special interest due to their high TL sensitivity, stability and low cost [1]. TL properties of rare earth doped CaSO₄, BaSO₄, SrSO₄, and MgSO₄ with single as well as multiple dopants were studied recently. TL studies of *Eu*-doped SrSO₄ compounds prepared via recrystallization method and irradiated by X-rays were done by J. Manam *et al.* [1]. Similarly, the TL performance of Eu doped SrSO₄ phosphors prepared through acid evaporation technique and irradiated with γ -rays were studied and reported by Q.Tang *et al.* [5]. Characteristics of the same host material prepared through a controlled chemical precipitation method by M. Karthikeyan *et al.* is also reported previously [6]. In many host lattices Mn is proved to be a best activator, when doped singly

or co-doped with rare earths [3,11,12]. Here the focus is on the TL properties of the SrSO₄:Eu nano phosphor co-doped with Mn. A much higher temperature TL emission is observed when the phosphor is subjected to X-rays. An attempt is made to estimate the activation energy corresponding to the trap from the geometry of the glow curve.

2. EXPERIMENTAL

SrSO₄:Eu,Mn nano phosphors were prepared by following the chemical precipitation technique described by Madhukumar *et al.* [7]. Analytical grade starting materials were used for the phosphor sample preparation. 0.5 mol% each of SrSO₄:Eu, SrSO₄:Mn and SrSO₄ were used for doping. After several washings, filtering and drying the precipitate was calcined at 400°C for 1 hour to eliminate the traces of any other compounds or acids. Further, the calcined material was ground well and then annealed at 3250°C in a programmable high temperature furnace for 10 hours in air atmosphere, to be required crystalline phase formation.

Subsequently, various characterization studies were carried out. The crystalline properties were studied from the X-ray diffraction taken from XPRT PRO Diffractometer using Cu K α radiation of $\lambda = 1.5406 \text{ \AA}$. SEM micrographs and EDS spectra obtained using JEOL 6390LV make Scanning Electron Microscope with EDS attachment were taken. Thereafter, the thermoluminescence glow curve at a heating rate of 5°C/s were recorded with a TL analyser TLD NUCLEONIX. About 5 mg of the phosphor powder was used all the time for recording the TL. In order to avoid any amount of phosphor sample influence the TL intensity, irradiations were made with Cu K α X-rays generated at 30-10mA from RADON make X-Ray unit before recording TL.

3. RESULTS AND DISCUSSION

A. Structure Analysis

Fig.1 shows the typical X-ray diffraction pattern of prepared SrSO₄:Eu,Mn nano phosphor. The spectrum shows orthorhombic lattice structure with Pnma 62 space group in accordance with the ICSD database of file number 0385. Observed and calculated d -values are in good agreement. The lattice parameters were found to be $a=4.32 \text{ \AA}$, $b=10.12 \text{ \AA}$ and $c=6.80 \text{ \AA}$, which are fairly in agreement with parameters reported for the undoped host lattice $a=4.33 \text{ \AA}$, $b=10.13 \text{ \AA}$, $c=6.84 \text{ \AA}$. The slight deviation in the parameters is

High temperature thermoluminescence emissions of SrSO₄ nano phosphors doped with Eu and Mn

Jayavelan S¹*, K. Madhukumar¹, C.M.K. Nair¹,
Ramesh G. Nair², V.M. Arunakumar²

¹Department of Physics,
Vignansarathi College
Thiruvananthapuram-695004, India
* jayvelan_india@yahoo.com

T.S. Eban²

²Regional Cancer Centre
Thiruvananthapuram-695011, India

Abstract— High temperature Thermoluminescence (TL) emissions of SrSO₄:Eu,Mn phosphor at 340°C is reported here for the first time. The nanocrystalline phosphors were prepared by wet chemical precipitation method. The glow curve shows an intense peak at 340°C, when the phosphor is subjected to X-irradiation. Co-doping with Mn enhances the trap depth and hence the TL emission temperature. Even though the luminescence intensity is found to be low, the phosphor becomes significant owing to its high temperature afterglow, which is one of the stringent requirements of a commercial thermoluminescence dosimeter (TLD). This phosphor appears to be fairly stable for TL measurements. Preliminary crystallographic and morphological studies of the phosphors were done using Powder X-ray Diffraction and Scanning Electron Microscopy (SEM). The phosphor has a single phase orthorhombic structure and the crystallites are sized in nano range. The dopant composition in the host matrix observed from the Energy Dispersive Spectra (EDS) were 8.18 atom% Eu and 8.15 atom% Mn. The single and well defined high temperature glow curve makes the phosphor suitable for high temperature radiation dosimetry applications.

Keywords— Thermoluminescence, Radiation dosimetry.

1. INTRODUCTION

Thermoluminescent (TL) phosphors were proved to be highly sensitive radiation detectors and are widely used for radiation dosimetry applications. Thermal ejection of relatively stable electrons trapped by means of ionizing radiation with X-ray, gamma ray, alpha, β -beam or other fast particles leads to TL. Studies are on in the search of suitable host-dopant combinations due to the constant need for high sensitivity TL dosimetry phosphors for different applications [1]. Recently, nanostructured materials are in focus, because of their potential impact in many areas such as electronics, photonics, catalysis and sensing [2-4]. Among the various phosphors alkaline earth sulphates are of special interest due to their high TL sensitivity, stability and low cost [1]. TL properties of rare earth doped CaSO₄, BaSO₄, SrSO₄, and MgSO₄ with single as well as multiple dopants were studied recently. TL studies of *Eu*-doped SrSO₄ compounds prepared via recrystallization method and irradiated by X-rays were done by J. Manam *et al.* [1]. Similarly, the TL performance of Eu doped SrSO₄ phosphors prepared through acid evaporation technique and irradiated with γ -rays were studied and reported by Q.Tang *et al.* [5]. Characteristics of the same host material prepared through a controlled chemical precipitation method by M. Karthikeyan *et al.* is also reported previously [6]. In many host lattices Mn is proved to be a best activator, when doped singly

or co-doped with rare earths [3,11,12]. Here the focus is on the TL properties of the SrSO₄:Eu nano phosphor co-doped with Mn. A much higher temperature TL emission is observed when the phosphor is subjected to X-rays. An attempt is made to estimate the activation energy corresponding to the trap from the geometry of the glow curve.

2. EXPERIMENTAL

SrSO₄:Eu,Mn nano phosphors were prepared by following the chemical precipitation technique described by Madhukumar *et al.* [7]. Analytical grade starting materials were used for the phosphor sample preparation. 0.5 mol% each of SrSO₄, Eu₂O₃ and MnO₂ were used for doping. After several washings, filtering and drying the precipitate was calcined at 400°C for 1 hour to eliminate the traces of any other compounds or acids. Further, the calcined material was ground well and then annealed at 3250°C in a programmable high temperature furnace for 10 hours in air atmosphere, to be required crystalline phase formation.

Subsequently, various characterization studies were carried out. The crystalline properties were studied from the X-ray diffraction taken from XPRT PRO Diffractometer using Cu K α radiation of $\lambda = 1.5406 \text{ \AA}$. SEM micrographs and EDS spectra obtained using JEOL 6390LV make Scanning Electron Microscope with EDS attachment were taken. Thereafter, the thermoluminescence glow curve at a heating rate of 5°C/s were recorded with a TL analyser TLD NUCLEONIX. About 5 mg of the phosphor powder was used all the time for recording the TL signal, such amount of phosphor sample influence the TL intensity. Irradiations were made with Cu K α X-rays generated at 30-10mA from RADON make X-Ray unit before recording TL.

3. RESULTS AND DISCUSSION

A. Structure Analysis

Fig.1 shows the typical X-ray diffraction pattern of prepared SrSO₄:Eu,Mn nano phosphor. The spectrum shows orthorhombic lattice structure with Pnma 62 space group in accordance with the ICSD database of the number 0885. Observed and calculated d -values are in good agreement. The lattice parameters were found to be $a=4.32 \text{ \AA}$, $b=10.10 \text{ \AA}$ and $c=6.80 \text{ \AA}$, which are fairly in agreement with parameters reported for the undoped host lattice $a=4.33 \text{ \AA}$, $b=10.10 \text{ \AA}$, $c=6.84 \text{ \AA}$. The slight deviation in the parameters is

modes, $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ possesses more than four Raman modes which indicate a lowering of symmetry from cubic. In accordance with observed number of modes and group theoretical predictions the most likely symmetry of $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ is monoclinic with the space group $P2_1/n$. The symmetry was further confirmed from the Rietveld refinement of the XRD pattern. The compound possesses band gap of 3.8 eV. The photoluminescence properties of $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ substituted with Eu^{3+} for four different concentrations (15, 10, 5 and 2.5 mol %) were also investigated and it was found that concentration quenching occurred at 15 mol % of Eu^{3+} substitution, due to the cross relaxation between two neighboring Eu^{3+} ions. Thermoluminescence spectra of Eu^{3+} substituted $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ presented three emission lines at 592, 611 and 633 nm corresponding to the magnetic dipole transition $^5\text{D}_0 - ^7\text{F}_1$, electric dipole transition $^5\text{D}_0 - ^7\text{F}_2$ and $^5\text{D}_0 - ^7\text{F}_3$ transitions of Eu^{3+} respectively. The chromaticity coordinates was found to be (0.629, 0.369) for 10 mol % Eu^{3+} substituted $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ which shows colour of emission in orange-red region.

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P 19

BIOGENIC SYNTHESIS OF SILVER NANOPARTICLES AND ITS CHARACTERISATION

**Remya G R¹, Lekshmi P Nair¹, Jayasudha S¹,
S Saravanakumar², Akhila S¹, Abhimanyu C M¹, Prabitha B Nair^{1*}**

¹Post Graduate and Research Department of Physics, Mahatma Gandhi College,
Thiruvananthapuram

²Department of Physics, NSS College, Pandalam

E-mail : prabibnair@gmail.com

Silver nanoparticles possess unique physical, chemical and biological properties due to which they exhibit catalytic, antimicrobial, anticancer and wound healing activity. In the present study silver nanoparticles are synthesized by reduction of silver salt with apple extract. The obtained silver nanoparticles are characterized using X-ray diffraction (XRD), FT-IR spectroscopy, micro Raman spectroscopy, Scanning Electron Microscopy (SEM) and UV-vis spectroscopy. Silver nanoparticles are in a state of tensile strain with an average particle size of 20 nm. The Surface Plasmon Resonance peak in the absorption spectra showed an absorbance maximum at 423 nm. The constancy in peak position with increasing time period indicates the stability of obtained silver nanoparticles.

Keywords : Nano particles, XRD, FT-IR, SEM

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GROWTH AND THERMAL CHARACTERISATION OF GEL GROWN CALCIUM MALEATE DIHYDRATE

PP-18

Lekshmi P. Nair¹, Bijini B. R.¹, Prasanna S.¹, Deepa M.², C. M. K. Nair¹, K. Rajendra Babu^{1*}

¹Postgraduate Department of Physics, M.G. College, Thiruvananthapuram, India-695004

²Department of Physics, All Saints' College, Thiruvananthapuram, India-695037

*Corres. author Tel. No: +91 9447963076, mgkrb1956@yahoo.co.in (K. Rajendra Babu)

Abstract: Calcium maleate dihydrate (CaMa) crystals are grown by gel method for the first time. Conditions for growing good quality crystals are optimized. Elemental analysis gives the formula of the compound as $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Thermal properties of the complex are analysed by TGA/DTA. Coats and Redfern method is utilised to obtain the kinetic and thermodynamic parameters of the complex.

Key words: Crystal growth, maleic acid, calcium maleate, gel method, TGA, DTA.

Introduction

Various metal carboxylate compounds strike the specific attention of the researchers due to their vast applications in science and technology. Maleic acid is biologically important and its interaction with different metal ions opens new potentialities with targeted properties. Calcium exhibits wide range of topologies and confirmations with co-ordination numbers ranging from 3 to 11¹. Calcium maleate is used as the substrate for enzymatic iodination process. As the gel method mimics the growth of crystals in human body, we are adopting the method of controlled diffusion of ionic species in hydrosilica gel medium to get quality crystals of this biologically important calcium maleate. The grown crystals are characterised by elemental analysis, TGA/DTA.

Experimental Procedure:

Growth Procedure:

The crystallisation of calcium maleate dihydrate was accomplished using gel diffusion technique. Crystals were grown in glass tubes of length 20cm and diameter 2.5cm. Silica gel of specific gravity 1.03 to 1.06g/cc was prepared by

dissolving sodium metasilicate (SMS) in double distilled water. Maleic acid (1M) was added to SMS to acidify it to get pH in the range 3 to 7. About 30ml of above solution was taken in each test tube and kept undisturbed for setting. Over the set gel, aqueous solution of calcium chloride (0.5 – 2M) was added as the top reagent, without damaging the gel system.

Results and discussion: Crystal Growth:

Crystals of CaMa were formed at the gel interface within two week. The growth process took three months for completion. Good quality crystals suitable for characterisation studies were grown in gel medium of pH 6.5 and density 1.04g/cc, 1M maleic acid, 1M calcium chloride. The crystals of CaMa were prone to decompose in air. The photograph of the grown crystal is shown in figure 1. Elemental analysis gives the formula of the compound as $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ (Experimental: C- 25.93%, H- 2.35% Calculated: C- 25.26%, H- 3.19%).

Thermal analysis:

Thermal analysis of the sample was carried out using Perkin Elmer Diamond TGA/DTA analyser with a heating rate of 10°C/min in the nitrogen atmosphere. The TGA/DTA results are shown in figure 2



Fig1: $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$

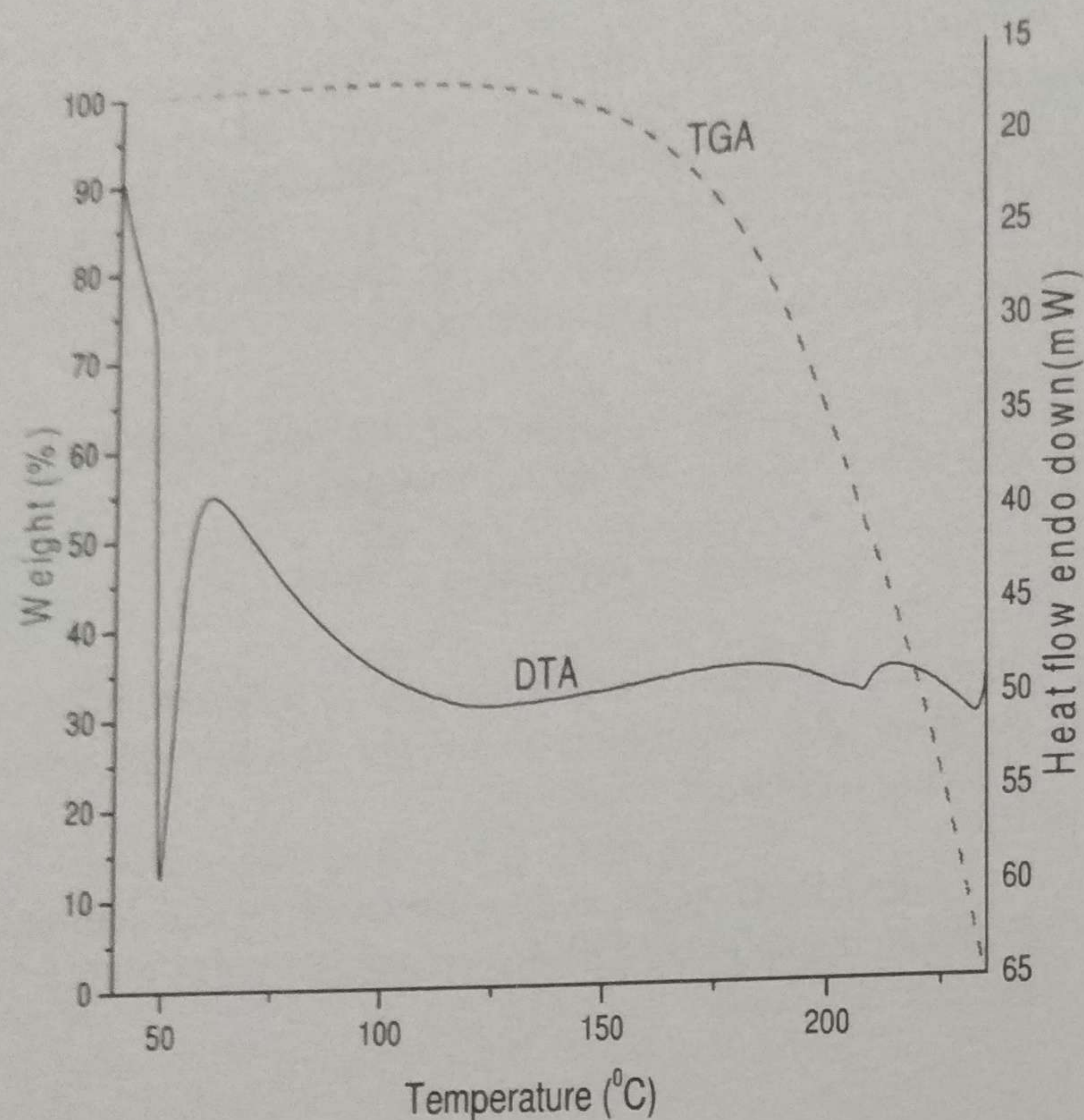


Fig. 4. TGA/DTA curves of Benzophenone crystal

IV. CONCLUSION

Good quality benzophenone crystals were grown by gel diffusion technique with optimum conditions of gel density 1.04 g/cc and pH value 6. FTIR spectrum has revealed the vibrational modes which identifies the grown crystal. The optical band gap of the crystal was determined as 3.18 eV from the UV visible spectrum. The crystal is having a good transparency region which makes it suitable for NLO applications. The crystal is thermally stable for 5% up to 150°C and the melting point was determined as 49.55°C.

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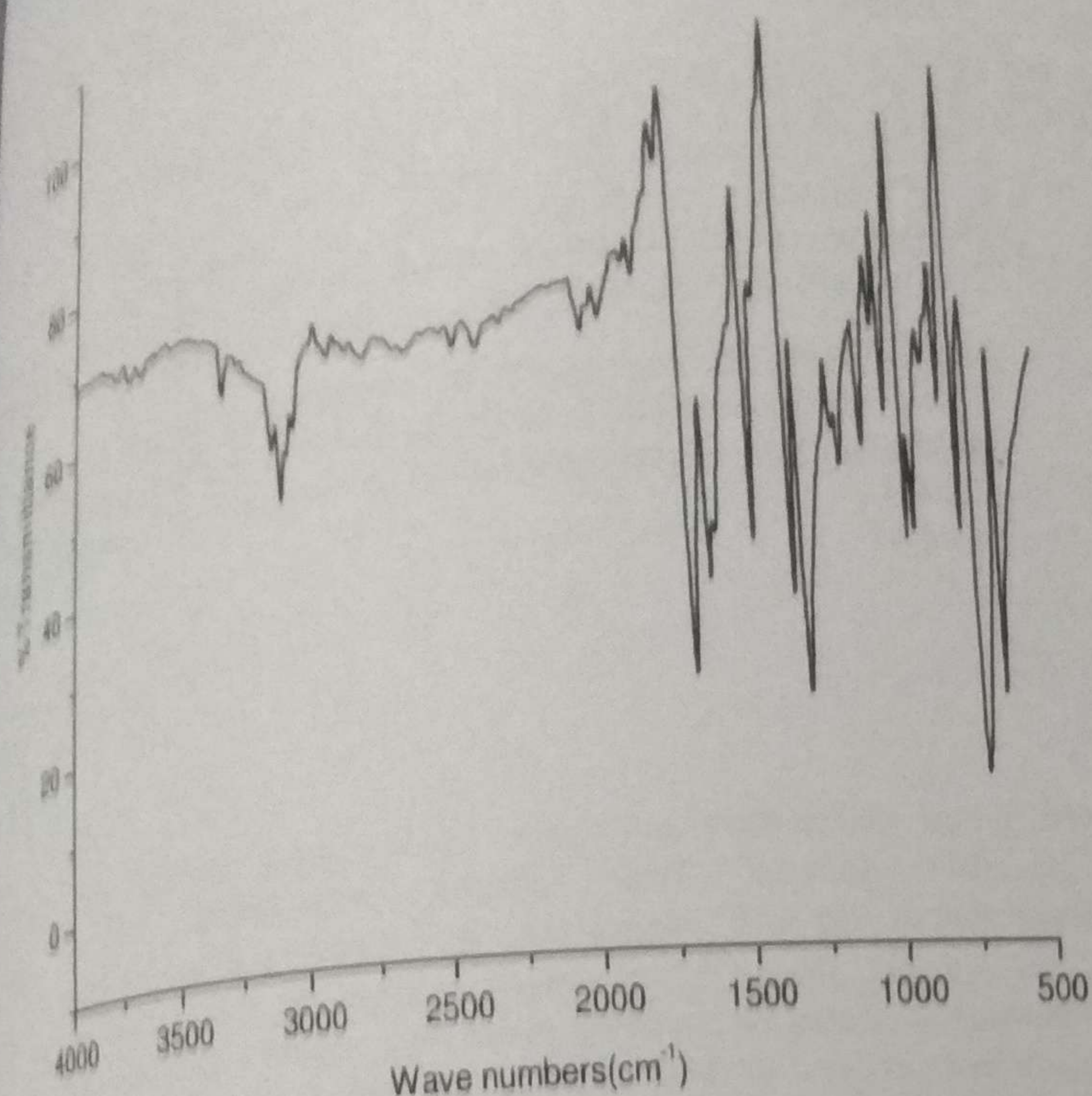


Fig. 1. FTIR spectrum of Benzophenone crystal

The region between 1274.65 and 1024.87 cm^{-1} represents the in plane bending modes of C-H while the peaks below 1000 cm^{-1} represents out of plane bending modes.

B. UV-Vis NIR spectral analysis

The UV-visible absorption spectrum of benzophenone crystal shown in Fig. 2 was recorded in the range 214 nm to 1200 nm using the instrument Varian Cary 5000 UV Vis NIR spectrometer.

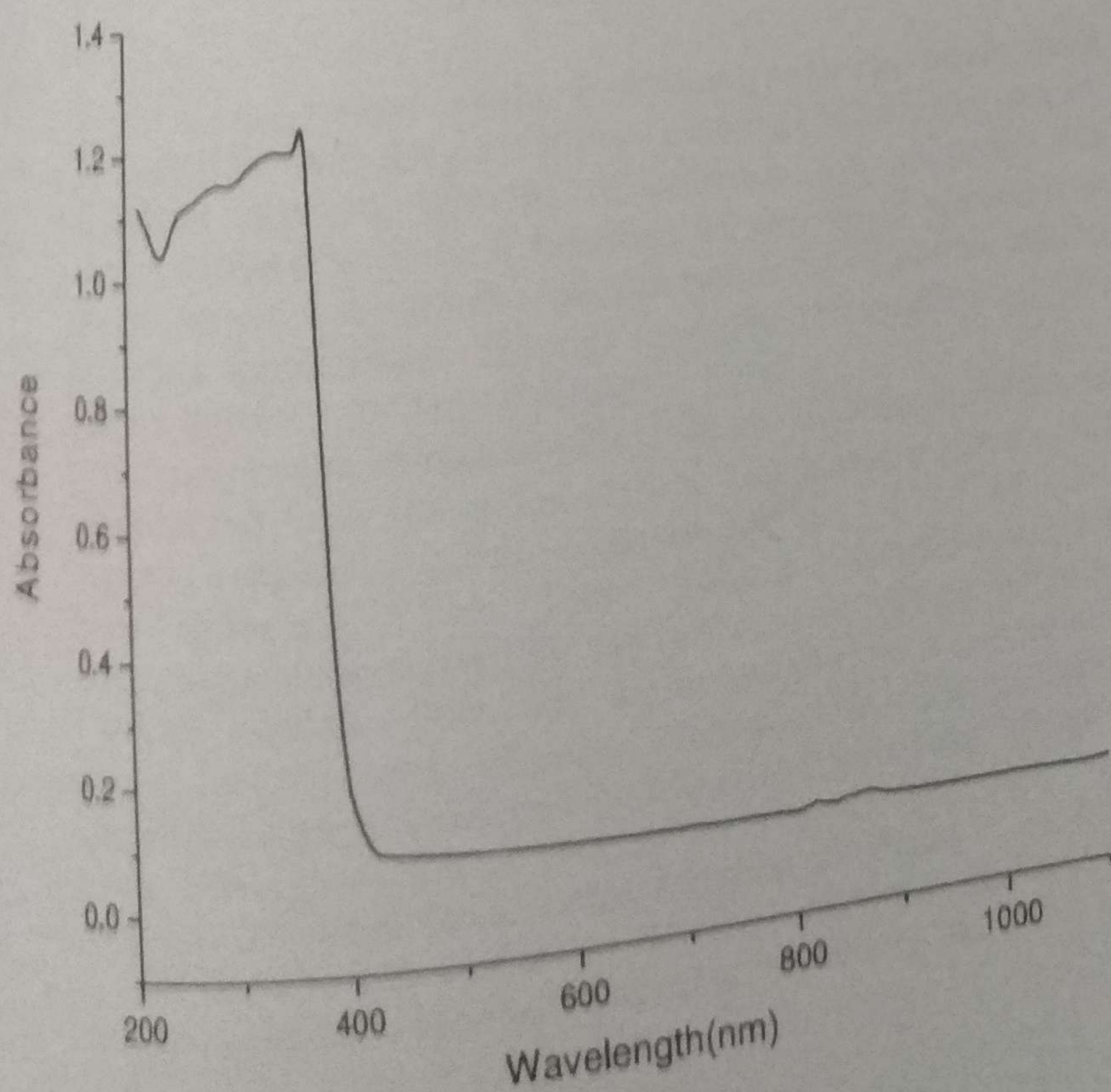


Fig. 2. UV visible spectrum of Benzophenone crystal

The transmission range and cut off wavelength of the crystals are very crucial in many important practical applications. Here a strong absorption is taking place at 377 nm, which is the lower cut off wavelength. There is no significant absorption in the visible range. This good transparency region makes the benzophenone crystal suitable for optoelectronic applications [8, 9].

The optical band gap E_g can be calculated from the absorption spectrum using the equation

$$(\alpha h\nu)^n = A(E_g - h\nu) \quad (1)$$

where A is a constant, E_g is the optical band gap, h Planck's constant and ν frequency of the incident photons, α absorption coefficient[10].

Fig. 3 shows a graph drawn between $(\alpha h\nu)^3$ versus $h\nu$. E_g is calculated as 3.18 eV by extrapolating the linear part of the graph.

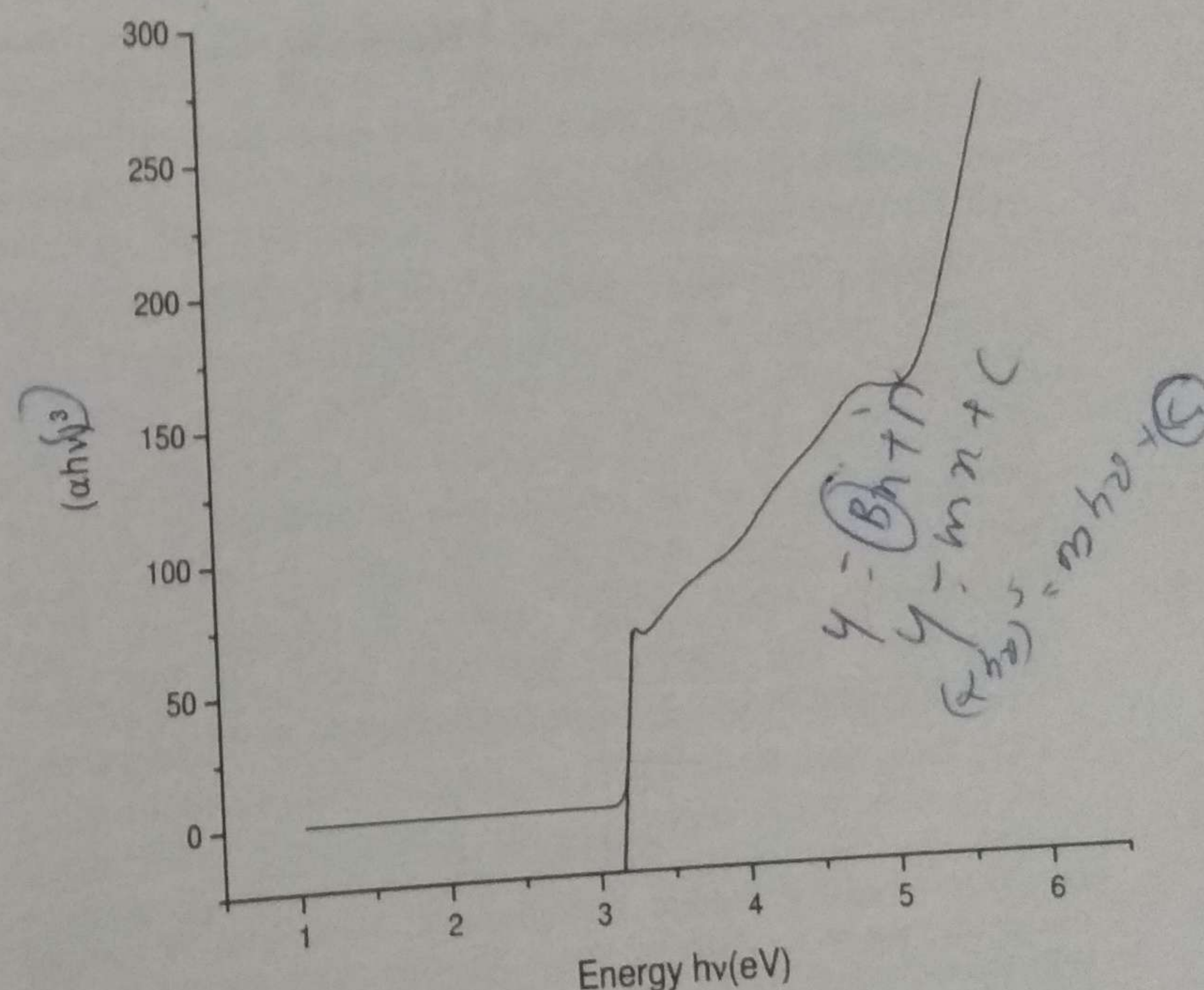


Fig. 3. Plot of $(\alpha h\nu)^3$ versus photon energy

C. Thermal Analysis

Thermo-gravimetric analysis (TGA) and Differential thermal analysis (DTA) were carried out for thermal studies. TGA and DTA curves are shown in Fig. 4.

In the DTA graph, the endothermic peak at 49.55°C corresponds to the melting point of the crystal. Here the melting point is found to be increased than the melting point of benzophenone crystals grown by other method (41.36°C) [6]. The sharpness of the endothermic curve shows good degree of crystallinity. The TGA graph shows that the crystal is thermally stable for 5% up to 150°C .

Spectral and thermal studies of gel grown Benzophenone crystal

Divya R, Lekshmi.P.Nair,
B.R.Bijini, K.Rajendra Babu
Department of Physics
MG College
Thiruvananthapuram, India

K.Rajendra Babu
Department of Science
Heera College of Engineering & Technology
Thiruvananthapuram, India

Abstract—Benzophenone has significant relevance in non linear optical applications. Benzophenone crystals had already been grown by several methods. In this work, single crystals of benzophenone were successfully grown by gel method. The grown crystal was subjected to FTIR spectral analysis to confirm the presence of functional groups. The optical band gap of the crystal was determined from the UV Visible NIR absorbance spectrum and found to be 3.18 eV. The nature of the spectrum shows its potential as an NLO material. Thermal properties and thermal stability were studied by conducting Thermo-gravimetric and Differential Thermal Analysis. Here the melting point was observed as 49.5 degree Celsius which is well matching with the theoretical value. It is also thermally stable for 5 percentage up to 150 degree Celsius.

Keywords—Benzophenone, gel growth, FTIR, UV-Vis-NIR spectral analysis, Thermal analysis

I. INTRODUCTION

Crystals play an inevitable role in modern technology. So crystal growth is a prominent area in the scientific and technological research. Since the crystal growth has immense applications, it is an interdisciplinary subject covering physics, chemistry, materials science, chemical engineering, metallurgy, crystallography, mineralogy etc. There is growing interest on crystal growth to meet the demand of materials for technological applications [1].

The growth of NLO materials has become trend in recent years. They are having technological importance in the field of optoelectronics, lasers, data storage systems and optical communication [2]. These materials should possess large second order optical non linearities, short transparency, cut off wavelength and thermal stability [3]. NLO response is larger in organic materials when compared to inorganic materials due to the presence of active π bonds [4]. So we focus our studies on organic materials.

Benzophenone is one of the most important organic materials showing NLO property [5]. It is an important compound in organic photochemistry and perfumery as well as in organic synthesis. It is also used a photo-initiator of UV curing applications in inks, adhesive and coatings, optical fiber as well as in printed circuit boards[5]. Rapid crystal growth of benzophenone by low temperature solution growth,

Unidirectional seeded single crystal growth from solution of benzophenone [5, 6] has already been reported.

Here we have grown benzophenone crystals by gel method to improve the quality of the crystals. The gel growth is simple in technique, effective in growing single crystals of compounds that cannot be easily grown by other methods [7]. In this paper, we are presenting the spectral and thermal studies of gel grown benzophenone crystals.

II. EXPERIMENTAL - GROWTH OF SINGLE CRYSTALS

Single crystals of benzophenone were formed by gel diffusion technique. The technique involves the setting of gel and addition of required top solution over the set gel. The crystallization apparatus for the growth consists of borosilicate glass test tube of length 20 cm and diameter 2.5 cm placed vertically on a stand. The solution for gel having specific gravity 1.03-1.05 g/cc was prepared by dissolving sodium meta silicate (SMS) in double distilled water. The solution was then acidified with 1M glacial acetic acid to get the pH in the range 4 - 7(in steps of 0.5) and taken about 30 ml of each in different test tubes. They were kept undisturbed for gel setting. Over the set gel, the top solution prepared by dissolving AR grade benzophenone in ethanol was added drop wise through the side of the test tube to prevent the gel breakage. The test tubes were covered with transparent plastic sheets to avoid evaporation and contamination of solution. The crystals were found growing over the gel surface within 1 day and the growth lasted for about 50 days. It is also found that pH = 6 and gel density 1.04 g/cc was the optimum condition for the growth of best quality benzophenone crystals.

III. RESULTS AND DISCUSSIONS

A. Fourier Transform Infrared Spectroscopic Studies (FTIR)

The FTIR spectrum of gel grown benzophenone crystal is shown in the Fig. 1. In the higher wavelength region, the peak at 3054.80 cm^{-1} is associated with aromatic C-H stretching. The peak at 1650 cm^{-1} represents C=O stretching. The skeletal vibrations are represented by the peaks 1591.44 cm^{-1} and 1443.87 cm^{-1} .

microcrystals was carried out between 200 nm and 1200nm. Fig. 5 shows the absorbance spectrum of the complex. The result is found to be transparent in the entire visible region which enables it to be a good candidate for optoelectronic application [8]. A graph is drawn between photon energy $h\nu$ versus $(\alpha h\nu)^2$, where α is the absorption coefficient, as shown in fig.6 and the electronic bandgap is estimated as 4.2 eV.

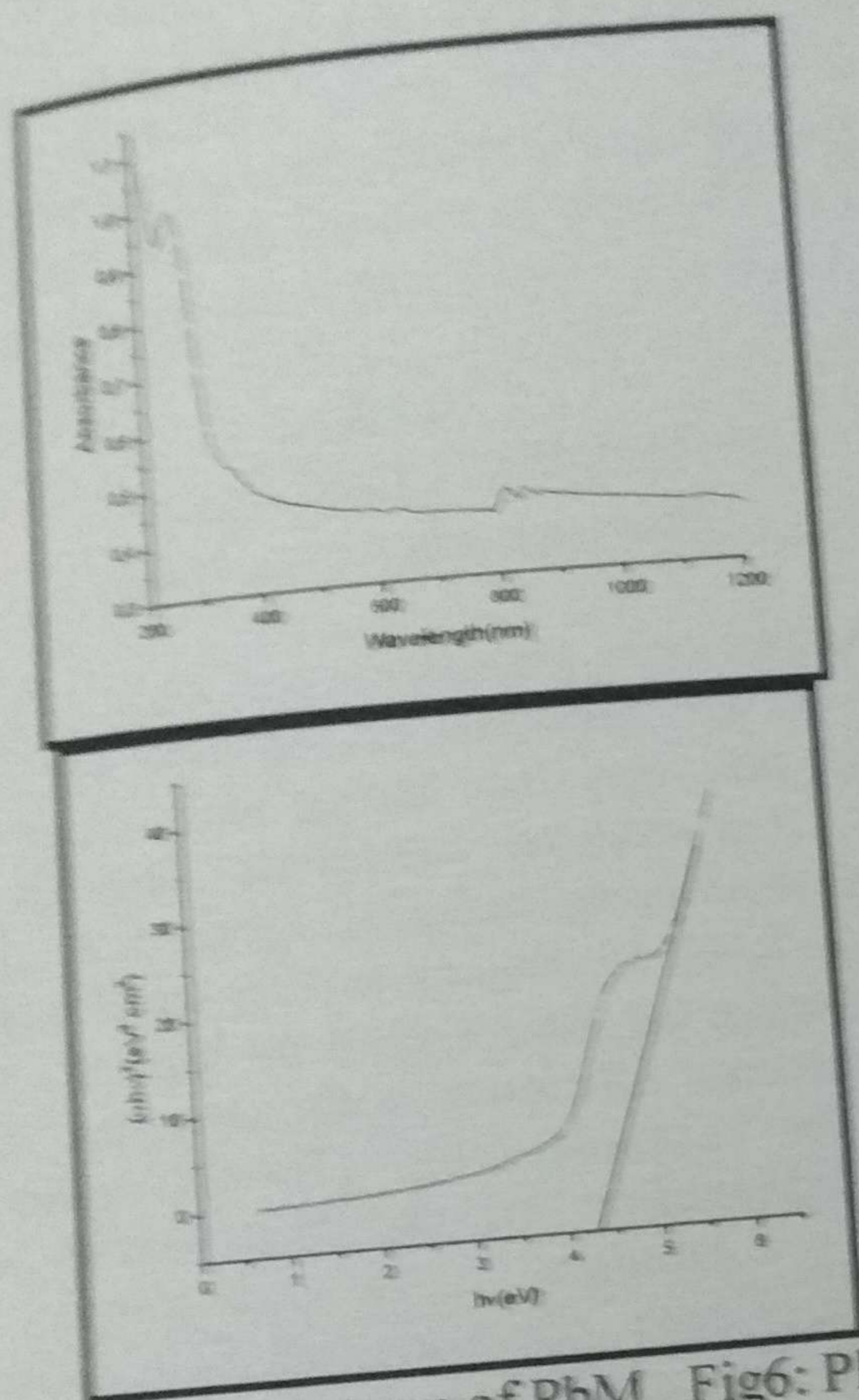


Fig5: Absorbance spectrum of PbM Fig6: Plot of alpha energy versus photon energy

4. CONCLUSIONS:

Single crystals of lead maleate are grown successfully by conventional gel method. Good quality single crystals belonging to monoclinic system, P21/C space group are grown from the gel medium of pH 5.5 and density 1.04g/cc. The crystal structure was same as that of the reported one. Thus in this case, the method of crystallization does not affect the crystal structure. The FTIR spectral analysis confirms the presence of various functional groups in the grown crystals. The elemental analysis is consistent with the chemical formula $PbC_2H_2(CO_2)_2$. The thermal stability of the complex is provided by the TGA/DTA. Wide transparency of PbM in the entire visible range makes it a suitable candidate for optoelectronic application. The porosity of the complex offers the potential for gas adsorption and storage.

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Using the crystallisation method described in section 2.1, crystals of PbM were formed at the gel interface within one week. The growth process took four weeks for completion. Good quality single crystals suitable for single crystal XRD studies were grown in gel medium of pH 5.5 and density 1.04g/cc with 1M maleic acid and 0.5M lead nitrate. The characteristic shape of the crystal is shown in Fig. 1.

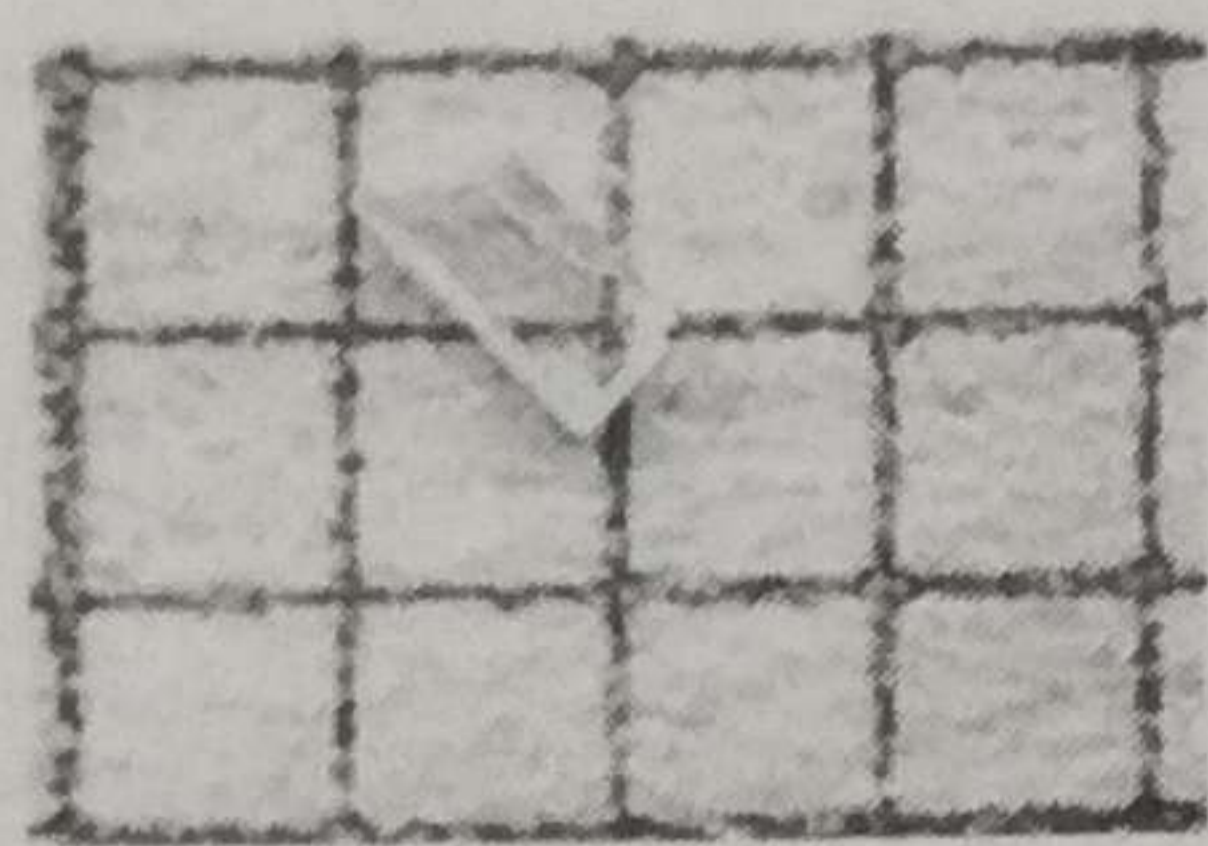


Fig. 1: Photo of grown PbM crystal.

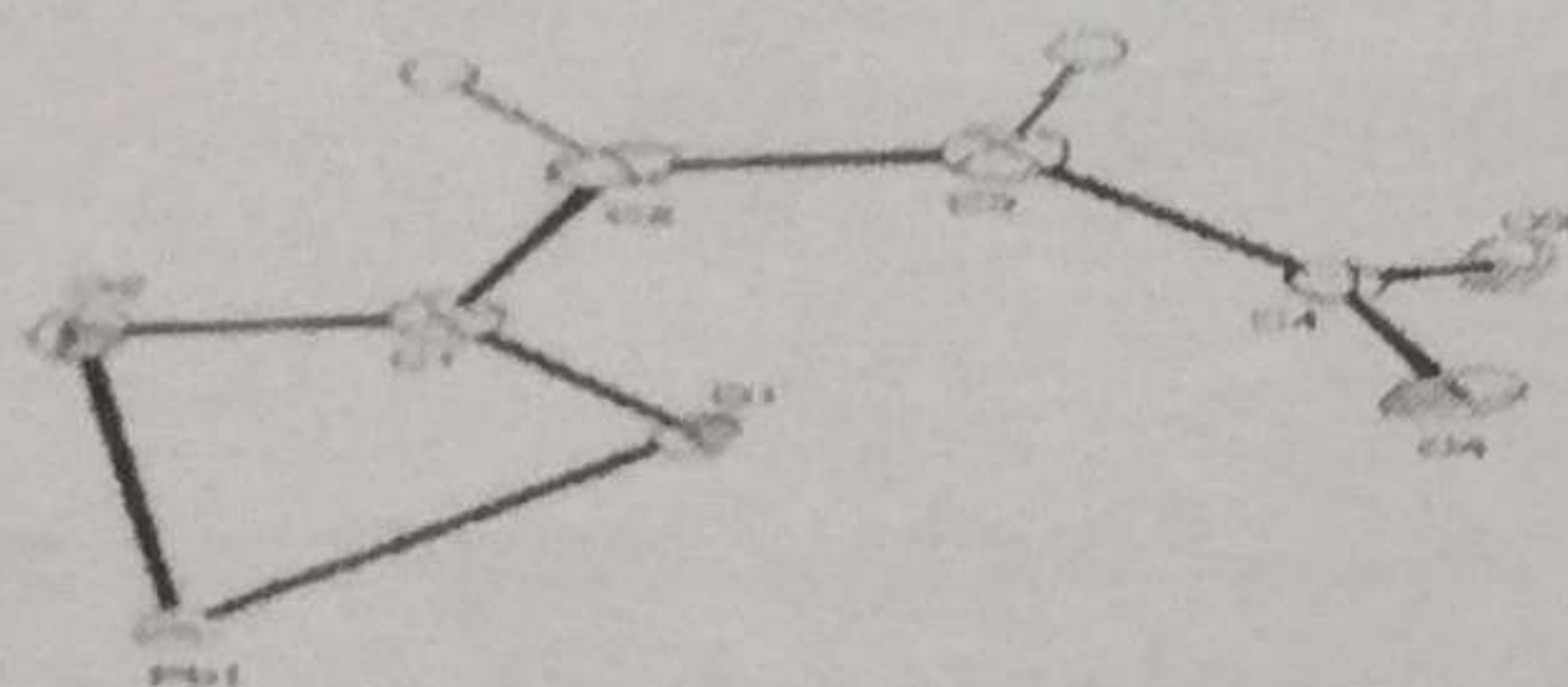


Fig2: Asymmetric unit of PbM.

3.2. CRYSTAL STRUCTURE:

A report on the structure of lead maleate grown at higher temperature is available [2]. The report on the growth of title complex at room temperature is not available so far. To ascertain whether the structure of the gel grown PbM is same as that of the reported one, the SXRD analysis is done. The single crystal XRD data of a well formed crystal were collected using Bruker AXS Kappa Apex2 CCD diffractometer with graphite monochromated Mo K α ($\lambda = 0.71073 \text{ \AA}$) radiation. The PbM crystals thus grown by gel method belongs to the space group P21/C with unit cell parameters $a = 9.8795(3) \text{ \AA}$, $b = 6.9537(3) \text{ \AA}$, $c = 8.2616(4) \text{ \AA}$, $\beta = 111.121(2)^\circ$. This is similar to the reported structure. Asymmetric unit of PbM is as shown in fig.2.

3.3. FT-IR SPECTRAL STUDIES:

The co-ordination of the metal ion with the organic linker is reflected as the shift in the vibrational frequency of the complex. The FTIR spectrum of PbM is shown in fig.3. The absence of broad band around 3400 cm^{-1} confirms the absence of water of ligation in the structure of PbM [4]. The bands of protonated carboxylic groups are usually expected in the range $1685\text{--}1715 \text{ cm}^{-1}$. These bands are absent in the PbM spectrum indicating the complete deprotonation of this group which is supported by SXRD. The band at 1642 cm^{-1} is assigned to the asymmetric stretch while the band at 1406 cm^{-1} and 1535 cm^{-1} is assigned to the symmetric stretch of the carboxylate group [5]. Thus the $\Delta\nu$ value of 236 cm^{-1} and 129 cm^{-1} corresponds to the unidentate and bidentate mode of co-ordination of the ligand with the metal, which is evident from the SXRD data. The band at 1530 cm^{-1} due to $\nu_{\text{C}=\text{C}}$ in the ligand spectrum shifts down to 1496 cm^{-1} in the complex spectrum. This

may be due to the C-H...O interaction in PbM. The band at 989 cm^{-1} in the ligand spectrum due to the C-H out of plane bending vibration shifts down to 973 cm^{-1} , which may be due to the presence of intermolecular hydrogen bonds. Pb-O stretching is identified by the band at 461 cm^{-1} [6].

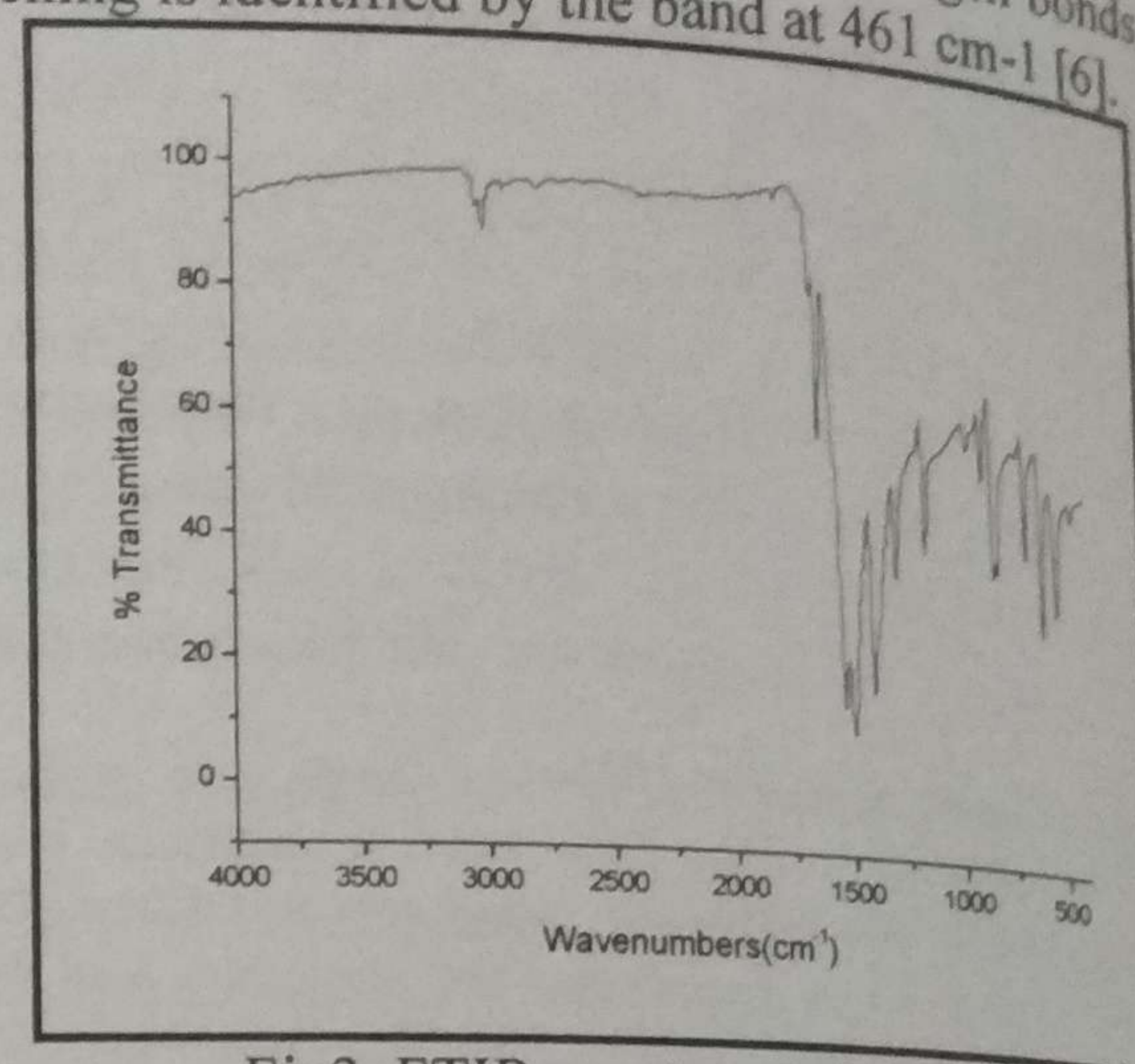


Fig3. FTIR spectrum of PbM

3.4. ELEMENTAL ANALYSIS:

The elemental composition of PbM crystals was determined both theoretically and experimentally. Both the values are in agreement with each other and the molecular formula is derived as $\text{PbC}_2\text{H}_2(\text{CO}_2)_2$.

Experimental: C- 14.81%, H- 0.69%; Calculated: C- 14.95%, H- 0.63%.

3.5. THERMAL ANALYSIS:

TGA/DTA data provides the details regarding the thermal stability of the complex. An amount of 15.5 mg is taken for the analysis. The results of TGA and DTA studies are given in Fig.6. PbM is thermally stable up to 250°C . This confirms the absence of lattice water and co-ordinated water molecules. This is followed by an endothermic peak at 337°C which indicates the elimination of organic ligand to form metal oxide, PbO and elemental carbon residue with a weight loss of 26 % (cal: 26.89%). Weight of the final residue PbO + C (74%) observed from thermal studies is found to be in agreement with the calculated residual weight of 73.11% [7].

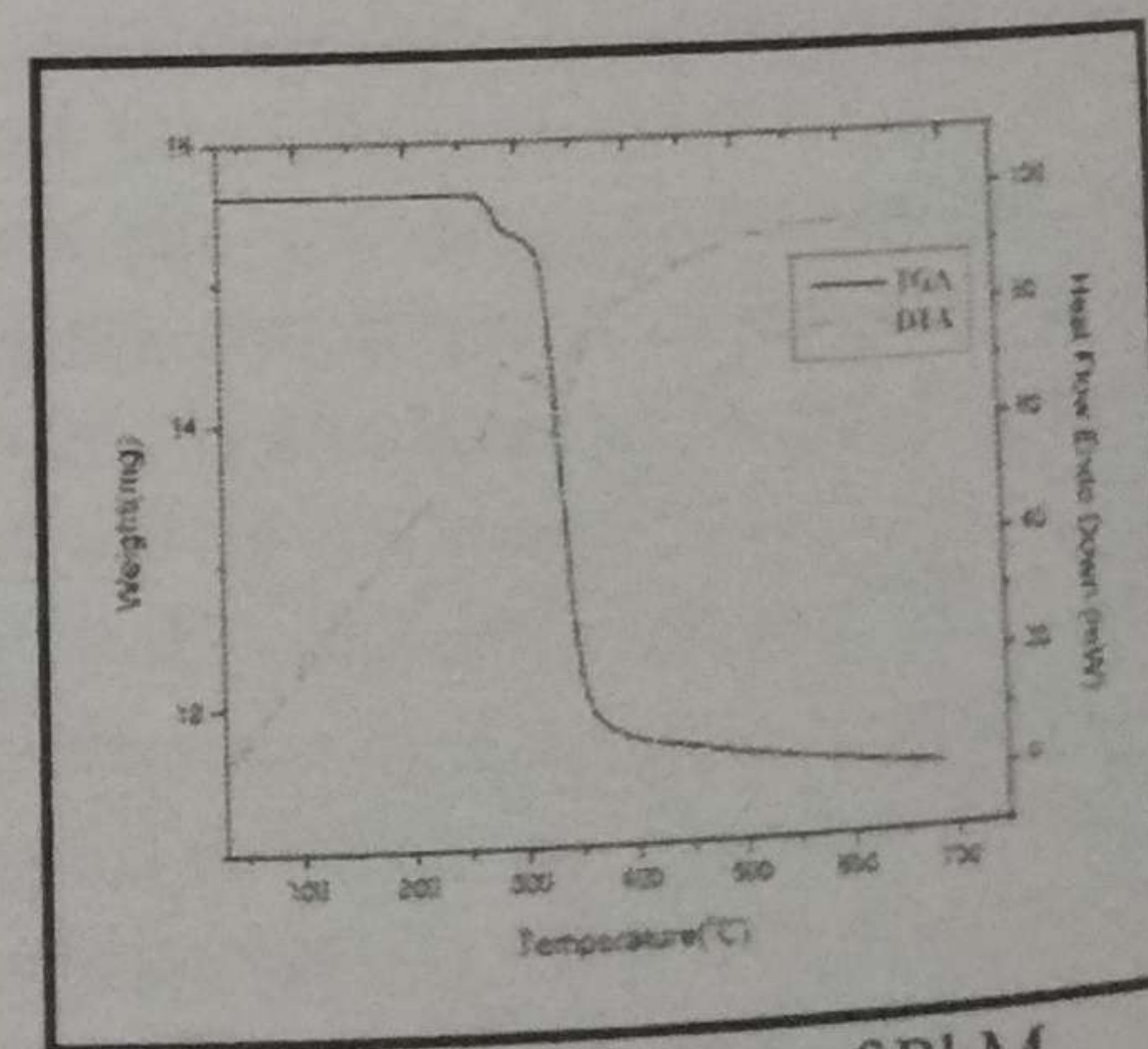


Fig4: TGA/DTA of PbM

3.6. UV- VIS SPECTRAL STUDIES:

To know the suitability of the material for optical applications, UV- Visible absorbance spectrum of

MARKET TIMING ABILITIES OF INDIAN MUTUAL FUND MANAGERS: AN EVALUATION

Kishore. H*

Abstract

Mutual funds play a crucial role in an economy by mobilizing savings from investors and invest the same in the stock-market, thereby establishing a direct link between savings and the capital market. The growth of mutual funds depends on the performance of the mutual fund schemes, which in turn, to a great extent depends on the ability of fund managers in generating superior returns on mutual fund schemes. The fund manager's efficiency is evaluated by looking into their stock selection skills and market timing abilities. The present study is an attempt to examine whether Indian mutual fund managers exploit market timing activities in generating superior returns on mutual fund schemes.

Mutual funds play a crucial role in an economy by mobilising savings from investors and invest the same in the stock-market, thereby establishing a direct link between savings and the capital market. Mutual fund is an investment avenue especially for those investors who want to participate in the stock market but who do not know the intricacies of the stock market. An average investor always prefers mutual fund investment rather than directly investing in stock market as it involves a huge amount of risk. An investor engaging directly in the stock market should have updated information and this information is

*Assistant Professor in Economics, Mahatma Gandhi College,
Thiruvananthapuram



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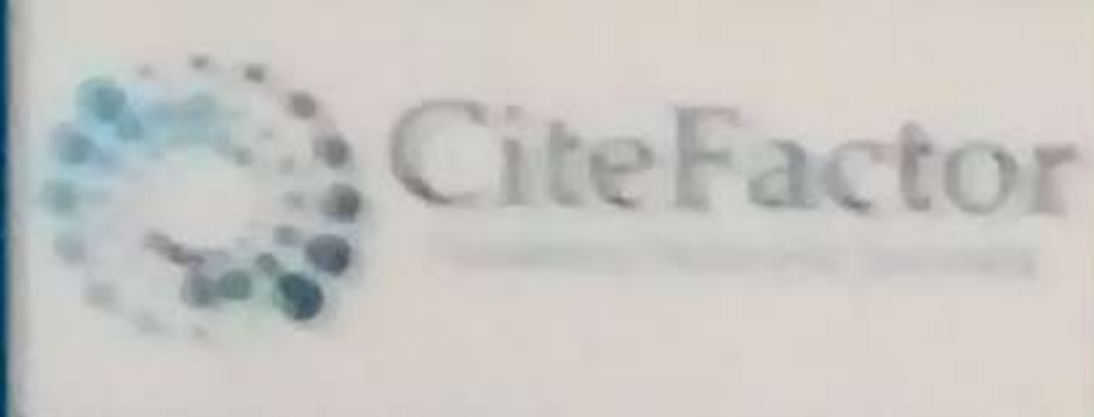
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MUTUAL FUND PERFORMANCE AND STRONG FORM EFFICIENCY OF INDIAN CAPITAL MARKET

Kishore*

Abstract

The Indian capital market has witnessed a fundamental institutional change since the reforms initiated by the Securities Exchanges Board (SEBI) of India during the 1990s. This paper attempts to test the strong form efficiency of Indian capital market by evaluating the performance of mutual funds over a period of ten years from April 1, 2000 to December 31, 2010 using monthly returns based on Net Asset Values (NAV) of 36 sample schemes. The index of NSE (i.e., S&P CNX Nifty) and that of BSE (i.e., SENSEX) is being used as benchmarks and the performance of mutual funds are compared with that of the benchmarks. The results of the study indicate that the Indian capital market is not strong form efficient and that the unethical practice of taking advantage of insider information prevails in the Indian capital market.

The Indian capital market has grown tremendously since the 1990s in terms of resource mobilisation, number of listed stocks, market capitalisation, trading volumes, turnover and investor base. The market has witnessed a fundamental institutional change since the reforms initiated by the Securities Exchanges Board (SEBI) of India during the 1990s. Capital market is the market for medium and long term funds. It mobilises the savings of the retail and institutional investors and channelise the same to the businesses, government and individuals. It induces economic growth by rationally allocating resources from conventional non-productive assets to productive assets. The capital market of a country is said to be efficient if it operates in such a way that the security prices reflect the current information in an unbiased manner and prices are determined on

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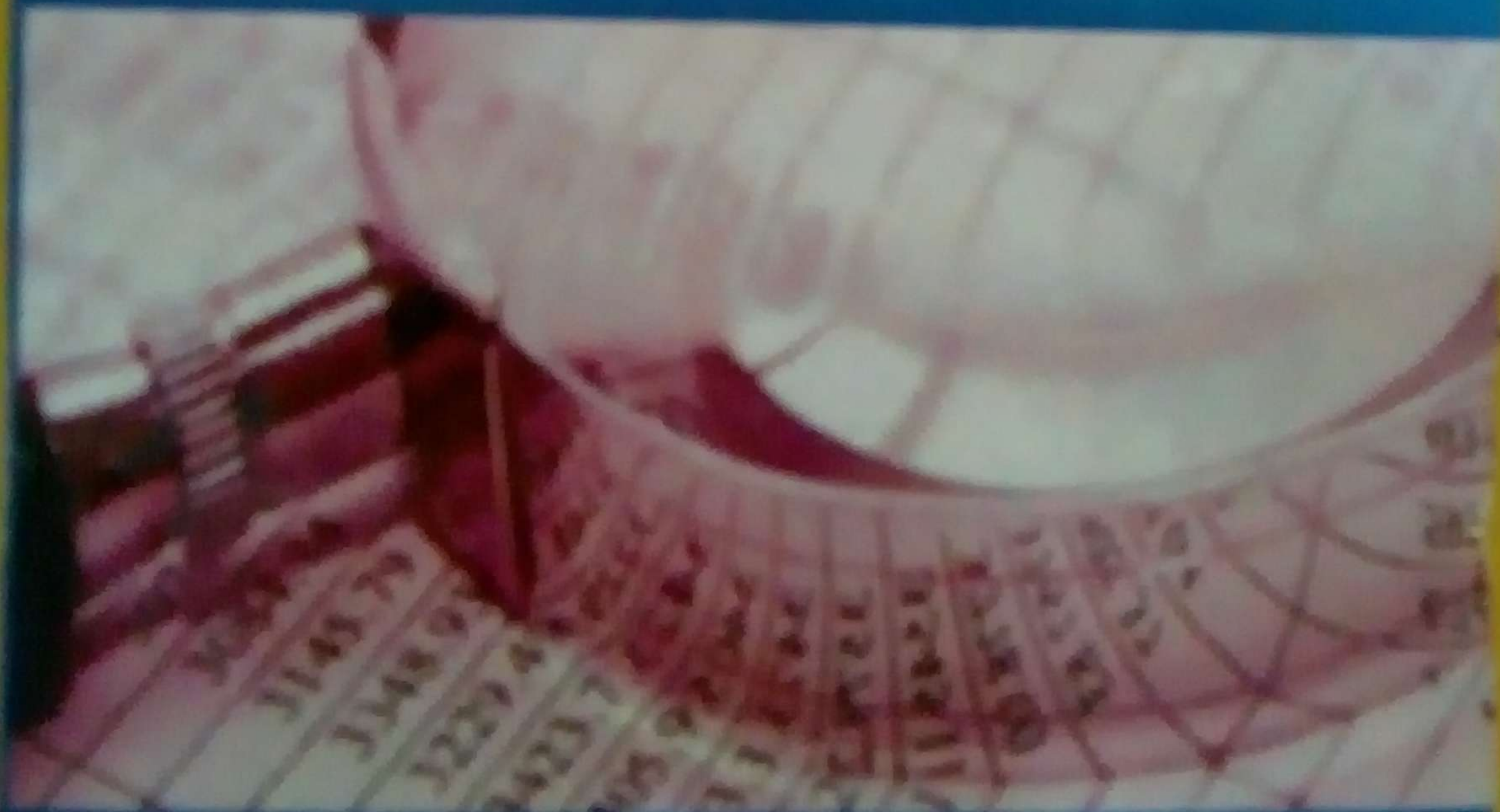
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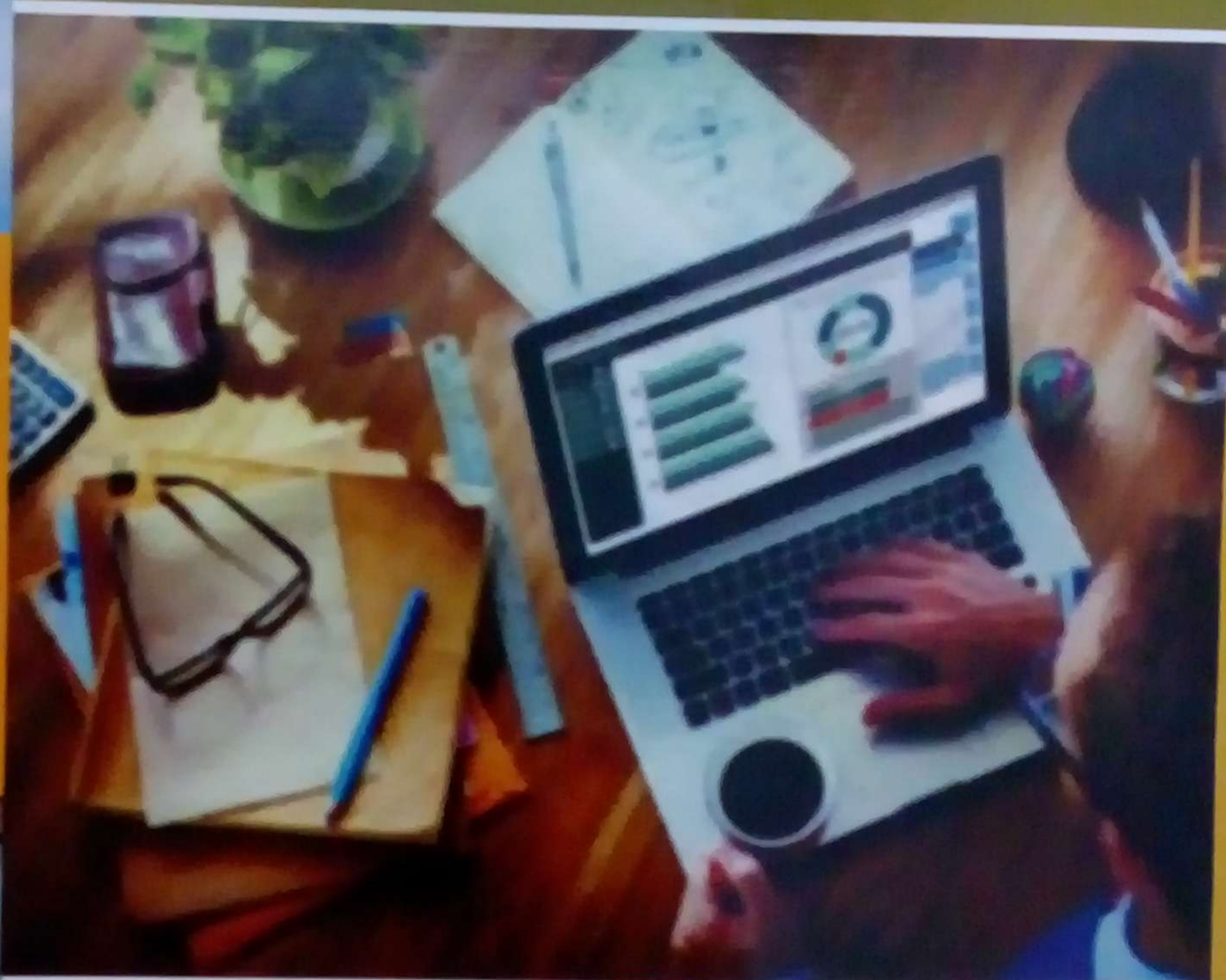
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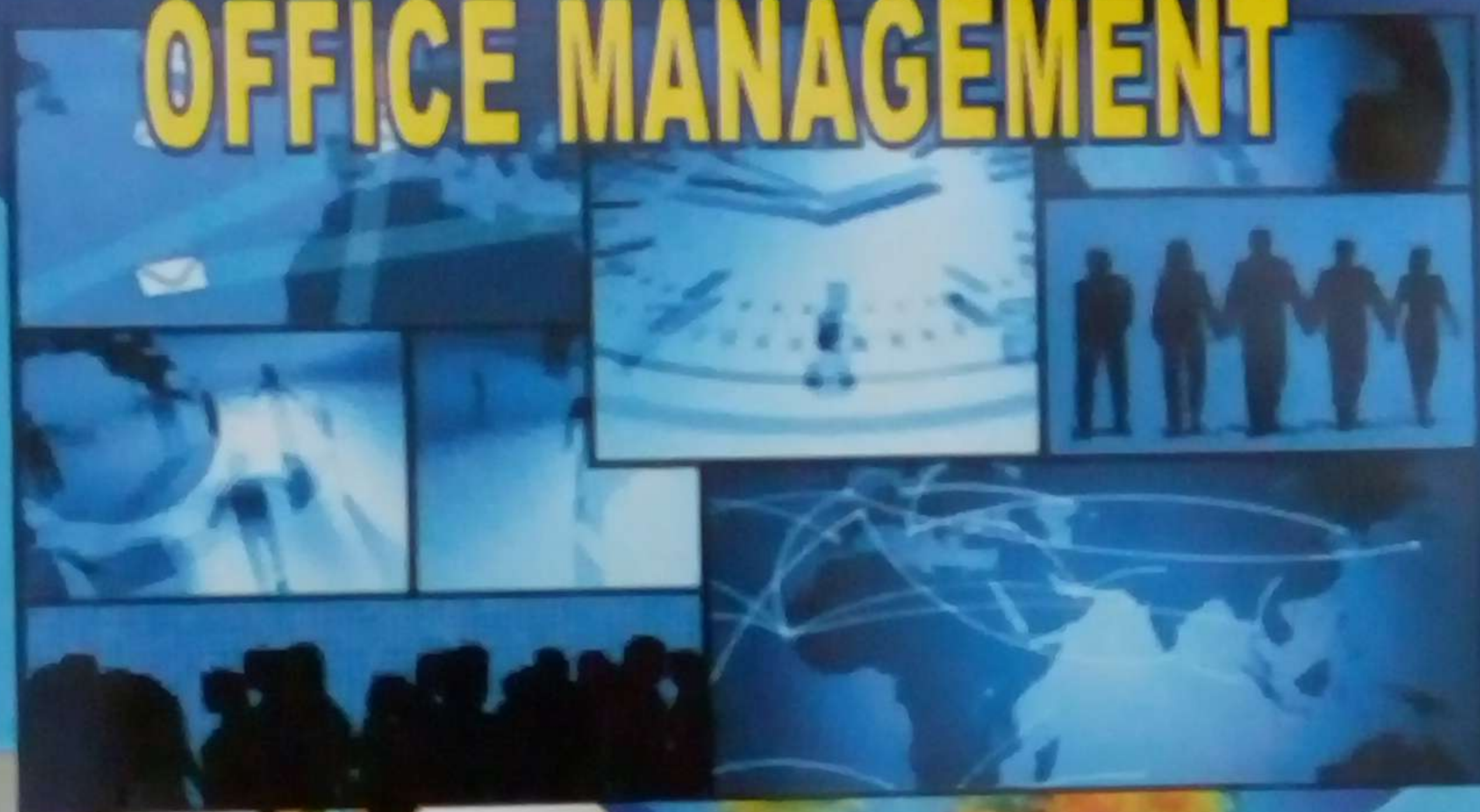
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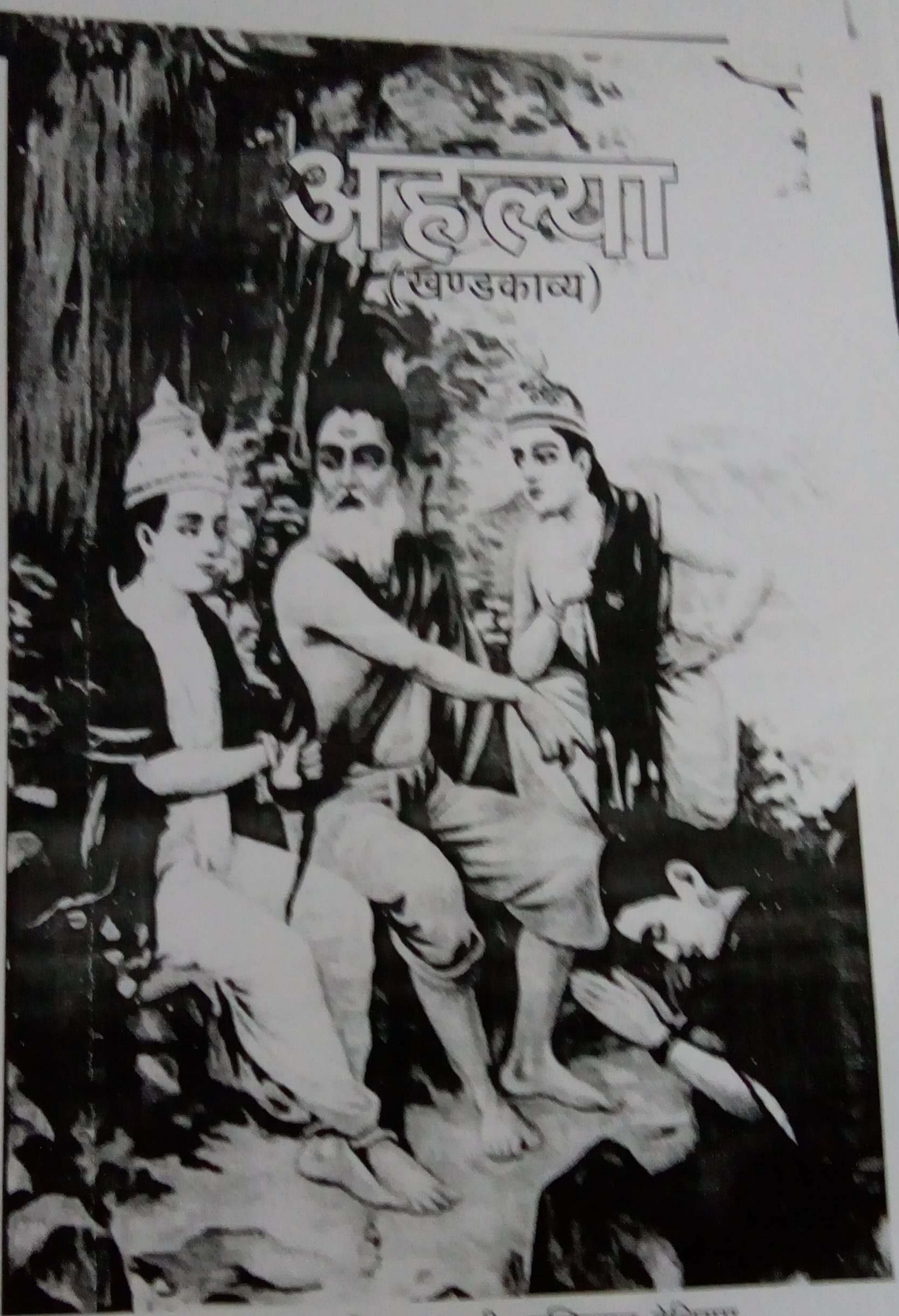
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OP14

SPECTROSCOPIC CHARACTERIZATION OF OXOVANADIUM(IV) COMPLEXES OF N(4)-PHENYLSEMICARBAZONES

V. L. Siji and M. R. Sudarsanakumar*

Department of Chemistry, All Saints' College, Thiruvananthapuram, Kerala, India

*Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala, India

E-mail: sijivl@yahoo.com

Abstract

Four oxovanadium(IV) complexes of benzaldehyde-N(4)-phenylsemicarbazone(HL¹) The complexes were characterized by different physicochemical techniques like partial chemical analyses, conductivity measurements, IR, electronic and EPR spectral techniques. All complexes are EPR active due to the presence of an unpaired electron. In frozen DMF at 77 K, the oxovanadium (IV) complexes, show axial anisotropy with two sets of circular dichroism patterns.

Keywords: Semicarbazones; Oxovanadium(IV) complexes; EPR spectra

Introduction

Semicarbazones are versatile compounds of considerable interest because of their chemical and potentially beneficial biological activities, such as antitumoral, antibacterial, antiviral and antimalarial effects. In the last decades, vanadium compounds have been widely studied because of their potential therapeutic applications. Vanadium is a wide spread trace element

Synthesis of [VOHL¹(SO₄)]

The complexes [VOHL¹(SO₄)] (1) and [VOL¹(OMe)] (2) were synthesized by reacting vanadylsulphate (1 mmol, 0.265 g) for (2) in methanol. The compounds formed were purified by vacuum.

[VOHL¹(SO₄)] (1): Yield 0.265 g, ϵ_{max} 10.39 cm²mol⁻¹, Anal. Calcd. (C, H, N, 10.39; S, 7.95).

[VOL¹(OMe)] (2): Yield 0.265 g, ϵ_{max} 10.39 cm²mol⁻¹, Anal. Calcd. (C, H, N, 10.39; S, 7.95).

Results and discussion

All newly synthesized complexes were soluble in DMF, DMSO etc. The molar conductivity values in the range, 10-16 ohm⁻¹cm²mol⁻¹.

Infrared spectra

The selected infrared spectra of the complexes are given in Table 1. Tentative assignments are given in parentheses.

Table 1 Selected infrared spectra

Compound	ν_{max} (cm ⁻¹)
HL ¹	1610 (C=O), 1510 (C=N), 1450 (C=C), 1380 (C=N), 1320 (C=C), 1280 (C=N), 1240 (C=C), 1180 (C=N), 1140 (C=C), 1080 (C=N), 1040 (C=C), 1000 (C=N), 960 (C=C), 920 (C=N), 880 (C=C), 840 (C=N), 800 (C=C), 760 (C=N), 720 (C=C), 680 (C=N), 640 (C=C), 600 (C=N), 560 (C=C), 520 (C=N), 480 (C=C), 440 (C=N), 400 (C=C), 360 (C=N), 320 (C=C), 280 (C=N), 240 (C=C), 200 (C=N), 160 (C=C), 120 (C=N), 80 (C=C).
[VOHL ¹ (SO ₄)] (1)	1610 (C=O), 1510 (C=N), 1450 (C=C), 1380 (C=N), 1320 (C=C), 1280 (C=N), 1240 (C=C), 1180 (C=N), 1140 (C=C), 1080 (C=N), 1040 (C=C), 1000 (C=N), 960 (C=C), 920 (C=N), 880 (C=C), 840 (C=N), 800 (C=C), 760 (C=N), 720 (C=C), 680 (C=N), 640 (C=C), 600 (C=N), 560 (C=C), 520 (C=N), 480 (C=C), 440 (C=N), 400 (C=C), 360 (C=N), 320 (C=C), 280 (C=N), 240 (C=C), 200 (C=N), 160 (C=C), 120 (C=N), 80 (C=C).
[VOL ¹ (OMe)] (2)	1610 (C=O), 1510 (C=N), 1450 (C=C), 1380 (C=N), 1320 (C=C), 1280 (C=N), 1240 (C=C), 1180 (C=N), 1140 (C=C), 1080 (C=N), 1040 (C=C), 1000 (C=N), 960 (C=C), 920 (C=N), 880 (C=C), 840 (C=N), 800 (C=C), 760 (C=N), 720 (C=C), 680 (C=N), 640 (C=C), 600 (C=N), 560 (C=C), 520 (C=N), 480 (C=C), 440 (C=N), 400 (C=C), 360 (C=N), 320 (C=C), 280 (C=N), 240 (C=C), 200 (C=N), 160 (C=C), 120 (C=N), 80 (C=C).

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OP-06

CRYSTAL STRUCTURE AND CHARACTERIZATION OF GEL GROWN DIAQUABISPICOLINATOZINC(II)DIHYDRATE

Remya M. Nair and M. R. Sudarsanakumar*

Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala
E-mail: sudarsanmr@gmail.com

Abstract

Metal complexes formed with biologically important N,O-donor ligands have received much attention over the past decades. Pyridine-2-carboxylate (also known as picolinic acid) is a very interesting ligand for chemists as well as biochemists as picolinic acid is the body's prime chelator and has important dietary and pharmacological applications. In the present study, we report the crystal structure of diaquabispicolinatozinc(II)dihydrate. The single crystals were obtained by gel diffusion technique. Sodium metasilicate was employed for gel preparation. The compound crystallizes in monoclinic space group $P2_1/n$ and possesses monomeric structure. The grown crystals were further characterized by elemental analysis, FT-IR and powder X-ray diffraction studies and UV-Visible spectroscopy.

Keywords: Gel growth, Single crystal X-ray diffraction, FT-IR, Powder XRD

Introduction

Metal complexes formed with biologically important N,O-donor ligands have received much attention over the past decades. Pyridine-2-carboxylate (also known as picolinic acid) is a very interesting ligand for chemists as well as biochemists as picolinic acid is the body's prime chelator and has important dietary and pharmacological applications^{1,2}. Picolinic acid can coordinate to the metal ions through nitrogen atom of the pyridine ring and oxygen atom of the carboxylate groups to give complexes with interesting topologies. Transition metal complexes of picolinic acid are particularly important as they can be employed for designing new metallopharmaceuticals. In the present study, we report the crystal structure of diaquabispicolinatozinc(II)dihydrate (ZNPI). The grown crystals were further characterized by elemental analysis, FT-IR and powder X-ray diffraction studies.

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OP-06

CRYSTAL STRUCTURE AND CHARACTERIZATION OF GEL GROWN DIAQUABISPICOLINATOZINC(II)DIHYDRATE

Reinya M. Nair and M. R. Sudarsanakumar*

Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala

E-mail: sudarsanmr@gmail.com

Abstract

Metal complexes formed with biologically important N,O-donor ligands have received much attention over the past decades. Pyridine-2-carboxylate (also known as picolinic acid) is a very interesting ligand for chemists as well as biochemists as picolinic acid is the body's prime chelator and has important dietary and pharmacological applications. In the present study, we report the crystal structure of diaquabispicolinatozinc(II) dihydrate. The single crystals were obtained by gel diffusion technique. Sodium metasilicate was employed for gel preparation. The compound crystallizes in monoclinic space group $P2_1/n$ and possesses monomeric structure. The grown crystals were further characterized by elemental analysis, FT-IR and powder X-ray diffraction studies and UV-Visible spectroscopy.

Keywords: Gel growth, Single crystal X-ray diffraction, FT-IR, Powder XRD

Introduction

Metal complexes formed with biologically important N,O-donor ligands have received much attention over the past decades. Pyridine-2-carboxylate (also known as picolinic acid) is a very interesting ligand for chemists as well as biochemists as picolinic acid is the body's prime chelator and has important dietary and pharmacological applications^{1,2}. Picolinic acid can coordinate to the metal ions through nitrogen atom of the pyridine ring and oxygen atom of the carboxylate groups to give complexes with interesting topologies. Transition metal complexes of picolinic acid are particularly important as they can be employed for designing new metallopharmaceuticals. In the present study, we report the crystal structure of diaquabispicolinatozinc(II) dihydrate (ZNPI). The grown crystals were further characterized by elemental analysis, FT-IR and powder X-ray diffraction studies.

mass corresponds to the dissociation of both ligand and acetate molecule with the oxidation of the metal to give the stable oxide ZnO. The residue obtained from TG data (18.95 %) is in agreement with the theoretical value (18.48 %).

Conclusions

The analytical and spectroscopic data suggest that all the metal complexes have the general formula (ZnLX) where L = ISH and X = Cl, ClO₄, CH₃COO. The ligand acts as tridentate chelating ligand coordinating through nitrogen and oxygen atoms. A tetrahedral geometry has been tentatively proposed for all the complexes.

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PP07

SPECTRAL, THERMAL AND CRYSTAL STRUCTURE OF BIS(GLYCOLATO) COPPER(II) SINGLE CRYSTALS

Drisya.R and M.R. Sudarsanakumar*

Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala

E-mail: sudarsanimr@gmail.com

Abstract

Single crystals of bis(glycolato)copper(II) have been successfully grown by gel diffusion technique. Sodium meta silicate was used to prepare the gel. It crystallizes in monoclinic system with space group P2₁/n. The cell parameters are a = 5.084(2) Å, b = 8.649(5) Å, c = 7.728(4) Å, α = 90.000°, β = 106.737(13)° and γ = 90.000°. The grown crystals were further characterized by using CHN analysis, FT-IR, UV-Vis spectroscopy, thermogravimetric and single crystal XRD.

Keywords: Gel diffusion technique, sodium meta silicate, single crystal XRD

Introduction

Alpha hydroxy carboxylic acid plays an important role in many biological processes. The simplest alpha hydroxy carboxylic acid is the glycolic acid. Glycolic acid and its derivatives are widely used in pharmaceutical, cosmetic, biological; food and general industrial chemical fields. Glycolic acid is also used to synthesize biomaterials, for instance, poly (D, L-lactic – co-glycolic acid), a polymer which is extensively utilized for drug delivery. The polymer has resorbable and biocompatible characteristics and hence can be used in biodegradable sutures and prostheses. More over glycolic acid is having strong antioxidant property.

Acknowledgements

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PP04

SYNTHESIS, CRYSTAL GROWTH, SPECTRAL CHARACTERIZATION AND BIOLOGICAL STUDIES OF VANILLIN-N(4)-PHENYLSEMICARBAZONE

Layana.S.R and M.R Sudarsanakumar*

Department of Chemistry, Mahatma Gandhi College, Thiruvananthapuram, Kerala,

Email: sudarsanmr@gmail.com

Abstract:

Vanillin-N(4)-phenylsemicarbazone (NVAN), a novel semicarbazone was synthesized by refluxing equimolar amounts of vanillin and N(4)-phenylsemicarbazide in presence of dilute acetic acid. By using slow evaporation technique, single crystals of NVAN were grown from methanol at room temperature. The grown crystals were characterized by single crystal X-ray diffraction (SCRD), FT-IR, FT-Raman, UV-Visible, ^1H NMR and ^{13}C NMR spectral studies. The title compound was screened for anti-bacterial and anti-fungal studies.

Keywords :

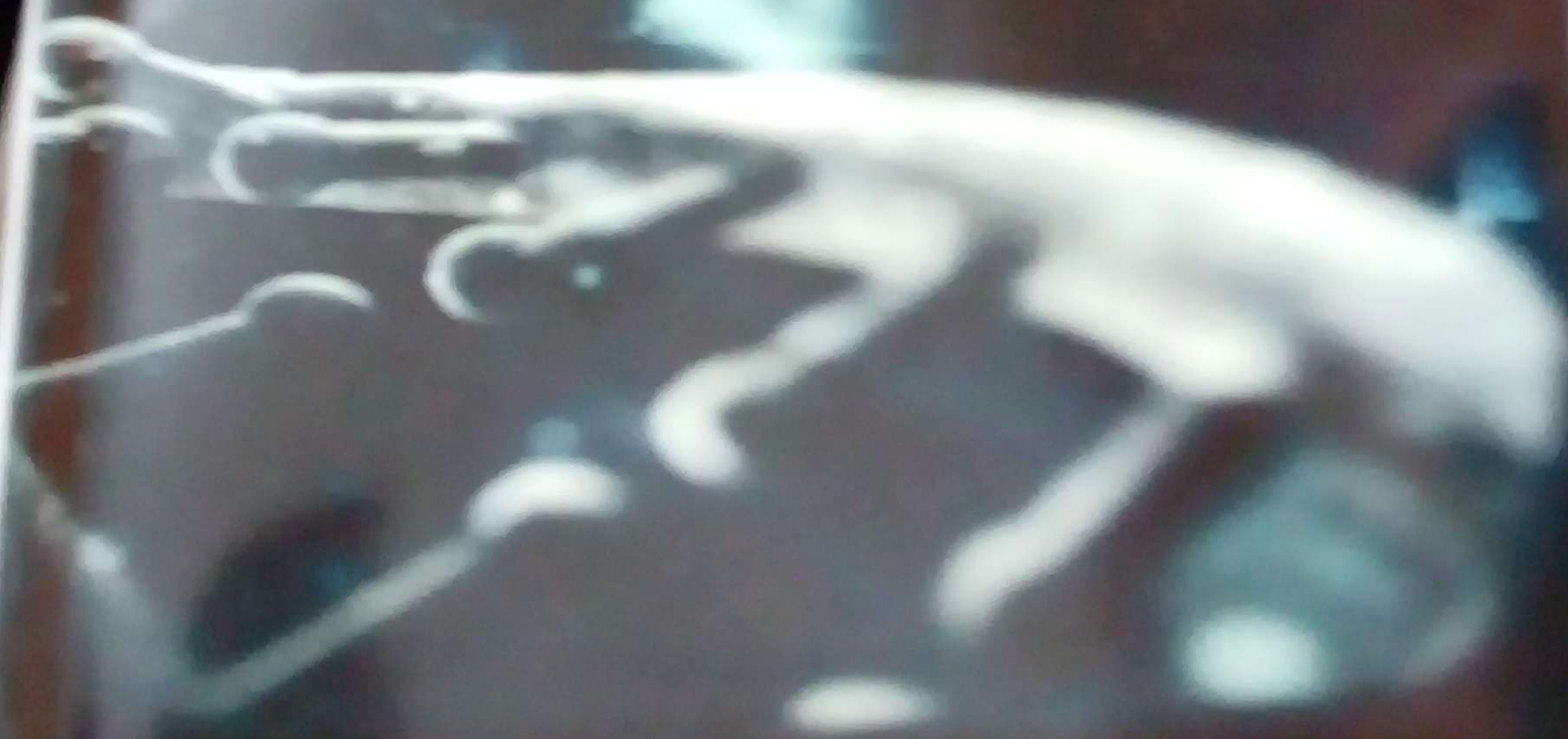
Vanillin-N(4)-phenylsemicarbazone, slow evaporation, single crystal X-ray diffraction, Anti microbial studies.

Introduction

Semicarbazones are synthesized by the condensation of an aldehyde/ a ketone with a semicarbazide. They possess the general formula $\text{R}_1\text{R}_2\text{C}=\text{N}-\text{NH}(\text{CO})-\text{NH}_2$. In recent years there has been considerable interest in semicarbazones due to their wide spectrum of biological applications and structural features. The chemistry of coordination of metals with semicarbazones has been of interest because of the different bonding modes shown by them. The presence of more electronegative nitrogen, oxygen or sulphur atoms on the ligand structure will enhance the coordinating possibilities of ligand. Semicarbazones can coordinate to the metal either as a neutral ligand or as a deprotonated anion and hence they form compounds with versatile structural features. Here we report the crystal structure of a novel semicarbazone, vanillin-N(4)-phenylsemicarbazone(NVAN). It is further characterized by elemental analysis,



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High temperature thermoluminescence emissions of SrSO₄ nano phosphors doped with Eu and Mn

Jayasudha S^{1*}, K. Madhukumar¹, C.M.K.Nair¹,
Resmi G. Nair¹, V.M. Anandakumar¹

¹Department of Physics,
Mahatma Gandhi College
Thiruvananthapuram-695004, India
* jsnair.india@gmail.com

T.S. Elias²

²Regional Cancer Centre
Thiruvananthapuram-695011, India

Abstract— High temperature Thermoluminescence (TL) emissions of SrSO₄:Eu,Mn phosphor at 346°C is reported here for the first time. The nanocrystalline phosphors were prepared by wet chemical precipitation method. The glow curve shows an intense peak at 346°C, when the phosphor is subjected to X-irradiation. Co-doping with Mn enhances the trap depth and hence the TL emission temperature. Even though the luminescence intensity is found to be less, the phosphor becomes significant owing to its high temperature afterglow, which is one of the stringent requirements of a commercial thermoluminescent dosimeter (TLD). This phosphor appears to be fairly stable for TL measurements. Preliminary crystallographic and morphological studies of the phosphors were done using Powder X-ray Diffractogram and Scanning Electron Microscopy (SEM). The phosphor has a single phase orthorhombic structure and the crystallites are sized in nano range. The dopant compositions in the host matrix observed from the Energy Dispersive Spectra (EDS) were 0.18 atom% Eu and 0.13 atom% Mn. The single and well defined high temperature glow curve makes the phosphor suitable for high temperature radiation dosimetry applications.

Keywords— Thermoluminescence, Radiation dosimetry.

I. INTRODUCTION

Thermoluminescent (TL) phosphors were proved to be highly sensitive radiation detectors and are widely used for radiation dosimetry applications. Thermal ejection of relatively stable electrons trapped by means of ionizing radiation with X-ray, gamma ray, alpha, e-beam or other fast particles leads to TL. Studies are on in the search of suitable host-dopant combinations due to the constant need for high sensitivity TL dosimetry phosphors for different applications [1]. Recently, nanostructured materials are on focus, because of their potential impact in many areas such as electronics, photonics, catalysis and sensing [2-4]. Among the various phosphors alkaline earth sulphates are of special interest due to their high TL sensitivity, stability and low cost [1]. TL properties of rare earth doped CaSO₄, BaSO₄, SrSO₄ and MgSO₄ with single as well as multiple dopants were studied recently. TL studies of Mn doped SrSO₄ compounds prepared via recrystallization method and irradiated by X-rays were done by J. Manam *et al.* [1]. Similarly, the TL performance of Eu doped SrSO₄ phosphors prepared through acid evaporation technique and irradiated with γ -rays were studied and reported by Q.Tang *et al.* [5]. Characteristics of the same host material prepared through a controlled chemical precipitation method by M. Kerikmäe *et al.* is also reported previously [6]. In many host lattices Mn is proved to be a best activator, when doped singly

or codoped with rare earths [1,11,13]. Here the focus is on TL properties of the SrSO₄:Eu nano phosphor co-activated with Mn. A much higher temperature TL emission is observed when the phosphor is subjected to X-rays. An attempt is made to estimate the activation energy corresponding to the trap from the geometry of the glow curve.

II. EXPERIMENTAL

SrSO₄:Eu,Mn nano phosphors were prepared by following the chemical precipitation technique described by Madhukumar *et al.* [7]. Analytical grade starting materials were used for the phosphor sample preparation. 0.5 mol% each of 99.995% pure Eu₂O₃ and MnO₂ were used for doping. After necessary washing, filtering and drying the precipitate was calcined at 400°C for 1 hour to eliminate the traces of any other compounds or acids. Further, the calcined material was ground well and then annealed at 1050°C in a programmable high temperature furnace for 3 hours in air atmosphere, for the required crystalline phase formation.

Subsequently, various characterization studies were carried out. The crystalline properties were studied from the X-ray diffractogram taken from XPERT PRO Diffractometer using Cu K α radiations of $\lambda = 1.5406 \text{ \AA}$. SEM micrographs and EDS spectra obtained using JEOL 6390LV make Scanning Electron Microscope with EDS attachment were analysed. Thereafter, the thermoluminescence glow curve at a heating rate of 5°C/s were recorded with a TL analyzer TL100 NUCLEONIX. About 5 mg of the phosphor powder sample was used all the time for recording the TL readout, since the amount of phosphor sample influence the TL intensity. Pre-irradiations were made with Cu K α X-rays generated at 20kV, 10mA from RADON make X-Ray unit before recording the TL.

III. RESULTS AND DISCUSSIONS

A. Structure Analysis

Fig.1 shows the typical X-ray diffraction pattern of the prepared SrSO₄:Eu,Mn nano phosphor. The spectrum shows orthorhombic lattice structure with Pnma 62 space group in accordance with the JCPDS database of file number 00-00-0885. Observed and calculated d -values are in good agreement. The lattice parameters were found to be $a = 8.32 \text{ \AA}$, $b = 5.32 \text{ \AA}$ and $c = 6.80 \text{ \AA}$, which are fairly in agreement with the parameters reported for the undoped host lattice, $a = 8.36 \text{ \AA}$, $b = 5.36 \text{ \AA}$, $c = 6.84 \text{ \AA}$. The slight deviation in the parameters may

Effect of lanthanum doping on barium alumino borosilicate glass

M.S. Salinigopal¹, N. Gopakumar² and P. S. Anjana^{1*}

¹Department of Physics, All Saints' College, Trivandrum, Kerala, India.

²Post Graduate Department of Physics, Mahatma Gandhi College, Trivandrum, Kerala, India.

Abstract - Rare earth doped $50\text{BaO}-(5-x)\text{Al}_2\text{O}_3-x\text{RO}-30\text{B}_2\text{O}_3-15\text{SiO}_2$ ($x = 0, 1, 3, 5$) glasses [$R = \text{La}$] has been prepared by conventional rapid melt quenching technique. The density of the as prepared glasses was measured using Archimedes method. Using the density values, molar volume and excess volume of each glass system was calculated. The amorphous nature of the glasses was confirmed using X-ray diffraction (XRD). Structural properties of these glass samples were studied using Fourier Transform Infrared (FTIR) Spectroscopy. FTIR spectra revealed the existence of various structural groups in the glasses and determined and differentiated the various vibrational modes in the structural changes.

Keywords: Glass, XRD, Density, FTIR

1. INTRODUCTION

Multi-component glasses have wide range of applications in the fields of optics, nuclear, electronics and constructions. Due to their manifold applications these glassy systems have drawn a lot of attention of researchers to investigate their structure [1]. The information to deep insight into the structure- properties relationship that can be exploited for the design of new materials like borosilicate based glasses [2]. Barium alumino borosilicate glasses are of great interest because of their good physical properties. Hence we have made a systematic investigation of La_2O_3 on the structure and physical properties of barium alumino borosilicate glass.

Density is one of the most important properties of the glass, which can be used for finding out the structure of different types of glass and also for the quality control in the glass industry. The density strongly depends on the composition and structure of the samples [3]. The technological relevance of glasses has been led to increased efforts to resolve their structures. The structural

earth into borosilicate glasses consolidates their structure and increases its density [4].

In the present work, the effect of La_2O_3 on $50\text{BaO}-(5-x)\text{Al}_2\text{O}_3-30\text{B}_2\text{O}_3-15\text{SiO}_2$ glass samples is studied.

2. EXPERIMENT

Glass samples of different compositions in $50\text{BaO}-(5-x)\text{Al}_2\text{O}_3-30\text{B}_2\text{O}_3-15\text{SiO}_2-x\text{La}_2\text{O}_3$ system with $x = 0, 1, 3, 5$ were prepared using the powders of BaCO_3 (Sigma Aldrich, 99.9%), Al_2O_3 (99%), B_2O_3 (99.9%), SiO_2 (99.9%) and La_2O_3 (Sigma Aldrich, 99.9%) with sample code BABS-G, BLBS-1G, BLBS-3G, BLBS-5G ($x=0, 1, 3, 5$) by normal melt quench method. Appropriate amounts of chemicals were weighed, thoroughly mixed and were dried using an oven. The dry powders were melted in the temperature range $1200-1260^\circ\text{C}$ for 2 hrs until a bubbled-free liquid was formed. The melt was then poured into a mold and then annealed it at an annealing temperature of 350°C for 2 hrs to avoid breaking the glass sample through residual internal strain.

The non-crystalline (amorphous) nature of the glass samples were analysed using XRD (Bruker AXS D8 Advance). Infrared absorption spectra of powdered glass samples were recorded in the range of $400-4000\text{ cm}^{-1}$ using FTIR spectrometer. Archimedes' method was employed to determine density of the annealed

*Corresponding author mail:
psanjanaa@yahoo.com

Spectral and thermal studies of gel grown Benzophenone crystal

Divya R, Lekshmi.P.Nair,
B.R.Bijini, K.Rajendra Babu
Department of Physics
MG College
Thiruvananthapuram, India

K.Rajendra Babu
Department of Science
Heera College of Engineering & Technology
Thiruvananthapuram, India

Abstract—Benzophenone has significant relevance in non linear optical applications. Benzophenone crystals had already been grown by several methods. In this work, single crystals of benzophenone were successfully grown by gel method. The grown crystal was subjected to FTIR spectral analysis to confirm the presence of functional groups. The optical band gap of the crystal was determined from the UV Visible NIR absorbance spectrum and found to be 3.18 eV. The nature of the spectrum shows its potential as an NLO material. Thermal properties and thermal stability were studied by conducting Thermo-gravimetric and Differential Thermal Analysis. Here the melting point was observed as 49.5 degree Celsius which is well matching with the theoretical value. It is also thermally stable for 5 percentage up to 150 degree Celsius.

Keywords—Benzophenone, gel growth, FTIR, UV-Vis-NIR spectral analysis, Thermal analysis

I. INTRODUCTION

Crystals play an inevitable role in modern technology. So crystal growth is a prominent area in the scientific and technological research. Since the crystal growth has immense applications, it is an interdisciplinary subject covering physics, chemistry, materials science, chemical engineering, metallurgy, crystallography, mineralogy etc. There is growing interest on crystal growth to meet the demand of materials for technological applications [1]. The growth of NLO materials has become trend in recent years. They are having technological importance in the field of optoelectronics, lasers, data storage systems and optical communication [2]. These materials should possess large second order optical non linearities, short transparency, cut off wavelength and thermal stability [3]. NLO response is larger in organic materials when compared to inorganic materials due to the presence of active π bonds [4]. So we focus our studies on organic materials. Benzophenone is one of the most important organic materials showing NLO property [5]. It is an important compound in organic photochemistry and perfumery as well as in organic synthesis. It is also used a photo-initiator of UV curing applications in inks, adhesive and coatings, optical fiber as well as in printed circuit boards[5]. Rapid crystal growth of benzophenone by low temperature solution growth,

Unidirectional seeded single crystal growth from solution benzophenone [5, 6] has already been reported.

Here we have grown benzophenone crystals by gel method to improve the quality of the crystals. The gel method is simple in technique, effective in growing single crystals of compounds that cannot be easily grown by other methods [7]. In this paper, we are presenting the spectral and thermal studies of gel grown benzophenone crystals.

II. EXPERIMENTAL - GROWTH OF SINGLE CRYSTALS

Single crystals of benzophenone were formed by diffusion technique. The technique involves the setting and addition of required top solution over the set gel crystallization apparatus for the growth consists borosilicate glass test tube of length 20 cm and diameter 1 cm placed vertically on a stand. The solution for gel has specific gravity 1.03-1.05 g/cc was prepared by dissolving sodium meta silicate (SMS) in double distilled water. The solution was then acidified with 1M glacial acetic acid to the pH in the range 4 - 7 (in steps of 0.5) and taken about 1 ml of each in different test tubes. They were kept undisturbed for gel setting. Over the set gel, the top solution prepared by dissolving AR grade benzophenone in ethanol was added drop wise through the side of the test tube to prevent breakage. The test tubes were covered with transparent plastic sheets to avoid evaporation and contamination of solution. The crystals were found growing over the surface within 1 day and the growth lasted for about 50 days. It is also found that pH = 6 and gel density 1.04 g/cc was optimum condition for the growth of best quality benzophenone crystals.

III. RESULTS AND DISCUSSIONS

A. Fourier Transform Infrared Spectroscopic Studies (FTIR)

The FTIR spectrum of gel grown benzophenone crystal is shown in the Fig. 1. In the higher wavelength region, a broad peak at 3054.80 cm^{-1} is associated with aromatic C-H stretching. The peak at 1650 cm^{-1} represents C=O stretching. The skeletal vibrations are represented by the peaks at 1510 cm^{-1} and 1443.87 cm^{-1} .

Structural and Optical properties of Co doped tin oxide nanoparticles

DHANYA CHANDRAN¹, LAKSHMI S. NAIR¹, BALACHANDRAN. S², RAJENDRA BABU. K¹ and DEEPA. M³

1. Department of Physics, Mahatma Gandhi College, Kerala University, Thiruvananthapuram, India
2. Department of Chemistry, Mahatma Gandhi College, Kerala University, Thiruvananthapuram, India
3. Department of Physics, All Saints' College, Kerala University, Thiruvananthapuram, India

Abstract

SnO₂ is an important wide-band-gap semiconductor and has widespread applications due to its tailor made properties. Pure and Co doped tin oxide (SnO₂) nanoparticles were synthesized by sol-gel method and characterized by X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), energy dispersive X-ray spectroscopy (EDAX) and UV-visible spectroscopy. The XRD analysis showed well crystallized tetragonal SnO₂ phase. The sizes are found to vary with doping. The diffuse reflectance spectroscopy measurements confirm red shift in the absorption edge of doped samples with respect to the bulk. The concentration of the dopants is determined from EDAX.

Keywords: Band gap narrowing; sol-gel process; Co-doped tin oxide;

1. INTRODUCTION

Tin oxide (SnO₂) is one of the most widely used n-type metal oxide semiconductor with a band gap of 3.6 eV ($E_g = 3.62$ eV, at room temperature). It has a regular octahedron coordination in which one tin (Sn) atom is surrounded by six oxygen (O) atoms. They have a wide range of applications in flat panel displays, transparent conducting electrodes, solar cells, gas sensors and rechargeable lithium ion batteries etc [1-3], due to its unique electrical, optical and electrochemical properties.

A variety of strategies have been employed for the synthesis of SnO₂ nanoparticles, such as sol-gel, chemical precipitation, microwave technique, gel combustion route, solvothermal, hydrothermal, sonochemical, mechanochemical, and solid state method [4-7]. Among them, sol-gel process offers several advantages over other methods, such as better homogeneity, controlled stoichiometry, high purity, phase-pure powders at a lower temperature and flexibility of forming dense monoliths, thin films or nanoparticles [3-4]. In the present paper pure and Cobalt doped SnO₂ nanoparticles have been

prepared through sol-gel method and the effect of doping in the structural and optical properties are discussed.

2. MATERIALS USED

The chemicals used in this study were tin(IV) chloride pentahydrate (SnCl₄·5H₂O, Sigma), ammonium hydroxide (NH₄OH 25%, Merck), Cobalt nitrate hexahydrate (Co(NO₃)₂·6H₂O, Merck) and ultra pure water. All reagents were used as received without any further purification.

3. EXPERIMENTAL

The pure and Co doped SnO₂ nanopowders were prepared by sol-gel method. Generally, tin(IV) chloride was added to 50 mL ultra pure water in a round bottom flask and was stirred for 20 min. A certain amount of ammonia solution (25%) was added into the mixture under a controlled feed rate with constant stirring. After 2 h of stirring, the sol was aged at room temperature for 24 hr. The resulting gel was then washed with ethanol until the pH of the solution became 7. After drying at 80°C for 24 hr in air, the obtained powder was ground using mortar and pestle. Co doped SnO₂ were prepared in a similar manner, by adding calculated amount of

GROWTH AND CHARACTERISATION OF GEL GROWN LEAD MALEATE

Lekshmi P. Nair¹, B.R. Bijini¹, R. Divya¹, S. Prasanna⁴, C.M.K. Nair¹, M. Deepa³, K. Rajendra Babu^{1*}
¹M.G. College, Thiruvananthapuram, India-695004
²Heera College of Engineering & Technology, Thiruvananthapuram, India-695568
³Department of Physics, All Saints' College, Thiruvananthapuram, India-695067
⁴Department of Physics, H.H.P.B.N.S.S. College, Thiruvananthapuram, India-695004
*Corresponding author Tel. No: +91 9447963076
E-mail address: mgkrl1956@yahoo.co.in (K. Rajendra Babu)

Abstract: Lead maleate (PbM) crystals are grown by gel diffusion method for the first time. Conditions for growing quality crystals are optimized. Single crystal X-Ray Diffraction analysis was done to determine the structure and the crystal belongs to monoclinic system, P21/C space group. Fourier Transform Infrared spectroscopic method was utilised for the analysis of various functional groups present in the complex. Thermal properties of the crystal were studied by TGA/DTA. Elemental analysis gives the formula of the compound as $PbC_2H_2(CO_2)_2$ and confirmed the stoichiometry of the complex. The UV-Visible spectral analysis was used to study the optical transparency of the crystal.

Key words: Crystal growth, SXRD, Lead maleate, FTIR, TGA/DTA.

1. INTRODUCTION:

Metal Organic Frameworks (M.O.F.) of dicarboxylic acids have potential application in fields like catalysis, drug design, gas storage, nonlinear optics and chemical sensing because of their structural diversity and interesting properties. Maleic acid (cis-butenedioic acid) is a dicarboxylic acid which is a multifunctional chemical intermediate that finds applications in nearly every field of industrial chemistry [1]. Maleic acid is extensively used in pharmaceutical industry for making maleate salts of drugs. Lead is one of the most used metals in industry, mainly in the production of electrical batteries for vehicles. Lead maleate is an active heat stabiliser for halogenated polymers [2]. It is used in wire insulation and jacketing.

M.O.Fs are produced mainly by hydrothermal or solvothermal techniques, where the crystals are slowly grown from hot solutions. A report on the growth of lead maleate from hot solution is available [2]. Our attempt was to grow PbM at ambient temperature by the gel method and to reinvestigate the crystal structure. Here we report the growth and characterisation of lead maleate crystals by gel method for the first time. Gel method is an inexpensive, effective and unique method for growing defect free crystals showing poor solubility in water by providing the advantages of controlled nucleation and convection less growth at ambient temperature [3]. The grown crystals are then subjected to Single Crystal XRD analysis for structure

determination and further characterised by elemental, thermal, FTIR and UV-Visible spectral analysis.

EXPERIMENTAL PROCEDURE:

2.1. GROWTH PROCEDURE:

The crystals of the lead complex of maleic acid were grown using gel diffusion technique. Good quality single crystals were obtained by controlled nucleation and convection less growth offered by gel technique. Single glass tubes of length 20 cm and diameter 2.5 cm are used for the growth procedure. Silica gel of specific gravity 1.05 to 1.06 g/cc was prepared by dissolving sodium meta silicate (SMS) in double distilled water. Maleic acid of particular molarity (0.5 M – 1.5 M) was added drop by drop to the continuously stirred SMS. The gel was then acidified with 1M glacial acetic acid to get pH in the range 3 to 7. About 30 ml of above solution was taken in each test tube and kept undisturbed for setting. Aqueous solution of lead nitrate (0.5 M – 1.5 M) was added as top reagent over the set gel without damaging the gel system. The open end of the test tubes was covered with transparent plastic sheets to avoid contamination of the solution. The experimental set up was kept undisturbed for crystallisation at ambient temperature.

2.2. CHARACTERIZATION:

The Single Crystal XRD analysis of the crystal was carried out using Bruker AXS Kappa Apex2 CCD diffractometer. FT-IR spectrum was recorded using KBr pellets on a Thermo Nicolet, Avatar 370 spectrometer with resolution of 0.9cm⁻¹, in the range 4000-400cm⁻¹. Absorption spectrum of the crystal was studied using Varian Cary 5000 UV-Vis-NIR spectrometer in the range 200-1200nm. TGA/DTA experiments were carried out in Perkin Elmer Diamond TG/DTG analyser instrument with a heating rate of 10°C/min in nitrogen atmosphere. The carbon, hydrogen, nitrogen and sulphur contents in the sample were determined using Elementor Vario-EL II CHNS Analyser.

3. RESULTS AND DISCUSSION:

3.1. CRYSTAL GROWTH:

Effect of Annealing Temperature on Thermoluminescence of Rare Earth Doped CaSO_4

Resmi Nairl*, Dr. K. Madhukumarl and
Jayasudha.Sl
Dept. of Physics
Mahatma Gandhi College
Thiruvananthapuram-695004, India
resminairl@gmail.com

T. S. Elias2
2Regional Cancer Centre
Thiruvananthapuram, India

Abstract - The thermoluminescence (TL) properties were found to be highly dependent on the method of preparation of the material. Variation of TL intensity of rare earth doped CaSO_4 phosphors with annealing temperature and dose of irradiation are discussed in this paper. The phosphors prepared through solid state synthesis were exposed to γ radiation from a $\text{Co } 60$ source with dose varying from 1 to 10 Gy. Samples annealed at 700°C gave the highest TL response for all doses of gamma irradiation. TL intensity is found to be decreased as preparation temperature is raised. Very less intense shoulder peaks were observed for phosphors of lower annealing temperatures while such shoulders were completely absent at higher temperature range. The peak intensity is less compared with that of the commercially available standard TL dosimeter (TLD). The observed favourable characteristics of the phosphors were ease of preparation, very high thermal stability, less fading and very high peak emission temperature which are the main requisites of a good TL dosimeter. The main TL emission temperature is 366°C which is very high compared to the standard TLD.

Keywords: Thermoluminescence, Dosimeter

I. INTRODUCTION

Thermoluminescence has applications in Archaeology, Geology, Biology, Forensic Science, Space Science etc and its most striking application is in Radiation Dosimetry [1]. The development of thermoluminescent dosimeters using CaSO_4 has a very long history due to its high sensitivity, simple structure, and good chemical and thermal stability. A large number of variants have been proposed from time to time. Rare earth doped CaSO_4 are excellent

thermoluminescent phosphors and CaSO_4 : Dy and CaSO_4 : Tm are important among them due to high sensitivity and very low fading when stored under standard environmental conditions. They are very useful in monitoring radiation levels from various sources [2, 3, 4]. Co doping in very small quantities while preparing the sample plays an important role in the luminescence efficiency of the phosphor. It may enhance or subside, the Thermoluminescence efficiency depending on the host dopant lattice matching. Attempts to improve the thermoluminescence characteristics of CaSO_4 : Dy and CaSO_4 : Tm, are sustained till date. During our investigations we came across a new phosphor with very high TL emission temperature. In this work we present the results of our research to improve the thermoluminescence efficiency of CaSO_4 : Tm by adding a very small quantity of co-dopant [3, 4].

II EXPERIMENTAL

The method used for preparation was Solid State Synthesis. All reactants were of analytic grade, Merck. Reactants were taken according to the stoichiometric ratio and were mixed properly in an agate for two hours using Acetone as the wetting medium. The mixture was then transferred to an Alumina crucible and heated at 500°C for three hours. After slow cooling the powder was again mixed properly and kept in the furnace for final heating. The final heating was done at different temperatures for three hours to fix the optimum temperature that give a good TL efficiency. After the final heating, finely powdered phosphor was used for various analysis.

Phase formation was confirmed by taking powder XRD. Thermoluminescence was measured using Nucleonix make TL Reader. For TL measurement, samples annealed at different temperatures were subjected to $\text{Co } 60$ Gamma radiation from 1 to 10 Gy.

BAND GAP ENGINEERING IN NI DOPED ZnO THIN FILMS FOR USE IN OPTOELECTRONIC DEVICES

Santhosh.V.S

Department of Physics, M.G.College
Thiruvananthapuram, Kerala, India
santhoshvs10@gmail.com

K.RajendraBabu

Department of Physics, M.G.College
Heera College of Engineering and Technology
Thiruvananthapuram, Kerala, India

Deepa.M

Department of Physics, All Saints' College
Thiruvananthapuram, Kerala, India

Pure and Ni doped ZnO thin films were deposited onto glass substrates by sol-gel spin coating method. $\text{Ni}^{2+} / \text{Zn}^{2+}$ content in the starting solution was varied from 0 to 0.5 at%. Structural, compositional, morphological, optical, luminescence and electrical properties of the films were analyzed using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), UV-vis spectroscopy, photoluminescence (PL) spectroscopy and four probe measurements respectively. All the films were preferentially oriented along the (002) plane and had a hexagonal wurtzite structure. Average crystallite size was found to increase with increase in Ni content. At higher Ni doping concentration of 0.4 and 0.5 at% the films were in a state of tensile stress. Significant changes in surface morphology were observed in the SEM images with increase in Ni content. Optical band gap was found to increase from 3.21 to 3.44 eV when Ni content in the films was varied from 0 to 0.5 at%. Porosity was found to decrease with increase in Ni content. Sharp UV emission was observed in the pure ZnO film. A blue shift in UV emission peak was observed upon Ni doping. Decrease in resistivity was observed with increase in Ni content which is correlated with increase in average crystallite size of the films.

Keywords: ZnO thin films, sol-gel spin coating, stress, optical properties, porosity photoluminescence

I. INTRODUCTION

Zinc oxide (ZnO) is a II – VI direct wide band gap semiconductor with a free exciton binding energy of 60 meV [1]. It has a variety of applications in gas sensors, piezoelectric devices, solar cells, transparent electrodes, varistors, photodetectors, spintronic devices, surface acoustic wave devices etc. ZnO thin films exhibit high conductivity and optical transparency in the visible range, which makes it

oxidation states and have different acceptor properties in a ZnO matrix, thus affecting the electronic surface band structure of ZnO.

Ni is an important dopant that can increase the magnetic properties of ZnO thin films. Ni^{2+} has the same valency as that of Zn^{2+} . Also, its ionic radius (0.069 nm) is close to that of Zn^{2+} (0.074 nm). Hence Ni^{2+} can replace Zn^{2+} in ZnO lattice. There are various reports in literature as to how structural and optical properties of ZnO thin films vary when doped with Ni [6-9]. However, these studies do not show a consistent variation in the optical and photoluminescence properties of ZnO thin films when doped with Ni. Optical band gap was found to increase with increasing Ni content as reported by some authors [6,7]. But Pandey et al. has reported that optical band gap decreases when doped with Ni [8]. Only UV emission is observed in Ni doped ZnO thin films as reported by some authors [7,9]. But, Farag et al. has reported that UV emission is absent and that a very weak visible emission is observed in Ni doped ZnO thin films [6]. This variation in reports has motivated the authors to conduct the present work. The effect of Ni doping on the structural, optical, photoluminescence and electrical properties of ZnO thin films deposited by sol-gel technique is investigated in the present study.

Undoped and doped ZnO thin films can be prepared by various deposition techniques such as RF magnetron sputtering [10], Molecular beam epitaxy (MBE) [11], metal organic chemical vapor deposition (MOCVD) [12], pulsed laser deposition (PLD) [13] and the sol-gel process [14-16]. The present study analyses the structural, compositional, optical, and electrical characteristics of pure and Ni doped ZnO thin films by sol-gel method as this is an easy technique that can produce good quality films with high homogeneity. The method also offers better control of film composition.

II. EXPERIMENTAL

films were deposited onto glass
0.5 M ethanolic

Mechanoluminescence properties of Europium(Eu) doped Barium Strontium Aluminate phosphors

S. J. Sajan¹, N. Gopakumar¹, P. S. Anjana²

¹Post Graduate Department of Physics, Mahatma Gandhi College, Thiruvananthapuram, Kerala, India
²Department of Physics, All Saints College, Thiruvananthapuram, Kerala, India

Abstract

The sample of required composition was prepared via high temperature solid state reaction method. The phase formation of the powder sample was confirmed by taking X ray Diffraction. The Mechano luminescence (ML) property of the sample by impact method was studied by using ML measuring apparatus. The variations in the ML peak intensity due to the variations in different parameters were also investigated.

I. INTRODUCTION

Mechanoluminescence is an interesting phenomenon, which is caused by mechanical stimuli such as grinding, cutting, collision, striking and friction. It is a defect related phenomenon, associated with trap involved process in which electrons (holes) dwell in the trap for some time and then recombine with the luminescence centre either by travelling in the conduction band or by electron(hole) tunneling.^[1] It is interesting to note that all solids do not exhibit ML. That means origin of ML in certain solids is related with the nature of materials^[2]. Earlier studies reported about the intense ML emission of rare earth doped strontium aluminate phosphors. Hence several researchers had conducted a lot of work to exploit the ML property of rare earth doped strontium aluminate for stress sensing applications^[3-8]. Akiyama et.al have reported ML intensity of strontium aluminate between different phases was so strong and the intensity strongly dependent on stress an suggested that the ML phenomena's are related to the movement of activated

doped strontium aluminates can be used for health monitoring of an aged bridge.^[10]

But only limited number of works were reported in the ML studies of barium based compounds^[1, 11, 12]. R.K.Rai et.al have reported the ML study of gamma irradiated BaAl₂O₄: Eu prepared via combustion synthesis method. To the best of our knowledge we are the first in reporting the ML studies of Eu doped barium aluminate phosphor prepared via high temperature solid state reaction method in air atmosphere.

II. EXPERIMENTAL

Stoichiometric weights of high purity (99.99%) BaCO₃, Al₂O₃, Eu₂O₃ were used as starting reagents. The stoichiometric weights of the reagents were taken using an electronic analytical balance (Schimadzu) and the mixture is thoroughly mixed for half hour without adding any mixing medium and then grounded well for one hour by adding double distilled water as mixing medium using a pestle and agate mortar. The well mixed mixture was dried in a hot air oven. The dried samples were preheated at 1050°C for 1 hour and then calcined at 6-4 hours.

Vehicle Sharing and Use of Bicycle for Travelling: An Effective Panacea to deal with Automobile Pollution

Santhosh Kumar, R., Lalithambika, R., Noor, S. Kumar and Ravendran, P.B.

Post Graduate Department and Research Centre of Botany, Mahatma Gandhi College, Thiruvananthapuram,
Post Graduate Department of Economics, Mahatma Gandhi College, Thiruvananthapuram, Kerala.

Abstract

Pollution is generally defined as the negative or undesirable alteration in the environment, usually the accumulation of something harmful or detrimental. Different developmental activities such as construction, transportation and manufacturing not only deplete the natural resources but also produce large amount of wastes that leads to various pollution to the environment. Pollution is thus direct or indirect changes in any component of the biosphere that is harmful to the biotic component in the ecosystem and in particular detrimental for human beings, affecting adversely the industrial level progress, cultural and natural assets or environment at local and global level. Transportation is one of the main causes for air pollution. In current situation a number peoples depends various vehicles or their travel or other transportation. In that situation a lot of unwanted carbon pollution is formed and transfer to the environment. In this present article, discussing a chance to introduce new methods to overcome the automobile pollution, including sharing of vehicles, use of cycle for short distance travelling. Cycling is not only help in travelling but also it is a good exercise as compared to other heavy exercise such running or reselling. New government policies are needed and to be implemented for the smooth functioning of such practices.

Introduction

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modes, $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ possesses more than four Raman modes which indicate a lowering of symmetry from cubic. In accordance with observed number of modes and group theoretical predictions the most likely symmetry of $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ is monoclinic with the space group $P2_1/n$. The symmetry was further confirmed from the Rietveld refinement of the XRD pattern. The compound possesses band gap of 3.8 eV. The photoluminescence properties of $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ substituted with Eu^{3+} for four different concentrations (15, 10, 5 and 2.5 mol %) were also investigated and it was found that concentration quenching occurred at 15 mol % of Eu^{3+} substitution, due to the cross relaxation between two neighboring Eu^{3+} ions. Thermoluminescence spectra of Eu^{3+} substituted $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ presented three emission lines at 592, 611 and 633 nm corresponding to the magnetic dipole transition $^5\text{D}_0 - ^7\text{F}_1$, electric dipole transition $^5\text{D}_0 - ^7\text{F}_2$ and $^5\text{D}_0 - ^7\text{F}_3$ transitions of Eu^{3+} respectively. The chromaticity coordinates was found to be (0.629, 0.369) for 10 mol % Eu^{3+} substituted $\text{Ba}_2\text{La}_{2/3}\text{TeO}_6$ which shows colour of emission in orange-red region.

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P 19

BIOGENIC SYNTHESIS OF SILVER NANOPARTICLES AND ITS CHARACTERISATION

**Remya G R¹, Lekshmi P Nair¹, Jayasudha S¹,
S Saravanakumar², Akhila S¹, Abhimanyu C M¹, Prabitha B Nair^{1*}**

¹Post Graduate and Research Department of Physics, Mahatma Gandhi College,
Thiruvananthapuram

²Department of Physics, NSS College, Pandalam

E-mail : prabibnair@gmail.com

Silver nanoparticles possess unique physical, chemical and biological properties due to which they exhibit catalytic, antimicrobial, anticancer and wound healing activity. In the present study silver nanoparticles are synthesized by reduction of silver salt with apple extract. The obtained silver nanoparticles are characterized using X-ray diffraction (XRD), FT-IR spectroscopy, micro Raman spectroscopy, Scanning Electron Microscopy (SEM) and UV-vis spectroscopy. Silver nanoparticles are in a state of tensile strain with an average particle size of 20 nm. The Surface Plasmon Resonance peak in the absorption spectra showed an absorbance maximum at 423 nm. The constancy in peak position with increasing time period indicates the stability of obtained silver nanoparticles.

Keywords : Nano particles, XRD, FT-IR, SEM

3. Results and discussion

The principal ligand acetone-N(4)-phenylsemicarbazone, (apsH), which is formed by direct condensation of N(4)-phenylsemicarbazide with acetone in methanol medium, was used for the synthesis of coordination complexes. During the synthesis of complex $[\text{Fe}(\text{apsH})_2(\text{CH}_3\text{OH})_2](\text{NO}_3)_2$ ferric(III) nitrate was reduced using hydroxylamine in acidic pH.

3.1. Crystal structures of $[\text{Fe}(\text{apsH})_2(\text{CH}_3\text{OH})_2](\text{NO}_3)_2$

The compound possesses a distorted octahedral geometry with two semicarbazone ligands (apsH) occupying four equatorial sites and two methanol molecules occupying the apical positions. The principal ligand apsH, behave as neutral bidentate N, O donor, coordinating via its carbonyl oxygen and azomethine nitrogen, resulting in five membered chelate ring [Fe1-N3-N2-C7-O1]. Two apsH ligands coordinate with same intraligand bite angle of 76.90° each, around iron(II) atom in the basal plane, while apical positions are occupied by methanol molecules at a distance of around 2.11 Å, almost orthogonal (91.9°) to the main plane.

The bond angles of O(1)-Fe(1)-O(1), O(2)-Fe(2)-O(2), N(3)-Fe(1)-N(3) are 180° , so the complex is centrosymmetric with respect to the coordinated ligands with Fe(II) situated on an inversion centre. The adjacent units are interconnected through H-bonding interactions involving O(4) and O(5) of the nitrate group with H(1N) and H(2N) of phenyl semicarbazone and H(2O) of methanol molecule. This nitrate group act as a bridge between molecules, in a one dimensional arrangement in the crystal structure, the complex molecules are arranged in face centered cubic lattice with nitrate ions interpenetrating the voids.

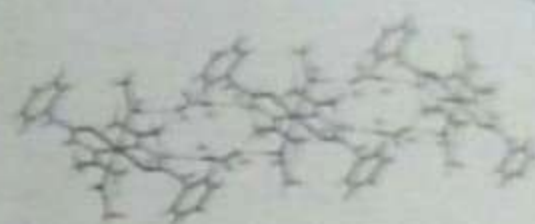


Figure 1. Bridging nitrate groups in one dimensional arrangement

Conclusion

The ligand acetone-N(4)-phenylsemicarbazone (apsH) was coordinated in neutral bidentate manner. Fe(III) has successfully reduced to Fe(II) before complexation, which is proved by X-ray diffraction studies. Intermolecular hydrogen bonding and other weak interactions contribute stability to the crystal. The Fe(II) complex exhibit a distorted octahedral geometry.

Acknowledgements

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Luminescence Properties of Rare Earth doped Calcium and Strontium Aluminate

Resmi G Nair*, Jayasudha. S and Dr. K. Madhukumar

Dept. of Physics, Mahatma Gandhi College, Thiruvananthapuram-695004.

PP-23

Abstract: Many aluminates have been employed as host materials for phosphors by doping rare earth elements. In this work Thermoluminescent (TL) and Photoluminescent properties of Calcium and

strontium aluminates, doped with Rare earths at varying concentrations, via combustion method have been studied systematically. All samples were examined by X-Ray diffraction to ascertain phase

High temperature thermoluminescence emissions of SrSO₄ nano phosphors doped with Eu and Mn

Jayashree S¹*, K. Madhukumar¹, C.M.K. Nair¹,
Ramesh G. Nair², V.M. Arunakumar²

¹Department of Physics,
Vidyanagar College
Thiruvananthapuram-695004, India
* jayashreeindia@gmail.com

T.S. Elmer²

²Regional Cancer Centre
Thiruvananthapuram-695011, India

Abstract— High temperature Thermoluminescence (TL) emissions of SrSO₄:Eu,Mn phosphor at 340°C is reported here for the first time. The nanocrystalline phosphors were prepared by wet chemical precipitation method. The glow curve shows an intense peak at 340°C, when the phosphor is subjected to X-irradiation. Co-doping with Mn enhances the trap depth and hence the TL emission temperature. Even though the luminescence intensity is found to be low, the phosphor becomes significant owing to its high temperature afterglow, which is one of the stringent requirements of a commercial thermoluminescent dosimeter (TLD). This phosphor appears to be fairly stable for TL measurements. Preliminary crystallographic and morphological studies of the phosphors were done using Powder X-ray Diffraction and Scanning Electron Microscopy (SEM). The phosphor has a single phase orthorhombic structure and the crystallites are sized in nano range. The dopant composition in the host matrix observed from the Energy Dispersive Spectra (EDS) were 8.18 atom% Eu and 8.15 atom% Mn. The single and well defined high temperature glow curve makes the phosphor suitable for high temperature radiation dosimetry applications.

Keywords— Thermoluminescence, Radiation dosimetry.

1. INTRODUCTION

Thermoluminescent (TL) phosphors were proved to be highly sensitive radiation detectors and are widely used for radiation dosimetry applications. Thermal ejection of relatively stable electrons trapped by means of ionizing radiation with X-ray, gamma ray, alpha, β -beam or other fast particles leads to TL. Studies are on in the search of suitable host-dopant combinations due to the constant need for high sensitivity TL dosimetry phosphors for different applications [1]. Recently, nanostructured materials are in focus, because of their potential impact in many areas such as electronics, photonics, catalysis and sensing [2-4]. Among the various phosphors alkaline earth sulphates are of special interest due to their high TL sensitivity, stability and low cost [1]. TL properties of rare earth doped CaSO₄, BaSO₄, SrSO₄, and MgSO₄ with single as well as multiple dopants were studied recently. TL studies of *Eu*-doped SrSO₄ compounds prepared via recrystallization method and irradiated by X-rays were done by J. Manam *et al.* [1]. Similarly, the TL performance of Eu doped SrSO₄ phosphors prepared through acid evaporation technique and irradiated with γ -rays were studied and reported by Q.Tang *et al.* [5]. Characteristics of the same host material prepared through a controlled chemical precipitation method by M. Karthikeyan *et al.* is also reported previously [6]. In many host lattices Mn is proved to be a best activator, when doped singly

or co-doped with rare earths [3,11,12]. Here the focus is on the TL properties of the SrSO₄:Eu nano phosphor co-doped with Mn. A much higher temperature TL emission is observed when the phosphor is subjected to X-rays. An attempt is made to estimate the activation energy corresponding to the trap from the geometry of the glow curve.

2. EXPERIMENTAL

SrSO₄:Eu,Mn nano phosphors were prepared by following the chemical precipitation technique described by Madhukumar *et al.* [7]. Analytical grade starting materials were used for the phosphor sample preparation. 0.5 mol% each of SrSO₄, Eu₂O₃ and MnO₂ were used for doping. After several washings, filtering and drying the precipitate was calcined at 400°C for 1 hour to eliminate the traces of any other compounds or acids. Further, the calcined material was ground well and then annealed at 3250°C in a programmable high temperature furnace for 10 hours in air atmosphere, to be required crystalline phase formation.

Subsequently, various characterization studies were carried out. The crystalline properties were studied from the X-ray diffraction taken from XPRT PRO Diffractometer using Cu K α radiation of $\lambda = 1.5406 \text{ \AA}$. SEM micrographs and EDS spectra obtained using JEOL 6390LV make Scanning Electron Microscope with EDS attachment were taken. Thereafter, the thermoluminescence glow curve at a heating rate of 5°C/s were recorded with a TL analyser TLD NUCLEONIX. About 5 mg of the phosphor powder was used all the time for recording the TL signal, such amount of phosphor sample influence the TL intensity. Irradiations were made with Cu K α X-rays generated at 30-10mA from RADON make X-Ray unit before recording TL.

3. RESULTS AND DISCUSSION

A. Structure Analysis

Fig.1 shows the typical X-ray diffraction pattern of prepared SrSO₄:Eu,Mn nano phosphor. The spectrum shows orthorhombic lattice structure with Pnma 62 space group in accordance with the ICSD database of the number 0885. Observed and calculated d -values are in good agreement. The lattice parameters were found to be $a=4.32 \text{ \AA}$, $b=10.10 \text{ \AA}$ and $c=6.80 \text{ \AA}$, which are fairly in agreement with parameters reported for the undoped host lattice $a=4.33 \text{ \AA}$, $b=10.10 \text{ \AA}$, $c=6.84 \text{ \AA}$. The slight deviation in the parameters is

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Jayashree S¹*, K. Madhukumar¹, C.M.K. Nair¹,
Ramesh G. Nair², V.M. Arunakumar²

¹Department of Physics,
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* jayashreeindia@gmail.com

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Thermally stimulated luminescence of SrSO₄:Eu,Mn phosphor under gamma excitation for TLD applications

Jayasudha S^{1*}, Dr. K. Madhukumar¹, Resmi G. Nair¹ & T.S. Elias²

¹*Department of Physics, Mahatma Gandhi College, Pattom P.O.,
Thiruvananthapuram-695004, India*

²*Regional Cancer Centre, Medical College P.O., Thiruvananthapuram-695011, India*

**jsnair.india@gmail.com*

Abstract - The thermoluminescence (TL) properties under gamma excitations of SrSO₄:Eu,Mn phosphor prepared via chemical precipitation technique is investigated. XRD pattern proved the orthorhombic structure and single phase of the host lattice. The line broadening of the peaks showed that the crystallites are nano in size. Uniformly distributed particles with different morphologies were observed in the SEM micrographs. The dopant compositions in the host matrix observed from the Energy Dispersive Spectra were 0.18 at% Eu and 0.3 at% Mn. The thermoluminescence studies of SrSO₄:Eu,Mn phosphor shows an emission at 306p C with a fairly high intensity, when the phosphor is subjected to gamma irradiation of 1Gy dose at room temperature from Co⁶⁰ buildup. This study is novel as the reported TL emission temperature of the widely used standard CaSO₄:Dy TLD is only 240p C. The high temperature emission of SrSO₄:Eu,Mn phosphor indicates its ability of long storage of trapped charge carriers at room temperature. The TL spectrum also shows the simple trap distribution of the lattice, which is desirable for dosimetric applications. The stability of the phosphor against gamma storage days were also investigated. An attempt is also made to calculate the activation energy of the traps by analyzing the kinetics of TL emission.

Keywords—Thermoluminescence, Radiation dosimetry.

oxidation, increases interlayer distance between graphitic layers, and reduces the crystalline size of GO.¹

We are also exploring the possibility of utilizing Metal Organic Frameworks (MOFs) for supercapacitor application. We have synthesised a cobalt based metal-organic-frameworks [CoNIm(RHO)] and the material was tested for supercapacitor application using electrochemical techniques such as cyclic voltammtery (CV), AC impedance, and chronopotentiometry. The MOF showed a specific capacitance value of 263 F/gm in KOH electrolyte.

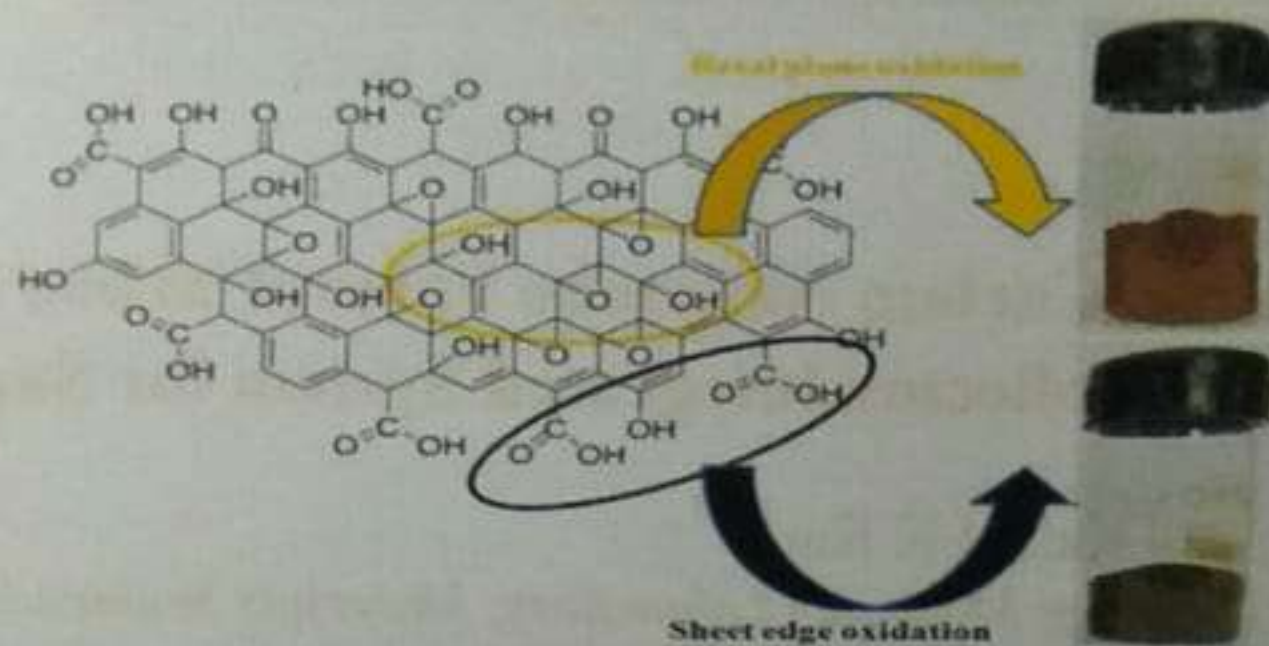


Figure 1. Graphite oxidation

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P 004 Influence of Al Co-Dopants on the Thermoluminescence Spectra of SrSO₄: Eu Phosphor Matrix

Jayasudha. S^{*1}, Resmi G Nair¹, Dr. K. Madhukumar¹, Dr.V.N. Praveen¹ and T.S. Elias²

¹Dept. of Physics, Mahatma Gandhi College, Thiruvananthapuram-695004.

²Regional Cancer Centre Thiruvananthapuram

Email: jsnair.india@gmail.com

Thermoluminescence Dosimetry is a powerful technique used for the estimation of both high and low ionising radiations. Various models of TL suggests that the impurities added can introduce high luminescence efficiency and to control the glow peak temperature. In the present work, the effect of codoping with Al in the SrSO₄ lattice is studied in detail. SrSO₄: Eu, Al phosphor have been irradiated using gamma-rays of Co⁶⁰ and the TL glow

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P 007 Study on the Dielectric Properties of Barium tetrakis (Maleate) Dihydrate

Lekshmi P. Nair^a, Dr. Bijini B. R.^a and Dr. Deepa M.^b

^aPost Graduate Department of Physics, M.G. College, Thiruvananthapuram.

^bDepartment of Physics, All Saints' College, Thiruvananthapuram.

E-mail: lekshmipadma@gmail.com

Metal co-ordination compounds of dicarboxylic acids are technologically very important as they have immense technological application. Maleic acid, a dicarboxylic acid, is biologically important and its interaction with different metal ions opens new potentialities with targeted properties. Barium complex of maleic acid (BM) is grown by gel method. Dielectric properties relate to the ability of a material to polarise under the influence of an external electromagnetic field. The study of dielectric property is concerned with the storage and dissipation of electric and magnetic energy in materials. The frequency dependent dielectric property of gel grown BM was studied at room temperature using a Hioki 3532 LCR Hitester meter. The variation of dielectric constant, dielectric loss, and ac conductivity with log frequency is plotted. From the spectrum it is observed that the dielectric loss and dielectric constant decreases with increase in frequency. The high value of dielectric constant at low frequency is attributed to the dipole and space charge polarisation. Using the results of Single crystal XRD, UV-Visible spectrum and the value of dielectric constant at higher frequencies, the Plasma energy, Penn Gap, Fermi energy and polarisability of the grown crystals are calculated and tabulated.

PP-032

Novel Calix[4]pyrrole receptor: Colorimetric sensing of Fluoride Ions

Keyur D. Bhatt^{1*}, Pooja Y. Raval¹, Sanjay D. Gupta¹, Bharat A. Makwana², Savan M. Darjee²

¹Department of Chemistry, B.V. Shah College of Science, C. U. Shah University, Wadhwan-city, Gujarat, India
²Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India
 *dkbhatt@outlook.com

A new calix[4]pyrrole receptor (meso-tetra(methyl) meso-tetra(4-hydroxy-3-methoxy-phenyl)-calix[4]pyrrole) HMCP, has been synthesized via conventional as well as microwave assisted methods. HMCP was characterized by ¹H-NMR, ¹³C-NMR, FTIR and by ESI-MS. The ion binding properties of calix[4]pyrrole with various anions were investigated using UV-Visible spectrophotometry. The red-shift in absorption band of HMCP was observed only in presence of fluoride ions. The results obtained from absorption spectra indicate that HMCP is linked with fluoride ions through hydrogen bonding. Among all the investigated anions, only fluoride ions showed sharp colour change from yellow to dark red, which was easily detectable by naked-eye even at very low concentration level of 1 µM.

PP-033

Crystal structure and dielectric study of Glycinium Maleate

B. R. Bijini^{1*}, K. Rajendra Babu²

¹Department of Physics, HHMSPB NSS College for women, Thiruvananthapuram, Kerala, India
²Post Graduate Department of Physics, M.G. College, Thiruvananthapuram, Kerala, India
 *bijiniyothis@gmail.com

Amino acids are vital components of a variety of biological, industrial and environmental samples. Glycine, the simplest amino acid is an important constituent of proteins, enzymes and a major inhibitory neurotransmitter in spinal cord and brainstem of vertebrate nervous system. In a strongly acidic medium Glycine exists in its protonated form (monocation) i.e. NH⁺₃CH₂COOH. Maleic acid, a dibasic unsaturated carboxylic acid is widely used in medicine. Glycinium maleate single crystals were grown by solution method. Good quality crystals were formed in solution of glycine and Maleic acid in the 1:1 molar ratio. The single crystal X-ray diffraction studies gave new insight into the crystal structure of the title compound. The study shows that the grown crystals belong to monoclinic system (C/c) with unit cell parameters a=17.9137(12) Å, b=5.6869(3) Å, c=17.4483(11) Å, β=112.710(5). Crystal structure reveals that the glycine molecule exists as a positively charged ion with protonated amino group. The anion is the singly negatively charged maleic acid in which one of the two carboxyl functional groups of maleic acid has been deprotonated. The Maleic acid is interconnected to glycine molecule through Hydrogen bonds. The crystal structure is stabilized by these hydrogen bonds between Glycine cation and Maleate anion. Fermi gap, Penn gap and Plasma energy of the grown crystals were calculated from unit cell parameters and dielectric studies.

PP-034

FT-IR and Raman spectroscopic studies of Thiosemicarbazide potassium chloride

Bincy Annie Philip¹, Anju Mary John¹, Shyamal Sreedhar¹, C. Ravikumar^{1*}

¹Department of Physics, CMS College, Kottayam-686 001, Kerala, India
 *rkz.ravi@gmail.com

The nonlinear optical (NLO) compound of interest Thiosemicarbazide potassium chloride crystal (TSPC) was grown by slow evaporation method. The molecular structure generated with the aid of density functional theory (DFT) Raman and IR spectra were recorded and analyzed. The harmonic wavenumbers and IR and Raman intensities were computed with the B3LYP method. The observed vibrational wavenumbers were compared with the theoretical values.

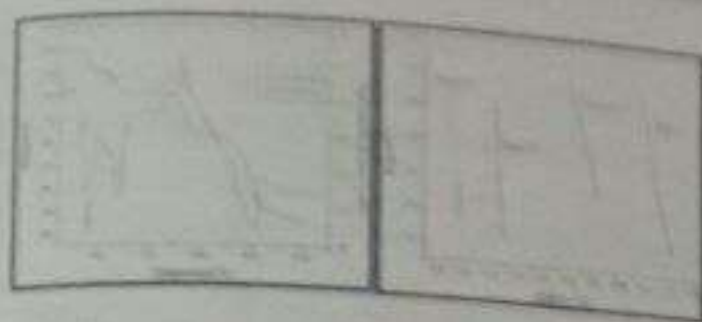


Fig 2: TGA/DTA curves plots

Fig 3: Coats and Redfern plots

The compound is thermally stable upto 100°C. The TGA curve shows a mass loss of 18.94 % within the temperature range 40-240°C, which corresponds to the loss of water molecules (calc-19.22%). Thus the two endothermic peaks upto 238.27°C indicates the loss of two water molecules. The anhydrous calcium maleate gets decomposed into calcium oxalate with the elimination of acetylene molecule, confirmed by the exothermic peak at 505°C in the DTA curve. Further heating results in the conversion of calcium oxalate to CaO with the evolution of CO and CO₂. The observed and calculated percent of weight loss in the temperature range 490°C - 790°C during the above said decomposition process is 49.5 and 50.75.

Kinetic parameters				Thermodynamic parameters		
Stage	n	E(KJ/mol)	logA(S ⁻¹)	ΔS(J/Kmol)	ΔH(KJ/mol)	ΔG(KJ/mol)
I	0.9	162.87	18.23	105	156.63	101.72
II	0.9	124.10	9.94	-58.49	115.74	145.15
III	0.9	516.54	31.60	352.78	503.58	228.69
IV	1.1	489.00	21.68	160.81	473.00	318.3

respectively. Coats and Redfern plots for the thermal decomposition stages are depicted in figure 3. Table 1 provides the kinetic and thermodynamic parameters of the compound.

Conclusion:

Calcium complex of maleic acid have been successfully grown by gel method. Sodium metasilicate of gel density 1.04g/cc and pH6.5 produced good quality crystals. Elemental analysis gives the formula of the compound as CaC₄H₂O₄·2H₂O. Thermal decomposition of the complex was studied by TGA/DTA.

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Screening of enzymatic activity in different bacterial isolates treated with phenol

Dr. J. K. Reshma¹, Anu Mathew^{1*}, Dr. V. Salom Gnana Thanga²

¹Post Graduate Department of Environmental Sciences, All Saints' College, Thiruvananthapuram, Kerala ²Department of Environmental Sciences, Kariavattom campus, Thiruvananthapuram, Kerala

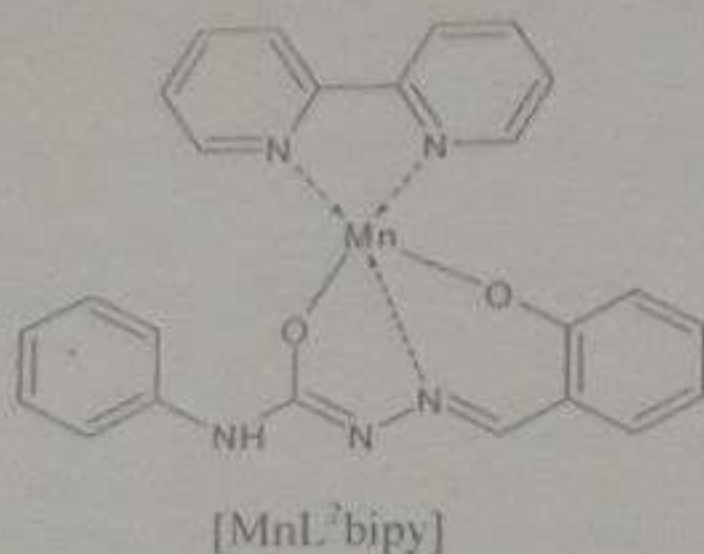
*Corresponding Author: anumathew85@yahoo.co.in

PP-19

Abstract

Coir-retting environment harbours a variety of potential microbes which can degrade phenols. Microorganisms capable of degrading phenol do so with the action of a variety of enzymes. So, a study

was carried out to analyse the enzymes present in Kadinamkulam retting area to highlight the importance of enzymes in degradation of phenol compounds. In this study phenol oxidase activity and cellulose enzyme complex (Cellulase, β-1,



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CRYSTAL STRUCTURE, SPECTRAL, THERMAL AND DIELECTRIC STUDIES OF A POLYMER OF SODIUM COMPLEX OF MALEIC ACID

Bijini B.R.¹, Lekshmi P Nair¹, Prasanna S.¹, Deepa M.², C.M.K. Nair¹ and Rajendra Babu K.^{1*}

¹Postgraduate Dept. of Physics, M.G.College, Thiruvananthapuram-695004, India

²Department of Physics, All Saints' College, Thiruvananthapuram-695037, India

*Corres.author: bijiniyothis@gmail.com,

PP-29

Abstract

Single crystals of sodium complex of maleic acid was grown in gel medium for the first time. Single crystal X-ray diffractometry reveals that the crystal lattice of the complex is triclinic (P-1) and the complex is in an 1D polymeric form. FT-IR spectral studies were used to identify the functional groups and the bonding sites of the ligand with the metal atoms.

Key words: Maleic acid, Sodium metasilicate gel, Crystal growth.

Introduction

Metal-organic frameworks (MOFs) constitute an emerging class of materials useful in gas storage, gas purification, separation applications and research on biomedical applications of MOFs is gaining momentum and this emerging new class of porous materials is likely to replace the traditional nanoporous materials in drug delivery and storage in the future¹. Maleic acid is widely used in medicine, in the preparation of drugs, in agriculture as the plant growth regulators, in food industry etc. Maleic acid is used extensively in the pharmaceutical industry for making maleate salts of drugs. Sodium is one of the four important biologically active cations.

Among many methods available for crystal growth, gel technique is commonly adopted due to its

simplicity and ability to suppress nucleation centers. Slow diffusion of reactants in the gel medium can be considered to mimic the growth of crystals in a human body². The principal aim of the present study mainly focuses on the growth of Sodium complex of maleic acid on sodium metasilicate gel.

Experimental procedure

Crystallization method

The apparatus used for crystallization of single crystals by gel technique consists of borosilicate glass tubes of length 20cm and diameter 2.5cm. Silica gel was prepared by adding a solution of sodium metasilicate to 20% maleic acid slowly with continuous stirring. The specific gravity of sodium metasilicate was varied between 1.04 g/cc and 1.05g/cc and pH was adjusted in the range 3 - 6. About 20ml of gel solution with the desired value of pH was then transferred to several test tubes and 5ml of acetone was added to each test tube to reduce solubility. Over the set gel, acetone was added.

Results and discussion

Crystal growth

Tiny crystals were observed at the gel solution interface in the third week after incorporation of the top solution. The optimum

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GROWTH AND THERMAL CHARACTERISATION OF GEL GROWN CALCIUM MALEATE DIHYDRATE PP-18

Lekshmi P. Nair¹, Bijini B. R.¹, Prasanna S.¹, Deepa M.², C. M. K. Nair¹, K. Rajendra Babu^{1*}

¹Postgraduate Department of Physics, M.G. College, Thiruvananthapuram, India-695004

²Department of Physics, All Saints' College, Thiruvananthapuram, India-695037

*Corres. author Tel. No: +91 9447963076, mgkrb1956@yahoo.co.in (K. Rajendra Babu)

Abstract: Calcium maleate dihydrate (CaMa) crystals are grown by gel method for the first time. Conditions for growing good quality crystals are optimized. Elemental analysis gives the formula of the compound as $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$. Thermal properties of the complex are analysed by TGA/DTA. Coats and Redfern method is utilised to obtain the kinetic and thermodynamic parameters of the complex.

Key words: Crystal growth, maleic acid, calcium maleate, gel method, TGA, DTA.

Introduction

Various metal carboxylate compounds strike the specific attention of the researchers due to their vast applications in science and technology. Maleic acid is biologically important and its interaction with different metal ions opens new potentialities with targeted properties. Calcium exhibits wide range of topologies and confirmations with co-ordination numbers ranging from 3 to 11¹. Calcium maleate is used as the substrate for enzymatic iodination process. As the gel method mimics the growth of crystals in human body, we are adopting the method of controlled diffusion of ionic species in hydrosilica gel medium to get quality crystals of this biologically important calcium maleate. The grown crystals are characterised by elemental analysis, TGA/DTA.

Experimental Procedure:

Growth Procedure:

The crystallisation of calcium maleate dihydrate was accomplished using gel diffusion technique. Crystals were grown in glass tubes of length 20cm and diameter 2.5cm. Silica gel of specific gravity 1.03 to 1.06g/cc was prepared by

dissolving sodium metasilicate (SMS) in double distilled water. Maleic acid (1M) was added to SMS to acidify it to get pH in the range 3 to 7. About 30ml of above solution was taken in each test tube and kept undisturbed for setting. Over the set gel, aqueous solution of calcium chloride (0.5 – 2M) was added as the top reagent, without damaging the gel system.

Results and discussion: Crystal Growth:

Crystals of CaMa were formed at the gel interface within two week. The growth process took three months for completion. Good quality crystals suitable for characterisation studies were grown in gel medium of pH 6.5 and density 1.04g/cc, 1M maleic acid, 1M calcium chloride. The crystals of CaMa were prone to decompose in air. The photograph of the grown crystal is shown in figure 1. Elemental analysis gives the formula of the compound as $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ (Experimental: C- 25.93%, H- 2.35% Calculated: C- 25.26%, H- 3.19%).

Thermal analysis:

Thermal analysis of the sample was carried out using Perkin Elmer Diamond TGA/DTA analyser with a heating rate of 10°C/min in the nitrogen atmosphere. The TGA/DTA results are shown in figure 2



Fig1: $\text{CaC}_4\text{H}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$

conditions to grow the best quality single crystals were at pH 5 and gel density, 1.04 g/cc.

Single crystal X-ray diffraction studies

The crystallographic data reveals that the crystal lattice of the complex is triclinic (P-1) with unit cell parameters $a=5.9512(3)\text{\AA}$, $b=6.3891(4)\text{\AA}$, $c=11.2178(7)\text{\AA}$, $\alpha=104.219(2)^\circ$, $\beta=91.490(2)^\circ$, $\gamma=100.165(2)^\circ$. Coordination environment of the complex with atom numbering scheme is shown in fig.1. The central Na atom is surrounded by six oxygen atoms and forms an octahedral environment. It means that the Na(I) is bonded to one maleate ligand with O(4)-Na(1) distance 2.373\AA and to five aqua oxygen atoms to form an octahedral environment. The bridging bond Na(1)-O(5) builds one dimensional polymeric structure.

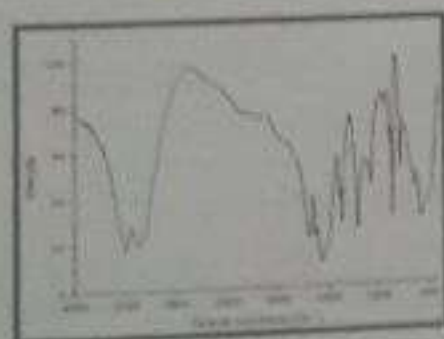
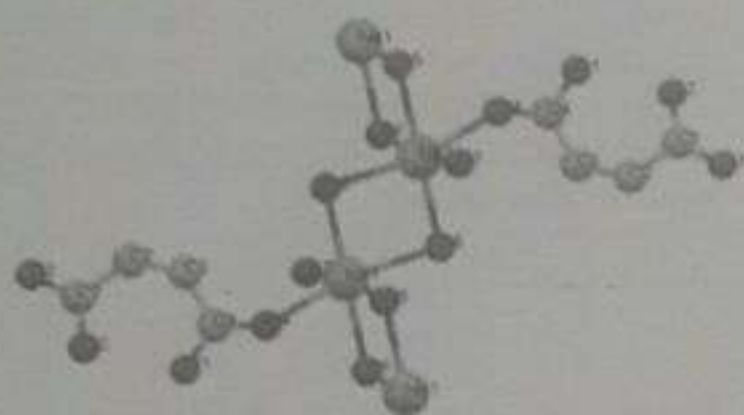


Fig.1 Molecular structure of $C_4H_4NaO_7$

Fig.2 FT- IR spectrum of the grown crystals

Fourier transform infrared (FTIR) spectra

The FT-IR spectrum of the grown crystal is as shown in fig. 2. The spectrum contains two sets of strong bands due to $\nu_{as}(\text{COO})$ at 1694, 1621 cm^{-1} and $\nu_s(\text{COO})$ at 1397, 1364 cm^{-1} of maleate ligand. For one of the carboxylate groups, the separation between $\nu_{as}(\text{COO})$ and $\nu_s(\text{COO})$ of 297 cm^{-1} is significantly larger than the value of 248 cm^{-1} for free maleic acid, indicating that one of the carboxylate groups coordinated to the central sodium ion in monodentate fashion. The band at 1214 cm^{-1} corresponds to C-O stretching which is shifted to lower frequency region with respect to the ligand (1261 cm^{-1}) due to the coordination with the central sodium atom.

Conclusions

Single crystals of Sodium complex of Maleic Acid have been successfully grown by gel diffusion method. Sodium metasilicate of gel density 1.04g/cc and pH 5 produced good quality crystals. X-ray diffraction study confirms that the grown crystals belong to triclinic system with unit cell parameters $a=5.951(3)\text{\AA}$, $b=6.389(4)\text{\AA}$, $c=11.217(7)\text{\AA}$, $\alpha=104.21(2)^\circ$, $\beta=91.49(2)^\circ$, $\gamma=100.16(2)^\circ$ and the molecules are built in a manner to form a polymerized infinite chain.

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STUDIES ON NEW COPPER (II) COMPLEXES OF N²-PHENYL-N⁴,N⁶-DI(THIAZOL-2-YL)-1,3,5-TRIAZINE-2,4,6-TRIAMINE

M.Vathananaruba^{*}, P.Tharmaraj^{*}, C.D.Sheela[#]

^{*} PG & Research Department of Chemistry, Thiagarajar College, Madurai-9

[#] PG & Research Department of Chemistry, The American College, Madurai-2

Email: ptharmaraj@rediffmail.com

PP-30

Abstract

A new series of copper(II) complexes of 1,3,5-triazine based NNN donor ligand, N²-phenyl-N⁴,N⁶-di(thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine have

been synthesized. The structural feature of the ligand and complexes has been arrived by elemental analysis, magnetic susceptibility measurements, molar conductance, spectral techniques. The free ligand and their metal complexes have been screened

Structural and spectroscopic characterization of DL-aluminium fumarate

V. K. Suma, D. Arul Dhas^{a,*}, I. Hubert Asa^b, S. Balakrishnan^c

^aDepartment of Physics, Nezamony Memorial Christian College, Marthandam
629165, Tamil Nadu, India

^bCentre for Molecular and Biophysics Research, Department of Physics, St
Ignace College, Thiruvananthapuram-695011, Kerala, India

^cDepartment of Chemistry, M. G. College, Thiruvananthapuram-695004
Kerala, India

*E-mail: arul_dhas_2004@yahoo.com

Abstract

In this work, the vibrational spectral analysis of the DL-aluminium fumarate compound was carried out by using FT-Raman and FT-IR spectroscopic techniques. The structure of the compound was optimized and the structural characteristics were determined by density functional theory (DFT) using B3LYP method with 6-311G(d,p) basis set. The observed vibrational wave numbers were compared with calculated results. The reactivity and bond strength has been investigated by applying the natural bond orbital analysis. The calculated HOMO and LUMO energies show that charge transfer occurs in molecule and other results observed shows the NLO active nature of DL-aluminium fumarate.

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PP-08

PNR SIZE DISTRIBUTION AND ELECTROLESS Ni-P STUDIES OF TIN OXIDE NANOPARTICLE SYNTHESIZED VIA WET CHEMICAL METHOD AND ITS INCORPORATION IN MILD STEEL PLATE

R. Sudha devi, S. Balachandran and S. Shoga

Department of Chemistry, Mahatma Gandhi college, University of Kerala,

Thiruvananthapuram, Kerala- 695004, India. Tel: +919495621360,

E-mail: sudhasudhadevi@gmail.com

Abstract

SnO_2 nanoparticles were synthesized by chemical precipitation method. Alkali neutralization method was used to determine the concentration of Sn-OH groups in the sample. The phase structure and chemical composition of prepared sample was analyzed using XRD. The broad peaks in the XRD patterns revealed the presence of rutile phase of SnO_2 . The optical absorption, the vibrational modes were evident from UV-visible, FTIR spectroscopic analysis respectively. The globular nature of nano SnO_2 was evident from SEM analysis. The SnO_2 having BET surface area 109.2318 revealed the better catalytic activity of nano SnO_2 . The pore size distribution was 22.8074Å. The results obtained from the above mentioned analysis reveal that the prepared nano tin oxide particles are of very small grain size with very fine characteristic properties. Amorphous metallic alloys like nickel-phosphorous alloys have the ability to generate high current per unit area of external surface and hence have been reported as an efficient electrode for further studies. The co-deposition of transition metal oxide nano particles of good electro catalytic activity improves the electrochemically active area of the Ni-P electrodes. The present study explored nano SnO_2 synthesized via wet chemical method, for the surface activation of electro less nickel coatings.

Key words: Nanomaterials, electrode, catalyst, co-deposition, electroless coating

Introduction

Semiconductor nanomaterials have interesting physical and chemical properties when compared with conventional bulk counter parts. Electro less nickel coatings are well known to exhibit good electro catalytic activity towards gas evolution reactions and play important roles in various electrochemical processes. Amorphous metallic alloys like nickel-phosphorous alloys have been reported as an efficient electrode. The co-deposition of transition metal oxide nano particles of good electro catalytic activity enhances the electrochemically active area of the Ni-P electrodes. The present study explored the development of nano SnO_2 incorporated electroless nickel coatings.

Experimental methods

In the present study, nanocrystalline SnO_2 sample was prepared by wet chemical method. For the preparation of $(\text{SnO}_2)_n$ in (II) salt solution, which was made by dissolving tin (II) chloride in isopropanol. The pH of the solution was maintained at a finite value. The precipitate obtained was centrifuged, washed several times with distilled water and the residue was air dried.

SYNTHESIS AND KINETIC STUDIES ON THE HYDROLYTIC STABILITY OF CURCUMIN BORON COMPLEXES

Jeenu John, Sudha Desai and Rajachandran P*

Department of Chemistry, Mahatma Gandhi College, Tiruvananthapuram-695004

INTRODUCTION

Curcumin is a biologically active compound isolated from the plant turmeric. About 2 to 8 % of turmeric by weight is curcumin. Curcumin is responsible for the bright yellow color of turmeric. It is commonly used as a spice in Indian cooking, a cosmetic agent for skin care and a traditional medicine for various diseases like cancer, Alzheimer's, various diseases, arthritis etc. The metal chelating ability of curcumin has been attracting researchers from wide ranging fields of physics, chemistry, biology and medicine. The ability of curcumin to form bright red colored complex with boron enable it to use as a spectrophotometric reagent for boron quantification and determination. Rosocyanin and Rubrocyanin are the two boron complexes of curcumin widely used for boron determination. One of the main drawbacks of this method is the rapid hydrolysis of these curcumin boron complexes. So attempts are there to synthesize a curcumin boron complex which resist hydrolysis in water mediated conditions. In the present work an attempt was made to synthesize different analogues of Rubrocyanin and to compare its hydrolytic stability in different aqueous water system with Rubrocyanin.

MATERIALS AND METHODS

Materials

A mixture of curcuminoid pigment from turmeric was obtained from Waco. The chemicals used were of reagent grade. The solvents used for kinetic study were chromatographic grade.

Methods

Curcuminoids were separated using column chromatography. Different curcumin boron complexes were prepared as per the procedure in literature (1). The synthesized compounds were

Scrub Typhus Fever –An Emerging Health Challenge in Kerala

Dr.Biju kumar.B.S

Assistant Professor, Department of Zoology
N.S.S College, Nilamel

Abstract

Scrub typhus fever is a disease caused by bacteria called *Orientia tsutsugamushi*. Scrub typhus fever occurs most commonly among people in contact with overgrown terrain, forest clearings, reforested areas etc. in many Asian countries including India. Scrub typhus fever is not directly spread from person-to-person. Disease is spread to people by the bite of a mite infected with the bacteria that causes scrub typhus fever. In India, it has been reported from northern, eastern, and southern India. In Kerala the disease was reported from many parts of Thiruvananthapuram District including Attingal and Nedumangadu. The diagnosis was based on the presence of eschar, a positive Weil-Felix test, and a positive rapid diagnostic test (immunochromatographic assay).

Key word: Scrub Typhus, *Orientia tsutsugamushi*

Introduction

Scrub typhus is a mite-borne infectious disease caused by *Orientia tsutsugamushi* (previously called *Rickettsia tsutsugamushi*). It is distributed throughout the Asia Pacific region, being endemic in Korea, China, Taiwan, Japan, Pakistan, India, Thailand, Malaysia, and northern portions of Australia. However, cases also occur in the United States, Canada, and Europe,

being imported by tourists returning from endemic regions. Scrub typhus is a public health problem in Asia, where about 1 million new cases are identified annually and 1 billion people may be at risk of this disease. In India, the presence of scrub typhus and other rickettsial diseases has been known for several decades [1].

Scrub typhus is manifested clinically by high fever, intense generalized headache, diffuse myalgias, and, in many patients, rash and an eschar at the site of the chigger bite. The diagnosis is suggested by the clinical history (including visit to an endemic area) and physical findings and confirmed by serologic testing or biopsy of an eschar.

Scrub typhus lasts for 14 to 21 days without treatment. Severe infections may be complicated by interstitial pneumonia, pulmonary edema, congestive heart failure, circulatory collapse, and a wide array of signs and symptoms of central nervous system dysfunction, including delirium, confusion, and seizures. Death may occur as a result of these complications, usually late in the second week of the illness [2].



Business Environment and Entrepreneurship Development

K. Manoharan Nair Anitha K.
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B. Com., 3rd Semester, Core Course Kerala & MG Universities

BUSINESS ENVIRONMENT AND ENTREPRENEURSHIP DEVELOPMENT

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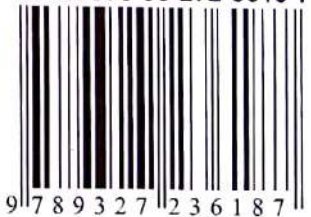


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Associate Professor

Post Graduate Department of Commerce and Research Centre

Mahatma Gandhi College, Thiruvananthapuram

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A.V. BIJU

Under the Supervision of

Dr. K. MANOHARAN NAIR

Associate Professor

Post Graduate & Research Department of Commerce, M.G College,
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ROLE OF ACCOUNTING DISCLOSURE IN FINANCIAL HEALTH: A STUDY WITH REFERENCE TO FINANCIAL INSTITUTIONS IN IRAN



Dr. K. Manoharan Nair

Dr. K. Manoharan Nair

Former Associate Professor and Head of the Post Graduate Dept of Commerce and Research Centre, Mahatma Gandhi College, Thiruvananthapuram.

Abstract: During the past two decades, various measures have been adopted to promote and advance accounting in Iran via harmonizing the domestic

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Scrub Typhus Fever –An Emerging Health Challenge in Kerala

Dr.Biju kumar.B.S

Assistant Professor, Department of Zoology
N.S.S College, Nilamel

Abstract

Scrub typhus fever is a disease caused by bacteria called *Orientia tsutsugamushi*. Scrub typhus fever occurs most commonly among people in contact with overgrown terrain, forest clearings, reforested areas etc. in many Asian countries including India. Scrub typhus fever is not directly spread from person-to-person. Disease is spread to people by the bite of a mite infected with the bacteria that causes scrub typhus fever. In India, it has been reported from northern, eastern, and southern India. In Kerala the disease was reported from many parts of Thiruvananthapuram District including Attingal and Nedumangadu. The diagnosis was based on the presence of eschar, a positive Weil-Felix test, and a positive rapid diagnostic test (immunochromatographic assay).

Key word: Scrub Typhus, *Orientia tsutsugamushi*

Introduction

Scrub typhus is a mite-borne infectious disease caused by *Orientia tsutsugamushi* (previously called *Rickettsia tsutsugamushi*). It is distributed throughout the Asia Pacific region, being endemic in Korea, China, Taiwan, Japan, Pakistan, India, Thailand, Malaysia, and northern portions of Australia. However, cases also occur in the United States, Canada, and Europe,

being imported by tourists returning from endemic regions. Scrub typhus is a public health problem in Asia, where about 1 million new cases are identified annually and 1 billion people may be at risk of this disease. In India, the presence of scrub typhus and other rickettsial diseases has been known for several decades [1].

Scrub typhus is manifested clinically by high fever, intense generalized headache, diffuse myalgias, and, in many patients, rash and an eschar at the site of the chigger bite. The diagnosis is suggested by the clinical history (including visit to an endemic area) and physical findings and confirmed by serologic testing or biopsy of an eschar.

Scrub typhus lasts for 14 to 21 days without treatment. Severe infections may be complicated by interstitial pneumonia, pulmonary edema, congestive heart failure, circulatory collapse, and a wide array of signs and symptoms of central nervous system dysfunction, including delirium, confusion, and seizures. Death may occur as a result of these complications, usually late in the second week of the illness [2].