

To,

20.07.2016

Prof. Ravindra R. Kamble Department of Chemistry Karnatak University Dharwad

Dear Dr. Kamble,

The pharmacological activity of drugs depends on how the drugs interact with proteins, enzymes, receptors, nucleic acid, or biomembranes. In this regard, I express my support for your research to analyze the genotoxicity, PDE inhibition studies etc., for the molecules designed and synthesized at your university. The focus of my responsibility is to carry out the above said activities for the molecules designed and synthesized at your university designed and synthesized at your research laboratory. Also, synthesizing the novel pharmacological scaffolds with required physical parameters is a very important starting point of our work as is the focus on obtaining the molecules with potential pharmacological property and clinical significance. Our laboratory is well equipped with basic facilities to test your novel compounds for the activities mentioned earlier. Our interdisciplinary collaborative work can make our research meaningful and hopefully lead to publications in reputed journals.

I look forward for continuing our collaboration.

Regards

dik

Dr Guruprasad Kalthur Professor & Head Division of Reproductive Biology Department of Reproductive Science Kasturba Medical College, Manipal Manipal - 576104, India



To,



15.08.2016

Prof. Ravindra R. Kamble Department of Chemistry Karnatak University Dharwad

Dear Dr. Kamble,

Molecular docking is a key tool in structural molecular biology and computer-assisted drug design. The goal of ligand-protein docking is to predict the predominant binding mode(s) of a ligand with a protein of known three-dimensional structure.

In view of the above, this letter is to express my support for your research to analyze docking score with the protein/enzyme for the molecules designed and synthesized at your university. The focus of my responsibility is to carry out the simulation study as I have been working for several years from now with a specific focus on addressing the possible interactions between previously unknown molecules with the target proteins/enzyme. Also, synthesizing the novel pharmacological scaffolds with required physical parameters is a very important starting point of our work as is the focus on obtaining the molecules with potential pharmacological property.

I look forward for continuing our collaboration.

Dr. Shrinivas D. Joshi Professor and Head, Department of Pharmaceutical Chemistry, SET's College of Pharmacy, Dharwad-580002, Karnataka Dr. Shrinivas D. Joshi Professor & Head Dept. of Pharm. Chemistry SET'S College of Pharmacy Dharwad. Karnataka





Dr. Pradeep Kumar Pujari Director Radiochemistry & Isotope Group B.A.R.C., Mumbai 400085.

Government of India BHABHA ATOMIC RESEARCH CENTRE Radiochemistry & Isotope Group Distinguished Scientist Senior Professor Homi Bhabha National Institute

To whomsoever it may concern

This is to certify that the research group headed by Dr. Rajashekhar F Bhajantri, Professor, Department of Physics, K.U. Dharwad has been carrying out collaborative research work on Positron Annihilation Studies of Polymer Nanocomposites from 2014-15 – till date with our research group at Radiochemistry & Isotope Group, Radiological Laboratories, Bhabha Atomic Research Centre, Mumbai. As I understand, presently they are working on synthesis of nanoparticles and polymer nanocomposites for energy storage devices. We will be able to carry out positron studies in the same materials.

(P.K. Pujari)

डॉ. प्रदीप कुमार पूजारी Dr. Pradeep Kumar Pujari Director / निदेशक रेडियो रासायनिक एवं आइसोटोप वर्ग, Radiochemistry & Isotope Group, भाभा परमाणु अनुसंधान केंद्र, Bhabha Atomic Research Centre Trombay, Mumbai - 400085.



BHABHA ATOMIC RESEARCH CENTRE Phone : + (91) (22) 2559 5326, 2559 2016, Res.: + (91) (22) 20850790 Mobile : + 91 9869279237, Fax : + 91 22 2550 5311 Email : pujari@barc.gov.in / pkpujari@yahoo.com



MANIPAL INSTITUTE OF TECHNOLOGY



(A constituent unit of MAHE, Manipal)

ANIPAL

22-12-2021 Manipal

To whomsoever it may concern

This is to certify that my research group has been carrying out research work on the research field *polymer physics* in collaboration with the reseach group headed by **Dr. Rajashekhar F Bhajantri**, Professor, Department of Studies in Physics, Karnatak University, Pavate Nagar, Dharwad-580 003, Karnataka, India **since 2014**.

Thanks and Regards,

Dr. Ismayil Assistant Professor (Selection Grade) Department of Physics Manipal Institute of Technology Manipal Academy of Higher Education Manipal, Karnataka - 576104, India Email ID - ismayil.mit@manipal.edu Phone Number - +91 9845497546



Manipal Institute of Technology, Manipal – 576 104, Karnataka, India *dir.* +91 820 2571060 *e-mails:* office.mit@manipal.edu; academic.section@manipal.edu www.manipal.edu



南京農業大學 NANJING AGRICULTURAL UNIVERSITY

NO. 1 Weigang, Nanjing 210095, Jiangsu Province P. R. China Tel: +86-25-84395754 Fax: +86-25-84396326 E-mail:ietc@njau.edu.cn Http://www.njau.edu.cn

College of Horticulture Nanjing Agricultural University Fax: 86-25-84395266 Phone: 86-25-84395217 Cellular: 86-015805162385 Email: fanggg@njau.edu.cn

January 4, 2017

Dr. Sudisha Jogaiah (Passport No. H3166225, Male) Department of Biotechnology and Microbiology Karnatak University, Dharwad Karnataka- 580003 India

Dear Dr. Sudisha:

With the establishment of our collaboration in fruit science and academy, I would like to invite you to come and visit Nanjing Agricultural University (NJAU) during 16 April – 15 July 2017, to carry out the research in my laboratory.

You are a famous scientist expert at plant physiology and molecular biology, your research work during your stay in China will be very important in improving our knowledge about the application of grape physiology and molecular biology in viticulture. I think both graduate students and some fruit scientists in China can be benefitted from our collaboration. I appreciate if you accept my invitation to visit NJAU.

I think we can have the following activities: i. Research work in my laboratory; ii. Visit laboratories and talk with graduate students about research art in fruit crop genomics and molecular biology iii. Attend the signing ceremony of collaboration in fruit crop science; iv. Exchange the experience in training graduate students; v. Visit NJAU and some other fruit institutes in China.

Looking forward to see you in Nanjing Agricultural University!

Sincerely Yours 52 Jinggui Fang Professor, Ph.D.





Dr. Lam-Son Phan Tran, Unit Leader Signaling Pathway Research Unit 1-7-22 Suehiro -cho, Tsurumi Yokohama, Japan 230-0045 Tel. (81)-45-503-9593 Fax (81)-45-503-9591 son.tran@riken.jp

August 15, 2017

To Whom It May Concern!

I have known Dr. Sudisha Jogaiah from Karnatak University, India as a research collaborator for the past 9 years. Dr. Jogaiah and I have shared successful scientific collaborations which have resulted in eight peer-reviewed papers having high impact factor.

Our collaborations spanning both his post-doctoral and professional days were very scientifically productive. It was his scientific intuition, meticulous planning, very well organized data collection and erudite interpretation which resulted in the success of the work jointly undertaken by us.

The fruitful research collaborations have been transformed into publications in reputed peer reviewed Journals with high impact factor have been appeared in e.g. in J. Expt. Botany (IF:6.9), Int. J. Mol. Science (IF: 5.9), Critical Rev. Biotechnology (IF: 8.4), Scientific Reports (IF: 4.3), Arabian J. of Chemistry (IF: 5.16), Molecular Plant Pathology (IF: 5.1), Plant Cell and Environment (IF: 7.3), Plant Cell Report (IF: 4.5) and others.

Sincerely,

enn

Lam-Son Phan Tran



सी एस आई आर - राष्ट्रीय समुद्र विज्ञान संस्थान (वैज्ञानिक एवं औद्योगिक अनुसंधान परिषद) दोना पावला, गोवा 403 004 भारत

CSIR - National Institute of Oceanography (Council of Scientific & Industrial Research) DONA PAULA, GOA - 403 004, India



CERTIFICATE

This is to certify that the dissertation work entitled "**Sponge diversity** from Karwar coast, Karnataka" is the original work done by Ms. Arpita Dutta for partial fulfillment of her M.Sc. Degree course during March 2017 to June, 2017 under my guidance at the Biological Oceanography Division, CSIR-National Institute of Oceanography, Dona Paula, Goa.

Dr. B.S. Ingole)

(Dr. B.S. Ingole) Professor & Chief Scientist Biological Oceanography Division, CSIR-National Institute of Oceanography, Dona Paula, Goa- 403004.

sĭ. बबन इंगोले / Dr. Baban Ingole मुख्य वैज्ञानिक / Chief Scientist सी.एस.आई.आर. - राष्ट्रीय समुद्र विज्ञान संस्थान CSIR - National Institute of Oceanography दोना पावला / Dona Paula - 403004 गोवा / Goa, भारत / India

Date: 17/05/2017 Place: Dona Paula, Goa



K.L.E. Society's



K.L.E. INSTITUTE OF TECHNOLOGY, HUBBALLI-580027

(Approved by AICTE, New Delhi and Affiliated to VTU, Belgaum)

Dr. P. S. Patil, M.Sc., Ph.D. Head, Dept. of Physics E-mail: <u>pspatilcrystal@gmail.com</u> Phone: (0836) 2232681 Fax: (0836) 2330688 Mobile: 9008979022

Date: 22-12-2021

LETTER OF COLLABORATION

To

Dr. Rajashekhar F Bhajantri Professor, Department of Studies in Physics Karnatak University, Pavate Nagar, Dharwad-580 003

Dear Dr. Rajashekhar Bhajantri,

The research group at Department of Engineering Physics, K.L.E Institute of Technology, Hubballi pleased to work together with your research group at Department of Studies in Physics, Karnatak University for the years 2019-20, 2020-21 and till date to investigate **Nonlinear Optical (NLO) properties** of thin films prepared by your Ph.D. research scholars. The department will provide necessary facilities to your students to carry out their Project/PhD work in our nonlinear optical laboratory.

Thanking you

Sincerely

Dr. P. S. Patil, M.Sc., Ph.D. Head, Department of Physics K.L.E. Institute of Technology, HUBBALLI-580 030.



Sub – Regional Science Centre, Karwar Department of Science and Technology, Govt. of Karnataka

Kaiga Nilaya, Kodibag, Karwar - 581 303



Telephone No: 08382 295540 En

Email: srsc.karwar@gmail.com Date: 10.6.2017

To, Dr. Shivakumar B. Haragi Assistant Professor Department of Marine Biology KUPG Centre, Karwar

Sir,

Sub: Request for Collaboration with Sub Regional Science Centre.

The Karnataka state Science and Technology department in collaboration with district administration Uttara Kannada has set up a Sub Regional Science Centre at Karwar, Karnataka. The main aim of the centre is to promote science and technology among students, teachers and civilians. Apart from this, the centre is also focusing on creating awareness about Oceans, Mangroves and depleting fishery resources. In this regard, I kindly request your collaboration with our centre to promote ocean science and sustainable environmental plans.

Thanking you.

Yours faithfully

Member Secretary Sub Regional Science Centre Karwar



GRASIM GR	SERVICE ORDER ORIGINAL PO Number : 8150004511 PO Date : 16.05.2018 ISO Doc No. :
Vendor Code : 2110000728 (Not Registered) M/S FISHERMAN'S GUIDANCE BUREAU UTTARA KANNADA	Your Ref. No. Offer mail dtd 16.5.18
KARWAR - 581301 Karnataka, India	
State Code : 29 Contact Person : Ph. No 9342700861 E-Mail ID - GSTIN :	Contact Person : Vivek Gunagi Phone : 08382-230174 E-Mail ID : vivek gunagi@adityabirla.com

Dear Sir,

We are pleased to place our order for the following material(s)/ service(s) subject to terms and conditions and instructions specified here and overleaf. Please address all Bills and correspondence mentioning our order No. & date to the HOD (Materials) Grasim Industries Limited/Chemical Division Karwar P.O Binaga - 581307, Karwar, Karnataka. Kindly mention our Item code & Purchase Order with applicable HSN/SAC Code on your Invoice.

SNo	Material/Service Code Code Description	HSN	SAC Code	Quantity UoM	Rate	Discount	Total Tax	Net Value
1	Plankton & Zooplanton Study			1.000 AU	50000.00 INR		0.00 %	50000.00
	11012964 - Plankton & Zooplankton	Study	2.00 NO	25000.00 INR				
	Collection of Plankton, Zooplankton different sites in Binaga bay, Karwal craft (boat). The first sampling site, discharge point in Binaga bay, (II) < located in Karwar and Arga bay res	and seawate r and Arga b (I) fixed at ou (>&<)> (III) r pectively	er samples from ay using mechar ir effluent eference points a	three hized are				
	Service Schedul Basic Price (Gross)	e			1.000	31.03.2019 50000.00		
Tota	I Value Excluding Taxes	ousand O	nlv.					50000.00
Pure	chase Order Terms and Cor	ditions						
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Con	signee Details							
GSTI	N : 29AAACG4464B3ZS sile - www.adityabirla.com					PAN No : AAA CIN No : L17	CG4464B 124MP1947PLC	000410

Remarks -Scope of work :

Collection of Plankton, Zooplankton and seawater samples from three different sites in Binaga bay, Karwar and Arga bay using mechanized craft (boat). The first sampling site, (I) fixed at our effluent discharge point in Binaga bay, (II) & (III) reference points are located in Karwar and Arga bay respectively. The plankton, zooplankton & seawater samples are to be collected and preserved in the field. Further, these samples are to be analysed in the laboratory by following standard methods of analysis. This study is to be conducted twice in a year. i. e. one during April/May 2018 and another during Sept/Oct.2018.

The study report is to be submitted to us in duplicate within two weeks time from the date of sampling.

Payment : 100% advance on receipt of intimation about collection of





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NO.1 Weigang, Nanjing 210095, Jiangsu Province P. R. China Tel: +86-25-84395754 Fax: +86-25-84396326 Email:ietc@njau.edu.cn Http://www.njau.edu.cn

NANJING AGRICULTURAL UNIVERSITY

Dr. Sudisha Jogaiah

Department of Biotechnology and Microbiology Karnatak University, Dharwad – 580 003 Karnataka State, India

April 25th, 2018

Dear Dr. Jogaiah,

With the establishment of our collaboration in fruit science and academy, I would like to invite you to visit Nanjing Agriculture University (NJAU), China for ten days (from 22nd to 31th May, 2018).

During your stay your presence will be highly appreciated as Molecular Biology expert in Viticulture for the discussion on the planned International Research Collaboration for establishment of Sino-Indo Grape Science and Technology Center under the One Route and One Belt concept. Also, I think we can have the following activities: i) Visit laboratories and talk with graduate students about research art in fruit crop genetics and breeding; ii) Discuss about the possibility to start some Sino-Israel fruit crop research center both for interesting research activities and graduate student training; iii) Visit Nanjing Agricultural University and some other fruit institutes and universities. This collaborative research project will be an initial step for creating long-term collaboration and mutually beneficial co-operation between our two universities

Your travel expenses and accommodations will be covered by Nanjing Agriculture University (NAU).

We look forward to seeing you in Nanjing.

Sincerely Yours,

Jinggui Fang, Professor, Ph.D. College of Horficulture Nanjing Agricultural University Cellular: +86-158 0516 2385 Email: fanggg@njau.edu.cn



UNIVERSIDADE ESTADUAL PAULISTA Institute of Science and Technology Department of Environmental Engineering

Sorocaba, February 15th, 2021.

To may whom it concerns

It is my pleasure to inform that I have a fruitful research cooperation with **Dr. Sudisha Jogaiah** (Karnatak University, India) since 2018 in development of project related to nanotechnology applied to agriculture in special with the topic of nanopesticides and nanofertilizers for sustainable crop improvement.

Please, if you need any additional information do not hesitate in contact me.

Sincerely,

Dr. Leonardo Fernandes Fraceto Associate Professor - UNESP/Sorocaba



Visvesvaraya National Institute of Technology

South Ambazari Road, Nagpur – 440 010 (INSTITUTE OF NATIONAL IMPORTANCE)

Dr. B.R. Sankapal Professor Department of Physics Former Assoc. Dean (Exam) E-mail: brsankapal@gmail.com Phone (off): +91-712-2801170

Web: <u>http://phy.vnit.ac.in/people/brsankapal/</u> 02.12.2019

To, Prof. Ravindra R. Kamble Department of Chemistry Karnatak University Dharwad

Dear Dr. Kamble,

This letter is to express my support for your research to analyze the Dye Sensitized Solar Cells for the previously unknown dyes synthesized at your university.

The focus of my responsibility is to fabricate the solar cells using either TiO_2/CdS nanowires as the semiconducting material and analyze the Incident Power Conversion Efficiency and the External Quantum Efficiency. I have been working for several years now with a specific focus on addressing the lacunae in organic photovoltaics and to improve the efficiency of solar cell device. Also, synthesizing novel organic dyes with required physical parameters is a very important starting point of our work as is the focus on obtaining the dyes of higher power conversion efficiency.

I have been struck by broad impact of your work through my involvement in the various conferences/workshops etc. In particular my collaboration with you so far has had an impact on the successful design of solar cells and the results of which will be communicated in near future for publication. I look forward for continuing our collaboration.

Truly Yours

Contopal

Prof. Babasaheb R. Sankapal (JSPS Fellow, Japan, Visiting Scientist: Germany, USA)



ವಲಯ ಅರಣ್ಯಾಧಿಕಾರಿ ಕಛೇರಿ ಕೋಸ್ಟಲ್ & ಮರೈನ್ ಇಕೋ ಸಿಸ್ಟಮ್ ಸೆಲ್, ಕಾರವಾರ. Email: rfocoastalmarinekarwar@gmail.com

Dr. Shivakumar Haragi, Assistant Professor, Department of Studies in Marine Biology, KUPG Centre Kodibag,Karwar.

Dear Sir,

Coastal and Marine Eco-system cell, Karwar, is a new wing established in Karnataka Forest Department on 19-02-2019 and started on 23-02-2021 to Conservation and Protection of Coastal & Marine eco-system. It's with extreme gratitude that the Karnataka University Post-graduation Centre of Marine Biology Karwar giving support on technical advice and assistance to us. And also, in collaboration with you it is possible to us to reach our Objectives.

Thank you Sir.

Date: 20-12-2021

Sincerely Eclaystem Cell Coastal & Karwar

"STUDY ON CORAL COMMUNITY STRUCTURE & ITS ASSOCIATED FISH FAUNA FROM THE ISLANDS OF CENTRAL WEST COAST OF INDIA"

The Thesis was submitted to

KARNATAK UNIVERSITY, DHARWAD

In partial fulfillment of requirement of the degree of

MASTERS OF SCIENCE

IN

MARINE BIOLOGY

By

PRANAY S. SAWANT

Under the guidance of

Dr. SHIVAKUMAR B HARAGI Asst. Professor

Dr. SREEKANTH G. B. Scientist, ICAR - CCARI, Goa

Dr. MANIKANDAN B. CSIR- National Institute of Oceanography. Dona Paula, Goa



DEPARTMENT OF STUDIES IN MARINE BIOLOGY KARNATAK UNIVERSITY POST GRADUATE CENTRE KODIBAG, KARWAR, KARNATAKA- 581303

2019

Reg.no:17S21008

KARNATAK



UNIVERSITY

DHARWAD

CERTIFICATE

This is to certify that the thesis entitled "STUDY ON CORAL COMMUNITY STRUCTURE & ITS ASSOCIATED FISH FAUNA FROM THE ISLANDS OF CENTRAL WEST COAST OF INDIA" submitted by MR. PRANAY S. SAWANT is in partial fulfillment of the course for the degree of Masters of Science in Marine Biology under the guidance of DR. SHIVAKUMAR B. HARAGI, Asst. Professor, Department of Marine Biology & Dr. SREEKANTH G. B. Scientist, ICAR - CCARI, Goa and Dr. MANIKANDAN B. CSIR- National Institute of Oceanography, Dona Paula, Goa.. This work is based on the observations and results of field studies carried out by her. The thesis is an original work done by the candidate under my supervision. The thesis or a part of thesis has not been previously submitted for any diploma or degree.

RESEARCH GUIDE Dr. Shivakumar B. Haragi

CHAIRMAN Dr. CHAIRMAN Department Of Studies in Marine Biology, K.U.P.G. Centre, Kodibag, KARWAR - 581303



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TRAINING CERTIFICATE

With the establishment of International collaboration in fruit science and academy together with Dr. Sudisha Jogaiah, Assistant Professor, PG Department of Biotechnology and Microbiology, Karnatak University, Dharwad, India, **Mr. SHIVAKANTKUMAR ADHIKARI** Ph.D. student of Dr. Jogaiah visited my Laboratory of Molecular Farming in Viticulture, College of Horticulture, Nanjing Agricultural University, China for a period of two months (7th May, 2019 to 05th July, 2019). During his two months stay at my laboratory, Mr. Shivakanthkumar Adhikari was trained in the field of Molecular Biology on the application of "MircoRNA mediated grapevine resistance to the Botrytis". The candidate was also given proper bench to learn physiological, biochemical and gene-expressional variations in grapevine under drought stress at my laboratory, Nanjing University, China.

July 5th, 2019

Best wishes

Jinggui Fang, Professor





南京農業大學 NANJING AGRICULTURAL UNIVERSITY

NO.1 Weigang, Nanjing 210095, Jiangsu Province P. R. China Tel: +86-25-84395754 Fax: +86-25-84396326 Email:ietc@njau.edu.cn Http://www.njau.edu.cn

Nanjing, March, 3rd, 2019

Mr. SHIVAKANTKUMAR ADHIKARI (Passport No. S9358012, Male) Department of Biotechnology and Microbiology Karnatak University, Dharwad – 580 003 Karnataka State, India Mobile No.: 00-91-9741485658

Dear Mr. S. ADHIKARI,

With the establishment of our collaboration in fruit science and academy with Dr. Sudisha Jogaiah, Project Leader, Laboratory of Plant Healthcare and Diagnostics, Department of Biotechnology and Microbiology, Karnatak University, Dharwad. I am pleased to invite you to join our research team 'Fruit Crop Genetics, Breeding and Genomics' in College of Horticulture, Nanjing Agricultural University as a visitor for three months. Your research project in which you will participate is called "MircoRNA mediated grapevine resistance to the Botrytis". I am really convinced that your participation is a route toward both self-enhancement and increasing the research collaboration between Nanjing Agricultural University, China and Karnatak University, India.

I am looking forward to welcome you in Nanjing.

Sincerely Yours,

Jinggui Fang, Professor, Ph.D.



College of Horticulture, Nanjing Agricultural University Cellular: +86-158 0516 2385 Email: <u>fangeg@njau.edu.en</u>



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Nanjing, March, 13th, 2019

Mr. MILAN VITHAL KAMBLE (Passport No. T1413874, Male) Department of Biotechnology and Microbiology Karnatak University, Dharwad – 580 003 Karnataka State, India Mobile No.: 00-91-7795961658

Dear Mr. M. V. KAMBLE,

With the establishment of our collaboration in fruit science and academy with Dr. Sudisha Jogaiah, Project Leader, Laboratory of Plant Healthcare and Diagnostics, Department of Biotechnology and Microbiology, Karnatak University, Dharwad. I am pleased to invite you to join our research team 'Fruit Crop Genetics, Breeding and Genomics' in College of Horticulture, Nanjing Agricultural University as a visitor for three months. Your research project in which you will participate is called "MircoRNA mediated grapevine resistance to the Botrytis". I am really convinced that your participation is a route toward both self-enhancement and increasing the research collaboration between Nanjing Agricultural University, China and Karnatak University, India.

I am looking forward to welcome you in Nanjing.

Sincerely Yours,

Jinggui Fang, Professor, Ph.D.



College of Horticulture, Nanjing Agricultural University Celhular: +86-158 0516 2385 Email: fangeg@njau.edu.en

/u/0/?pli=1#search/CMFRI/FMfcgxwKkHdxGJNgXWzRPMtmXJkDFjnJ aps 莊 Q X CMFRI ÷ ~ . 19 63 Ø. Cetacean budget D Inbox × S.R.Krupesh Sharma <krupeshsharma@gmail.com> @ Wed, Dec 30, 202 to me -Dear Shivakumar PL c d attached file. The budget was prepared to establish a cetacean stranding management and training centre. Best of Luck! Thanks Krupesh Dr. Krupesha Sharma S.R., M.V.Sc, Ph.D, ARS (Veterinary Pathology) **Principal Scientist** Marine Biotechnology Division **ICAR-Central Marine Fisheries Research Institute** (Indian Council of Agricultural Research) Ernakulam North PO Kochi-682018; Kerala, India Cell: 9449810746; E mail: krupeshsharma@gmail.com krupesh.sharma@icar.gov.in 片 33°C Sunny ^ D 0

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GRASIM GR	SERVICE ORDER ORIGINAL PO Number : 8150007176 PO Date : 29.10.2020 ISO Doc No. :
E-Mail ID - grasim.karwar@adityabiha.com Vendor Code : 2110000728 (Not Registered) M/S FISHERMAN'S GUIDANCE BUREAU UTTARA KANNADA	Ref. No.: Offer dtd 13.10.2020 Date :
KARWAR - 581301 Karnataka, India State Code : 29	Contact Person : Vivek Gunagi
Contact Person : Ph. No 9342700861 E-Mail ID - kupgcntrkarwar@gmail.com GSTIN :	E-Mail ID : vivek.gunagl@adityabirla.com

mal/goods/equipment etc. shall be strictly in accordance with the description, specifications and in full conformity with the Purchase Order and of

Dear Sir.

We are pleased to place our order for the following material(s)/ service(s) subject to terms and conditions and instructions specified here and overleaf. Please address all Bills and correspondence mentioning our order No. & date to the HOD (Materials) Grasim Industries Limited/Chemical Division Karwar P.O Binaga - 581307, Karwar, Karnataka. Kindly mention our Item code & Purchase Order with applicable HSN/SAC Code on your Invoice. Order with applicable HSN/SAC Code on your Invoice.

	Material/Service Code Code Description	HSN / SAC Code	Quantity UoM	Rate	Discount	Total Tax	Net Value
1	Detailled Nutrient Marine Blology study	998719	1.000 AU	350000.00 INR		0.00 %	350000.00
	11025588 - Detailed study on nutrient a in r	nalysis 1.00 GRO	350000.00 INR				
	Scope of work: During the recent years	frequent occurrence of a	Igal				
	blooms are reported in the Karwar and I	Binaga shore, therefore, i	l is				
	necessary to conduct a comprehensive	detailed study on hydrolo	gical,				
	biological and nutrient analysis in order	to comply the suggestion	s made				
	of Kamataka State Pollution Control Bos	ard. Proposed study will p	provide				
	Information regarding existing conditions	status prevailing in the					
	discharge and adjacent sites in the in se	3					
	Service Schedule			1.000	31.03.2021		
	Basic Price (Gross)				350000.00		
Tota	I Value Excluding Taxes						350000.00
		FIG. Th					
Amo	ount in Words: Rupees Three Lakh	Fiπy inousand Only					
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Amo Purc INCO Insu	bunt in Words: Rupees Three Lakh hase Order Terms and Condit D Terms : FOR - BINAGA,KA rance : Consigner oht	ons RWAR	7. D	Dispatch From	m Je		
Amo Purc INCO Insu Freig Payr Disp	bunt in Words: Rupees Three Lakh chase Order Terms and Condition O Terms : FOR - BINAGA,KA irance : Consigner ght ment Terms : Payment Terms as batch Through	ons RWAR mentioned in text	/- D	Dispatch From	m Je		
Amo Purc INCO Insu Freig Payr Disp	bunt in Words: Rupees Three Lakh chase Order Terms and Condition D Terms : FOR - BINAGA,KA irance : Consigner ght ment Terms : Payment Terms as batch Through signee Details	ons RWAR mentioned in text	,. D	Dispatch From	m Je		
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Remarks -The unit rates shall remain firm and fix till completion of work and no escalation shall be allowed on whatsoever ground

Scope of work: comprehensive detailed study on hydrological, biological and nutrient analysis in order to comply the suggestions made of Karnataka State Pollution Control Board. Proposed study will provide information regarding existing conditions/status prevailing in the discharge and adjacent sites in the sea.

Detailed study Nutrient analysis in correlation to Plankton studies along the Karwar Coast as per Planktons and Zooplanktons population studies in Binaga bay by Fisherman#s Guidance Bureau, Dept. of Studies in









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Spectroscopic investigations on the interaction of biologically active 4-aryloxymethyl coumarins with TiO₂ nanoparticles

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Keywords: Coumarin TiO₂ nanoparticles Fluorescence quenching Binding constant Electron transfer

ABSTRACT

The interaction of four biologically active 4-aryloxymethyl coumarin dyes 4-*p*-tolyloxymethyl-benzo[*h*]coumarin (4PTMBC), 1-(4-iodophenoxymethyl)-benzo[*f*]coumarin (1IPMBC), 4-(4-iodo-phenoxymethyl)-benzo[*h*]coumarin (4IPMBC) and 4-(4-iodo-phenoxymethyl)-6-methoxy coumarin (4IPMMC) with colloidal TiO₂ nanoparticles has been investigated using absorption, steady state and time resolved fluorescence. The size of TiO₂ nanoparticles has been found to be 50 nm from SEM measurements. The absorption spectral changes of dyes in the presence of TiO₂ nanoparticles suggest their possible interaction. The apparent association constants of the interaction are estimated using Benesi-Hildebrand model. Fluorescence quenching has been observed for all the dyes with the addition of colloidal TiO₂ nanoparticles and Stern-Volmer plots of fluorescence surements indicate the presence of static quenching mechanism. The binding constants and the number of binding sites have been estimated from fluorescence data. The role of electron transfer process in fluorescence quenching mechanism has been discussed.

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1. Introduction

Colloidal semiconductor nanoparticles have drawn considerable attention of researchers because of their excellent size dependent electronic and optical properties [1,2]. Among several semiconductor nanoparticles, titanium dioxide (TiO₂) nanoparticles are much investigated ones owing to their application in pharmaceuticals [3–5], carriers of photosensitizers like porphyrins [6] and treatment of cancer [7], catalysis, electrochromism and sensors [8]. Dye sensitized TiO₂ has been used effectively in photo electrochemical devices for producing electricity from visible light [9] and also in photo degradation contaminants in the visible region [10]. TiO₂ nanoparticles also find applications in medical field because of their photoreactivity [11]. It has been reported that TiO₂ nanoparticles interact with lactate dehydrogenase (LDH), superoxide dismutase (SOD) in vitro and caused DNA damage in vivo [12–16]. Further, interaction of TiO₂ nanoparticles with biomacromolecules namely lysozyme and albumins has been reported [17]. Such studies throw more light on interaction mechanisms between nanoscale materials and biomacromolecules which in turn helps in development of biotechnological applications.

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Coumarin molecules investigated in the present study are reported to be exhibiting excellent properties such as antimicrobial activity, long range coupling and centrosymmetric nature [18,19]. Lately, it has been reported that 4-aryloxymethyl coumarin 4-p-tolyloxymethylbenzo[h]coumarin (4PTMBC) exhibited good antibacterial and antifungal activities [20], whereas iodinated 4-aryloxymethyl coumarins 1-(4-iodo phenoxymethyl)-benzo[f]coumarin (1IPMBC), 4-(4iodo-phenoxymethyl)-benzo[h]coumarin (4IPMBC) and 4-(4-iodophenoxymethyl)-6-methoxy coumarin (4IPMMC) exhibited better anticancer and anti-mycobacterial activities [21]. The biological importance of compounds substituted with iodine has been well reported in literature such as binding ability and cannabinoid receptor antagonists [22]. Recently, we have reported the effect of pure solvents, solvent mixture and silver nanoparticles on absorption and fluorescence characteristics of these dyes [23–26]. It has been observed that they are sensitive to solvents, solvent mixture and their fluorescence is quenched by silver nanoparticles. The sensitivity of these molecules to solvents could be used in sensor applications. The biological activities exhibited by these coumarin molecules could be used in pharmaceutical field. Therefore owing to their excellent biological activities, studies on the interaction between TiO₂ nanoparticles and these coumarin dyes would help to explain the interactions between biomacromolecules and nanoparticles. Also, coumarin derivatives in general and investigated 4-aryloxymethyl coumarins in particular because of their excellent

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ORIGINAL ARTICLE



Solvent Effects on the Electronic Absorption and Fluorescence Spectra of HNP: Estimation of Ground and Excited State Dipole Moments

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Abstract We report the effect of solvents on absorption and fluorescence spectra of biologically active 3(2H)-pyridazinone namely 5-(2-hydroxy-naphthalen-1-yl)-2-phenyl-2Hpyridazin-3-one (HNP) in different solvents at room temperature. The ground and the excited state dipole moments of HNP molecule was estimated from Lippert's, Bakshiev's and Kawski-Chamma-Viallet's equations using the solvatochromic shift method. The ground state dipole moment (μ_g) was also estimated by Guggenheim and Higasi method using the dielectric constant and refractive index of solute at different concentrations, the μ_g value obtained from these two methods are comparable to the μ_g value obtained by the solvatochromic shift method. The excited state dipole moment (μ_e) is greater than the ground state dipole moment (μ_g) , which indicates that the excited state is more polar than the ground state. Further, we have evaluated the change in dipole moment ($\Delta \mu$) from the solvatochromic shift method and on the basis of molecularmicroscopic solvent polarity parameter (E_T^N) , later on the values were compared.

Keywords 3(2H)-pyridazinone · Solvatochromic shift method · Molecular-microscopic solvent polarity parameter · Guggenheim method · Higasi method

Introduction

The 3(2H)-pyridazinones are the pyridazine derivatives contain two adjacent nitrogen atoms at the 1 and 2 positions in a six-membered ring and a carbonyl group at the 3 position and they have different functionalities in their structure [1, 2]. A substantial number of pyridazinones in the recent past have been reported to possess antimicrobial, antitubercular, analgesic, anti-inflammatory, cyclooxygenase inhibitor, antidiabetic, antihypertensive, antiplatelet, anticancer, antifungal, antidepressant-anxiolytic, anticonvulsant, bronchodilatory (for asthma) and anti-allergic, antifeedant, inhibition of linolenic acid, activity for neurological disorders and many other properties. Some of the major pyridazinone derivatives which have appeared in a market are indolidan, bemoradan, pimobendan, levosimendan as antihypertensive, minaprine as antidepressant, emorfazone as anti-inflammatory and azanrinone as a cardiotonic [3].

Recently, spectroscopic and quantum chemical investigations on 3(2H)-pyridazinone derivatives such as levosimendan and bromopyrazone compounds have been reported in the literature [4, 5]. Furthermore, the detailed structural, conformational, spectroscopic, electronic and nonlinear optical properties of the 3(2H)-pyridazinone derivatives namely flufenpyr (used in agriculture as a herbicide) and amipizone (designed to be antithrombotics and an inhibitor for platelet aggregations and the cardiovascular system) compounds have been studied using B3LYP, B3PW91 and HSEH1PBE levels of theory with the 6-311G (d, p) basis set [6]. Soliman et.al reported the molecular structure, spectroscopic properties, NLO, HOMO–LUMO and NBO analyses of 6-hydroxy-3(2H)-pyridazinone [7].

The effect of solvents on the absorption and fluorescence properties of organic molecules has been a subject of several investigations [8–13]. These investigations have considerable

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Fluorescence quenching of DMB by aniline in benzene–acetonitrile mixture

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Keywords: Fluorescence quenching, sphere of action static quenching model, finite sink approximation model.

Abstract. The fluorescence quenching of coumarin dye namely 4-(2, 6-dibromo-4-methylphenoxymethyl)-benzo[h]chromen-2-one [DMB] has been studied by aniline, in a different solvent mixture of benzene (BN) and acetonitrile (AN) at room temperature. The quenching is found to be appreciable and shows positive deviation from linearity in the Stern-Volmer (S-V) plots for all the solvent mixtures. The various rate parameters responsible for fluorescence quenching have been determined using a sphere of action static quenching model and finite sink approximation model. The magnitudes of these rate parameters indicate that positive deviation in the S-V plot is due to both static and dynamic quenching processes.

1. Introduction

Derivatives of coumarin are well-known for their photochemical and photophysical properties, as well as for their interesting second-order nonlinearities [1]. They are extensively studied due to their widespread industrial use as dye lasers [2]. Now a day, there has been drive to synthesize coumarin-based organic dyes for use in high-efficiency dye-sensitized solar cells (DSCs) [3-4]. Coumarin and its derivatives have attracted significant interest in pharmaceutical research areas such as anti-inflammatory, hepatoprotective, antiviral, anticarcinogenic and anticoagulant activities [5-6].

The fluorescence quenching of organic molecules in solution by various quenchers like aniline, carbon tetrachloride, halides ions, ethyltriocarbonate, CdSe nanoparticles, oxygen etc has been studied by several investigators [7-12]. In all most all cases the experimental results follow the linear Stern-Volmer equation given by

$$\frac{I_0}{I} = 1 + K_{SV}[Q]$$
(1)

 $K_{SV}=k_q\tau_0$ called S-V constant. Where I₀, I, k_q , τ_0 and [Q] are the fluorescence intensities in the absence and presence of the quencher, bimolecular quenching rate parameter, lifetime of the excited solute molecule in the absence of quencher and quencher concentration respectively. But in few cases, it has been observed that the experimental results show positive deviation from a linear S-V relation [13-15]. This positive deviation was attribute to various processes like singlet to triplet excitation, static and dynamic quenching, the formation of charge transfer complexes both at the ground and excited states. Apart from this, the polarity of the solvent medium and the range of quencher concentration are also except to play a part in this mechanism.

In the present work, we have studied the steady state fluorescence quenching of the newly synthesised coumarin derivative DMB using aniline as a quencher in a different mixture of benzene and acetonitrile at room temperature. The various rate constants responsible for fluorescence quenching mechanisms have been estimated using a sphere of action static quenching model and a finite sink approximation model.





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Steady state absorption and fluorescence study: Estimation of ground and excited state dipole moments of newly synthesized pyridazin-3(2*H*)-one derivatives

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Highlights

- Pyridazin-3(2*H*)-one derivatives (HMP, BHP and CHP) were shows the solvatochromism.
- HMP and BHP molecules shows $\pi \to \pi^*$ transitions and CHP molecule shows $n \to \pi^*$ transition.
- The excited state dipole moment is greater than the ground state dipole moment.
- The ground and excited state dipole moments are parallel.
- The molecules show less sensitive to hydrogen bonding effect of solvents.

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Identification of mineral compositions in some *renal calculi* by FT Raman and IR spectral analysis



SPECTROCHIMICA ACTA

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ABSTRACT

We present in this paper accurate and reliable Raman and IR spectral identification of mineral constituents in nine samples of *renal calculi* (kidney stones) removed from patients suffering from nephrolithiasis. The identified mineral components include Calcium Oxalate Monohydrate (COM, whewellite), Calcium Oxalate Dihydrate (COD, weddellite), Magnesium Ammonium Phosphate Hexahydrate (MAPH, struvite), Calcium Hydrogen Phosphate Dihydrate (CHPD, brushite), Pentacalcium Hydroxy Triphosphate (PCHT, hydroxyapatite) and Uric Acid (UA). The identification is based on a satisfactory assignment of all the observed IR and Raman bands (3500–400 cm⁻¹) to chemical functional groups of mineral components in the samples, aided by spectral analysis of pure materials of COM, MAPH, CHPD and UA. It is found that the eight samples are composed of COM as the common component, the other mineral species as common components are: MAPH in five samples, PCHT in three samples, COD in three samples, UA in three samples and CHPD in two samples. One sample is wholly composed of UA as a single component; this inference is supported by the good agreement between ab initio density functional theoretical spectra and experimental spectral measurements of both sample and pure material. A combined application of Raman and IR techniques has shown that, where the IR is ambiguous, the Raman analysis can differentiate COD from COM and PCHT from MAPH.

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1. Introduction

Stone disease (Nephrolithiasis) in men and women is common health problem and the incidence is growing worldwide [1]. This disease most commonly affects 20-40 years age group resulting in significant morbidity and loss of work. There has been significant progress in the treatment of calculi over the last two to three decades and the estimated cost of treatment, for instance, is two billion dollars per year in the US [2,3]. With probably 5-7 million patients suffering in India too, the incidence is more prevalent over the upper western geographical region referred to as 'stone belt' though it is not uncommon in other regions [4]. Recurrence of stone is the biggest challenge in the management of patients suffering from Nephrolithiasis. It is estimated that 50% of the patients will experience recurrent stone disease within 10 years [5]. Knowing the type of stone helps in preventing the recurrence by modifying the diet and other risk factors. Hence it is an important determinant in management of stone disease. Various techniques of stone analysis are available ranging from the traditional wet chemical analysis to

* Corresponding author. *E-mail address:* jrtonannavar@kud.ac.in (J. Tonannavar). sophisticated techniques like FTIR, X-Ray diffraction, SEM, thermal analysis [6,7]. We discuss in the present paper Raman and FTIR spectroscopic analysis of nine kidney stones, identifying six different molecular mineral species distributed over the samples.

While the chemical wet method, TA and SEM provide information on chemical composition, all the other methods give mineralogical composition, and SEM and PM provide surface morphology as well. It must be pointed out that XRD and IR spectroscopy give complete information of mineralogical content compared to other methods. With its advantage of no sample preparation, the Raman technique is strongly complementary to IR and in some cases it can even be a substitute [8–11]. Fundamentally, both IR and Raman give the same information on the characteristic vibrational frequencies and structural aspects of chemical functional groups. IR radiation is absorbed by the vibrating chemical functional groups that make up a sample, producing characteristic absorption bands which facilitate identification of the functional groups. While Raman technique is based on the scattering of light radiation by the chemical functional groups and produces characteristic Raman bands which facilitate identification of the functional groups as in IR, it is more structure sensitive with the ability to differentiate spectral aspects [12].

In the present work, a batch of nine *renal calculi* (kidney stone samples) surgically removed from patients suffering from Nephrolithiasis

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Studies on Electrical and Magnetic Properties of Mg-Substituted Nickel Ferrites

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Abstract

The semiconducting polycrystalline ferrite materials with the general formula Ni_{1-x} Mg x Fe₂O₄ were synthesized by using the solid state reaction method. X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectrographs, and atomic force microscopy techniques were utilized to study the structural parameters. XRD confirms the formation of single phase cubic spinel structure of the ferrites. The crystallite sizes of ferrites determined using the Debye–Scherer formula ranges from 0.963 µm to 1.069 µm. The cation distribution of ferrite shows that Mg^{2+} ions occupy a tetrahedral site (A-site) and the Ni²⁺ ion occupy an octahedral site (B-site) whereas Fe^{3+} ions occupies an octahedral as well as a tetrahedral site. The study of elastic parameters such as the longitudinal modulus, rigidity modulus, Young's modulus, bulk modulus, and Debye temperature were estimated using the FTIR technique. The decrease of direct current (DC) resistivity with increase in temperature indicates the semiconducting nature of ferrites. The dielectric constant as well as loss tangent decreases with increase in frequency, and at still higher frequencies, they are almost constant. This shows usual dielectric dispersion behavior attributed to the Maxwell-Wagner type of interfacial polarization and is in accordance with Koop's phenomenological theory. The linear increase of alternating current conductivity with increase of frequency shows the small polaron hopping type of conduction mechanism in all the ferrites. The magnetic properties such as saturation magnetization (M_s) , magnetic moment, coercivity, remnant magnetization (M_r) , and the ratio of M_r/M_s was estimated using the M–H loop.



Research Article

Thermal and Dielectric Behavior Studies of Poly(Arylene Ether Sulfone)s with Sulfonated and Phosphonated Pendants

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The present paper discusses the aspects of the synthesizing valeric acid based poly(ether sulfone)s with active carboxylic acid pendants (VALPSU) from solution polymerization technique via nucleophilic displacement polycondensation reaction among 4,4'-dichlorodiphenyl sulfone (DCDPS) and 4,4'-bis(4-hydroxyphenyl) valeric acid (BHPA). The conditions necessary to synthesize and purify the polymer were investigated in some detail. The synthesized poly(ether sulfone)s comprise sulfone and ether linkages in addition to reactive carboxylic acid functionality; these active carboxylic acid functional groups were exploited to hold the phenyl sulphonic acid and phenyl phosphonic acid pendants. The phenyl sulphonic acid pendants in VALPSU were easily constructed by altering active carboxylic acid moieties by sulfanilic acid using N,N'-dicyclohexylcarbodiimide (DCC) mediated mild synthetic route, whereas the latter one was built in two steps. Initially, polyphosphoric acid condensation with VALPSU by 4-bromoaniline and next straightforward palladium catalyzed synthetic route, in both of which acidic pendants are clenched by polymer backbone via amide linkage. Without impairing the primary polymeric backbone modified polymers were prepared by varying the stoichiometric ratios of respective combinations. All the polymers were physicochemically characterized and pressed into tablets; electrical contacts were established to study the dielectric properties. Finally, the influence of the acidic pendants on the dielectric properties was examined.

1. Introduction

Ionomers aim to control the dielectric properties in supramolecular assemblies [1–6]. Many attempts were noticed recently to synthesize ions containing polymers hanging to the macromolecular systems via amide linkages [7, 8], with expected dielectric properties owing to the flexibility of molecular chemistry and the subtleties of supramolecular interactions [9–11]. Several challenges were overcome recently, such as aromatic poly(ether ketone)s with pendant sulfonic acid phenyl groups [12], synthesis of highly sulfonated poly(arylene ether sulfone) random (statistical) copolymers via direct polymerization [13], comb-shaped poly(arylene ether sulfone)s [14], and phosphonic acid containing poly-(arylene ether)s [15]; mild and effective protocols to modify the polymer chains at room temperature opened new prospects as well [16]. The covalent linkages of these different classes of molecules to a single linear polymer chain can produce reactive and functional polymeric systems [17–19] with different physical properties and functions.

Aromatic poly(ether sulfone)s have been paid much attention as high performance polymers and they have been widely used [20, 21] by developing new types of bisphenol monomers [22], with sulfonic and phosphonic acid pendants

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Research paper

Measurement of the radiative L₃-M vacancy transfer probabilities of some 4f elements and compounds using Indus-2 synchrotron radiation

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1. Introduction

It is well known that in radiative process, the accurate values of L shell fluorescence parameters are needed to check the validity of theoretical models used in X-ray emission spectroscopy. It is interesting to study the L shell X-ray fluorescence parameters as the L shell consists of three subshells namely L₁, L₂ and L₃ which have different binding energies and total angular momenta. The primary vacancies created in this L subshell may be filled not only by radiative process but also non-radiative. Whereas the contribution of non-radiative process may be weak, it must be taken into account while determining the L subshell parameters. The L shell fluorescence parameters of some medium and high Z elements and their compounds have been determined by many researchers using proton beam, gamma radiation as well as synchrotron radiations [1–18]. From the survey of literature we notice that the measured L shell fluorescence parameters are strongly influenced by various chemical environments such as oxidation state, electronegativity, crystal structure and chemical bonding. Bonzi [1] has measured radiative vacancy transfer probabilities from the L₃ to M and to N shells for W, Re and Pb using synchrotron radiation. Porikli [10] has measured FWHM as well as intensity ratios of L X-ray photons of La, Ce, Pr elemental and compound targets using 59.5 keV gamma rays from ²⁴¹Am. They have observed the

ABSTRACT

The L X-ray intensity ratios $(I_{L\alpha}/I_{Li}, I_{L\alpha}/I_{Lp}, I_{L\alpha}/I_{Lp})$ and the radiative L₃-M vacancy transfer probabilities (η_{L3-M}) of some 4f elements such as Gd, Tb, Ho and compounds; Pr₂O₃, Pr₂(CO₃)₃·8H₂O, Nd₂O₃, Sm₂O₃, Sm₂(CO₃)₃·2.85H₂O, Sm₂(SO₄)₃·8H₂O, Gd₂(CO₃)₃, Tb₂O₃, Dy₂(SO₄)₃. Ho₂O₃ and HoF₃ have been measured using Indus-2 synchrotron radiation. The elements and compounds are excited by synchrotron radiation and the emitted characteristic L X-ray photons are measured with high resolution silicon drift detector. The measured intensity ratios of compounds are not influenced by the chemical environment. However, the η_{L3-M} values of compound targets indicate the effect of crystal structure.

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correlation between observed spectral features with oxidation state and molecular symmetry. Durdu and Kucukonder [11] have measured L X-ray fluorescence cross-sections, intensity ratios and fluorescence parameters of Sm and Eu in halogen compounds by exciting the target with 59.54 keV gamma radiations. From their experimental results they have concluded that the above parameters depend on the quantity of unpaired 4f electrons in the atom. Kumar and Puri [12] have measured LX-ray intensity ratios of some compounds of Dy by creating L shell vacancy with 22.6 keV and 59.4 keV gamma photons to understand the chemical environment on intensity ratios and also dependence of intensity ratios on excitation energy. Turhan et al. [13] have measured LX-ray fluorescence parameters of Ho, Lu, W, Hg and Bi using EDXRF technique. They have determined L X-ray fluorescence cross-sections, L sub-shell fluorescence yields and level widths and radiative vacancy transfer probabilities of L sub-shells to M_i, N_i and O_i sub-shells. The obtained results are in good agreement with theoretical and other experimental values. Recently, Aylikci et al. [15] have determined empirical and semi-empirical interpolated L X-ray fluorescence parameters for elements in the atomic range $50 \le Z \le 92$ by exciting the targets with gamma photons from ⁵⁵Fe and ²⁴¹Am radioactive source. Wang et al. [16] have measured the L X-ray intensity ratios of Ta, W, Au and Pb by 13.1 keV bremsstrahlung radiations. They have observed good agreement between theory and experimental values. But the L₃ subshell ionization cross-section of Ta and W are increased with the variation of excitation energy from 59.5 keV to 13.1 keV. Krishnananda et al. [18] have shown that the







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Gamma-ray and neutron shielding efficiency of Pb-free gadolinium-based glasses

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Abstract The radiation shielding efficiency of material depends upon photon attenuation, exposure buildup factors and neutron removal capacity. A newly developed Pb-free gadolinium-based glasses in compositions (80-x) B_2O_3 - $10SiO_2 - 10CaO - xGd_2O_3$ (where x = 15, 20, 25, 30 and 35 mol%) had completely been investigated for their shielding efficiency with Geant4 simulation for mass attenuation coefficients and neutron total macroscopic cross section and by calculating exposure buildup factors. The exposure buildup factors for photon energy from 0.015 to 15 MeV had been calculated up to 40 mean free paths using five factors geometric progression method. The mass attenuation coefficients of the Pb-free glasses were simulated for energies from 223 to 2614 keV and compared with the possible available experimental results. The neutron shielding efficiency of these glasses was discussed by calculating neutron total macroscopic cross section for

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energies from 1 eV to 14.1 MeV. Present investigations are found to be very useful for applications in nuclear engineering.

Keywords Gadolinium · Neutron · Glass · Buildup factor · Geant4 simulation

1 Introduction

Radiation protection in nuclear installations has prime importance for personnel safety from the ionizing radiation. Shielding of radiation source to control radiation exposure is the area of radiological safety engineering in nuclear technology, which is considered and implemented during reactor design. Therefore, choice of appropriate radiation shielding is extremely crucial to fulfill the requirements of exposure control. Nowadays, radiation is associated with our life in power production, industries, agriculture, medical, petroleum, research work, etc. Initially lead (Pb) was considered as the best available radiation shielding materials for gamma-rays while low-Z materials (water, boron, lithium, hydrogenous, etc.) are commonly applied for neutron shielding. A common shielding material for both gamma-ray and neutron is mixture of low- and high-Z elements and are being used in nuclear reactors for core shielding. Transparent window (viewing window) in nuclear installations is required for visual inspection of high radiation components or equipment prepared using Pb and Pb-equivalent shielding materials. However, Pb has been found to be very hazardous material which required immediate attention. Over the past few years, there have been great deals of expressed concern about the toxicity of the Pb and reduction in the

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ಪ್ರಾಧ್ಯಾಪಕರು



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Date: 22-12-2021

To Whom So ever It may Concern

This is to certify that Prof. Rajashekar Bhajentri, Department of Physics, Karnataka University, Dharwad had research collaboration with us since from 2014-15 to 2021-22 in terms of exchange the research facilities available both sides, as a Co-Principal Investigator in research projects, and other possible extended support from each side.

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Ionic conductivity and free volume related microstructural properties of LiClO₄/PVA/NaAlg polymer composites: Positron annihilation spectroscopic studies



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Keywords: Poly(vinyl alcohol) Sodium Alginate Positronium Free Volume Conductivity Mechanical properties

ABSTRACT

Poly(vinyl alcohol) (PVA)/sodium alginate (NaAlg) polymer composites were prepared by doping with lithium perchlorate salt (LiClO₄) using solution casting method. The miscibility, crystallinity, conductivity, thermal behavior, mechanical strength and free volume properties have been examined. The FTIR results reveal that the dopant (Li⁺) ions interact strongly with polymer chains through hydrogen bonding. X-ray diffraction patterns show a variation in the degree of crystallinity with increase in LiClO₄ concentration. The dc conductivity increases with addition of LiClO₄ salt concentration at room temperature and is attributed to increase in the number of mobile charge carriers (Li⁺ and ClO₄⁻) and degree of dissociation of salt in the composites. The variations in the mechanical properties are observed upon doping. The differential scanning calorimetric (DSC) study shows a single glass transition temperature (T_g) and reveals the compatibility and variation in the decomposition temperature (T_d). Thermogravimetric analyses (TGA) shows a decrease in the decomposition temperature with addition of lithium salt concentration. The positron annihilation lifetime spectroscopy (PALS) and Doppler broadening measurements were carried out for all the samples in terms of positron annihilation and positronium formation. The *S*-parameter shows a similar behavior as that of the o-Ps lifetime and o-Ps intensity. The correlation between carrier concentration and ionic conductivity with Ps formation was observed in this particular system. The conductivity versus temperature plot was found to follow an Arrhenius nature.

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1. Introduction

The synthetic and biodegradable polymers are major portion in investigations, as they have gained much attention due to non-environmental friendly effects [1–2]. The combinations of synthetic, biodegradable natural polymer composites have been studied significantly [3]. They have many applications in electrochemical devices such as supercapacitors, fuel cells, and solar cells when an appropriate salt dissolved in such polymer matrix to form a suitable composite [4–5]. Recently many researchers reported that the ionic conduction usually appears in amorphous phase of the polymeric material [1–6].

The ionic dissociation and transport phenomena in doped polymer blends are also understood based on the mechanism of the charge transport in the amorphous portion of the composites. This is mainly due to the fact that the conductivity depends on the macromolecular chain

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dynamics and the degree of ion aggregation. Most of the studies in this field are devoted to Poly (ethylene oxide) (PEO) and poly (propylene oxide) (PPO) based polymer electrolytes using alkali metal salts [3– 5]. In recent years, blending of polymers is one of the simple and low cost methods of developing new material with improved properties for the desired application. In polymer blends, the miscibility is the indication of the specific interaction between polymer segments, particularly for improving mechanical properties [6].

Poly (vinyl alcohol) (PVA) is a semicrystalline polymer studied extensively due to its many interesting physical properties, which are mainly arise from the presence of —OH groups and the hydrogen bonding formation and another polymer Sodium Alginate (NaAlg) is one of the polysaccharides extracted from seaweed, found to have an excellent performance as a membrane material for pervaporation and can be used as electrolyte material. In many cases, the microstructural properties of natural polymers do not fit for specific applications due to their weak mechanical properties. To overcome this problem, the blending of natural polymers with synthetic polymer like PVA has been focused [7–9]. Hindaws Publishing Corporation International Journal of Medicinal Chemistry Volume 2016, Article ID 9890630, 18 pages http://dx.doi.org/10.1155/2016/9890630



Research Article

Design and Microwave Assisted Synthesis of Coumarin Derivatives as PDE Inhibitors

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Commarins appended to benzimidazole through privatele are designed and synthesized using intervorave irradiation. These compounds were analyzed for phosphodiesterase (PDE) inhibition indirectly by motility pattern in human spermatozoa. Some of the synthesized compounds, namely, 5d, 5e, 5f, 5g, 5h, and 5k, have exhibited potent inhibitory activity on PDE.

1. Introduction

The development of simple, mild, practicable, cheap ecobenign method for the synthesis of heterocycles has grabbed the attention of researchers. In particular, microwave assisted organic synthesis has become a rapidly growing field in organic chemistry as this technique makes reaction time shorter and tolerates wide range reactions which are best suited to the increased demands of industry [1] and some of the synthesized compounds were screened by PDE.

PDE inhibitors are therapeutic agents which target PDE isoenzymes and inhibit the catabolism of the secondary messengers such as cyclic adenosine monophosphate (cAMP) and cyclic guanosine monophosphate (cGMP), thus prolonging the biological effect determined by the type of cell invivied. Cyclic nucleotide phosphodiesterases (PDEs) catalyze the hydrolysis of cAMP and/or cGMP. They function in conjunction with *adenylyl* and *guareylyl* cyclaser to regulate the amplitude and duration of cell signaling mechanisms mediated via cAMP and cGMP. They therefore serve to regulate a range of biological responses to first messengers such as light vascular resistance, cardiac output, visceral motility. immune response [2], inflammation [3], neuroplasticity, vision [4], and reproduction [5]. Phisphodiesterases (PDEs) modulate the activity of cyclic nucleotides by regulating their degradation. PDEs are critical determinants for modulation of cellular levels of cAMP and/or cGMP by many stimuli [6]. Thus, the ubiquitously present PDEs play a pivotal role in regulating cell signaling the breakdown of cAMP and cGMP.

The fold selectivity for PDE5 over PDE11A4 for Sildenafil (1000-fold selectivity) and Vardenafil (9000-fold selectivity) reveals that these drugs are very unlikely to cross-react with PDE11A4 in patients treated with these medications. On the contrary, it was suggested to use the newest PDE5 inhibitor Tadalafil with caution. In fact, the 40-fold selectivity ratio of Tadalafil for PDE5 over PDE11A4 is significantly lower than those reported with the other two drugs and is nearly the same as that reported for Sildenafil over PDE1 (41-fold). In this case, it has been suggested that the 41-fold selectivity of Sildenafil for PDE5 over PDE1 may induce vasodilatation, fushing, and tachycardia. Within human PDE11A family, the alternative splicing leads to generation of proteins which display unique properties [7, 8]. Received: 06 December 2015,

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Spectroscopic investigation of water-soluble alloyed QDs with bovine serum albumin

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ABSTRACT: We present here a systematic investigation on the interaction between a water-soluble alloyed semiconductor quantum dot and bovine serum albumin using various spectroscopic techniques i.e. fluorescence quenching, resonance light scattering and synchronous fluorescence spectroscopy. The analysis of fluorescence spectrum and fluorescence intensity indicates that the intrinsic fluorescence of bovine serum albumin (BSA) gets quenched by both static and dynamic quenching mechanism. The Stern-Volmer quenching constants, energy transfer efficiency parameters, binding parameters and corresponding thermodynamic parameters (ΔH^0 , ΔS^0 and ΔG^0) have been evaluated by using van 't Hoff equation at different temperatures. A positive entropy change with a positive enthalpy change was observed suggesting that the binding process was an entropy-driven, endothermic process associated with the hydrophobic effect. The intermolecular distance (r) between donor (BSA) and acceptor (CdSeS/ZnS quantum dots) was estimated according to Förster's theory of non-radiative energy transfer. The synchronous fluorescence spectra revealed a blue shift in the emission maxima of tryptophan which is indicative of increasing hydrophobicity. Negative ΔG^0 values implied that the binding process was spontaneous. It was found that hydrophobic forces played a role in the quenching process. Copyright © 2016 John Wiley & Sons, Ltd.

Keywords: QDs; bovine serum albumin; synchronous fluorescence scan; resonance light scattering; fluorescence quenching; FRET

Introduction

Nanotechnology, an extremely powerful emerging technology, is expected to have a substantial impact on the field of pharmaceutical and medical diagnostics. As such there is an enhanced interest in the studies on interaction between nanomaterials and biomolecules such as proteins (1–7). Nanomaterials can influence the structural and functional properties of proteins and as such there is increasing interest to understand the effects of various nanomaterials on their interaction with biomolecules.

Bovine serum albumin (BSA) is one of the most studied proteins and makes up a high percentage of the total plasma proteins. Serum albumin is the most abundant protein in blood plasma and its major physiological role is to carry various ligands to their respective target organs (8,9). These proteins manage transportation of drug and nutrition throughout the human body (10). They maintain the pH of blood and greatly contribute to maintaining colloidal osmotic pressure (11). Therefore, binding of ligands to serum albumin is an important determinant of their distribution and fate in the body (12). BSA has been considered as a model protein due to its water-soluble nature, which is important for interaction with nanoparticles. Albumins also possess catalytic activity for a broad range of organic molecules such as esters, amides, phosphates, etc. BSA contains 582 amino-acid residues with a molecular weight of 66 kDa. It has two tryptophan moieties at positions 134 and 212 as well as tyrosine and phenylalanine, while the intrinsic fluorescence of BSA is due to aromatic amino-acid residues (13,14).

Nanoparticle (NP) probes act as biosensors and have extensive applications. Generally, three types of NPs are used in biochemical analysis: gold nanoparticles (15), silica nanoparticles (16) and luminescent quantum dots (QDs) (17,18). Depending on the size and shape of NPs/QDs, one can broadly assign three distinct kinds of molecular interactions between NP/QD surfaces and proteins, namely electrostatic, hydrophobic and hydrogen bond interactions. The above probes have been applied to ultrasensitive detection of proteins, DNA sequencing, clinical diagnostics, etc. Absorption spectroscopy and fluorescence spectroscopy are the most powerful techniques to investigate the interaction between nanoparticles and biological molecules.

Semiconductor QDs have emerged as better and preferred candidates for optoelectronic and biomedical applications compared with organic dyes (19–21). They have unique spectral properties such as size-dependent tunable photoluminescence (PL) with broad excitation spectra and narrow emission bandwidths, which allow simultaneous excitation of particles of different sizes at a single wavelength. In addition, their high

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Abbreviations: BSA, bovine serum albumin; FRET, fluorescence resonance energy transfer; QD, quantum dots; RET, resonance energy transfer; RLS, resonance light scattering; SFS, synchronous fluorescence spectra; SV, Stern-Volmer; TCSPC, time correlated single photon counting; UV, ultraviolet



Journal of Luminescence Volume 190, October 2017, Pages 161-170

Time-resolved fluorescence and absence of Förster resonance energy transfer in ferroelectric liquid crystal-quantum dots composites

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Abstract

The present article deals with the interaction of octadecylamine (ODA) capped <u>cadmium selenide</u> <u>quantum dots</u> (CdSe QDs) and two <u>ferroelectric liquid crystals</u> (FLCs) having different values of spontaneous polarization (Ps). The pristine FLCs and FLC-QDs composites have been investigated by using steady-state and time-resolved fluorescence spectroscopic techniques. Stokes shift and the preferred alignment of FLC molecules in the presence of QDs are found to depend on the secondary order parameter of FLCs (i.e. Ps). The secondary <u>fluorescence emissions</u> have been strongly influenced by the concentration of QDs. The Förster <u>resonance energy</u> <u>Transfer</u> (FRET) was absent in both the composites. This article discloses the role of various factors, like relative orientation, <u>dipolar interaction</u> between donor and acceptor and the proximity of QDs (>10 nm), which might be responsible for the absence of FRET. FLC-QDs composites do not form a new class of <u>luminescent material</u> though the fluorescence properties of host FLCs are tailored in the presence of QDs by means of the change in <u>molecular alignment</u>. The change in lifetimes of FLC-QDs composites has not been observed.

Graphical abstract

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Estimation of ground and excited state dipole moment of laser dyes C504T and C521T using solvatochromic shifts of absorption and fluorescence spectra



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1. Introduction

Coumarin is a member of benzopyrone family of compounds, which consist of a benzene ring joined to a pyrone ring. Coumarins are well known laser dyes in the blue-green spectral region and they establish a family of dyes, which are applicable in physics, chemistry, biology and medicine [1–7]. The strong solvent dependence of various substituted coumarins was exploited for photo initiators, probes, photosensitizing agents in the biological study and photodimerization in polar and non-polar solvents in chemistry [8]. Coumarins are also widely used as fluorescent indicators [9], sunburn preventives [10], for estimation of enzymes, [11] etc.

The study of effect of solvents on absorption and fluorescence characteristics of organic compounds has been a subject of interesting investigations, since, the physical and chemical processes are influenced by the properties of solvents in which they carried out [12,13]. It is observed that the spectral shift such as blue shift or red shift occurs due to effects of various solvents with polar or non-polar nature [14–16], at different temperature [17,18] and at different pH values [19]. Also, the fluorescence characteristics can be altered by the substitution at various positions in the parent coumarin molecule. From the literature survey, we noticed that the substituted coumarins have electron donating and withdrawing groups attached at different positions and these substituents alter their spectral shifts in various solvents [20–23]. In general, electron donating

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ABSTRACT

The absorption and fluorescence spectra of laser dyes: coumarin 504T (C504T) and coumarin 521T (C521T) have been recorded at room temperature in a series of non-polar and polar solvents. The spectra of these dyes showed bathochromic shift with increasing in solvent polarity indicating the involvement of $\pi \rightarrow \pi^*$ transition. Kamlet– Taft and Catalan solvent parameters were used to analyze the effect of solvents on C504T and C521T molecules. The study reveals that both general solute–solvent interactions and specific interactions are operative in these two systems. The ground state dipole moment was estimated using Guggenheim's method and also by quantum mechanical calculations. The solvatochromic data were used to determine the excited state dipole moment (μ_e). It is observed that dipole moment value of excited state (μ_e) is higher than that of the ground state in both the laser dyes indicating that these dyes are more polar in nature in the excited state than in the ground state. © 2015 Elsevier B.V. All rights reserved.

> substituent tends to enhance the fluorescence intensity while electron withdrawing substituents tend to diminish it. These spectral changes impart a substantial alteration of the optical properties of the solute, for example, change in degree of polarization, quantum yield, excited state lifetime, excited state dipole moment, etc.

> One of the important physical parameters of any organic molecules, which describe the distribution of electrons around them is quantitatively known as dipole moment. In the ground and excited state, the dipole moments are different due to change in electron density in these states. The ground state (μ_g) and excited (μ_e) state dipole moments of organic (dyes) molecules reveal information on electronic and geometrical structure of the molecule in the excited state. A prior knowledge of the dipole moment of electronically excited species is often useful in the design of non-linear optical materials and elucidation of the nature of the excited state as well as the course of any photochemical transformation [24].

Several methods are used to determine the dipole moment of the singlet excited state, namely electronic polarization of fluorescence [25], electric dichroism [26], microwave conductivity [27] and Stark splitting [28,29]. Solvatochromism is the simplified and popular method, employed to determine the excited state dipole moment. Because, it shows a linear correlation between the wave number of the absorption and fluorescence maxima with solvent polarity functions $f(\varepsilon,n)$. Therefore, this method is informative and proves fruitful in studying the excited state behavior of the molecules [30–36]. As a part of our research on laser dyes, in the present paper, we have studied the effect of solvent polarity on absorption and fluorescence characteristics of two coumarin laser dyes: C504T and C521T and estimated the ground and



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This is to certify that the research group headed by Dr. Rajashekhar F Bhajantri, Professor, Department of Physics, Karnatak University Dharwad has carried out collaborative research work on Polymer Nanocomposites for the years 2014-15 till date with our research group at Department of Chemistry, Mangalore University, Mangalagangotri. Presently we are working on synthesis of nanoparticles and studies on polymer nanocomposites for energy storage devices.

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TO WHOM SO EVER IT MAY CONCERN

I hereby inform you that I have research collaboration in the field of **Positron annihilation** and **Dielectric Studies of polymer nanocomposites** with **Prof. Rajashekhar F Bhajantri**, **Department of Studies in Physics, Karnatak University, Dharwad** from 2014 till date.

23/12/21 Dr. H. B. Ravikumar Associate Professor Department of Physics Managemootri, University of Mysone Mysors - 570 006



Date: 24-12-2021 Place: Mangalore

TO WHOMSOEVER IT MAY CONCERN

This is to certify that the research group headed by Dr. Rajashekhar F Bhajantri, Professor, Department of Physics, K.U. Dharwad has carried out collaborative research work with our research group on synthesis of nanoparticles and studies on polymer nanocomposites for energy storage devices for the years 2014-15, 2015-16 and till date.

With Regards

Dr Vincent Crasta Dean – Academic Affairs Professor – Department of Physics <u>vincentc@sjec.ac.in</u>

ORIGINAL ARTICLE



Photophysical Properties of a Novel and Biologically Active 3(2H)-Pyridazinone Derivative Using Solvatochromic Approach

Vani R. Desai¹ · Shirajahammad M. Hunagund¹ · Malatesh S. Pujar¹ · Mahantesha Basanagouda² · Jagadish S. Kadadevarmath¹ · Ashok H. Sidarai¹

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Abstract Herein, we report photophysical properties of a novel and biologically active 3(2H)-pyridazinone derivative 5-(4-chloro-2-hydoxy-phenyl)-2-phenyl-2H-pyridazin-3-one [CHP] molecule using solvatochromic approaches. Absorption and fluorescence spectra of CHP molecule have been measured at room temperature in various solvents of different polarities. From this, it is observed that the positions, intensities and shapes of the absorption and emission bands are usually modified. Experimentally, the ground and excited state dipole moments are estimated using solvatochromic shift method which involves Lippert's, Bakshiev's and Kawski-Chamma-Viallet's equations. Theoretically, the ground state dipole moment was estimated using the Gaussian-09 program. The value of ground state dipole moment estimated using experimental and theoretical methods are well correlated. This inference that the molecular geometry is taken for CHP molecule under theoretical and experimental methods are similar. Further, we observed that the excited state dipole moment (μ_e) is greater than the ground state dipole moment (μ_o) which indicates that the excited state is more polar than the ground state. Furthermore, we have estimated an angle between the ground and excited state dipole moments. In addition, we have estimated the fluorescence quantum yield of CHP molecule using Rhodamine B as a standard reference in different solvents.

Keywords 3(2H)-pyridazinone · Dipole moment · Fluorescence quantum yield · Gaussian-09 program · Solvatochromic approach · Stoke's shift

Introduction

The 3(2H)-pyridazinones are the pyridazine derivatives contain two adjacent nitrogen atoms at the one and second positions in a six-membered ring and a carbonyl group at the third position and they have different functionalities in their structure [1, 2]. These derivatives generally exhibit broad spectrum showing biological activities such as anticancer, antimicrobial, analgesic, anti-inflammatory, antituberculosis, antipyretic, antiplatelet, adrenoreceptor antagonist, antidiabetic, COX inhibitors and acetylcholinesterase activities [3]. They are also known as weedicidal and muticidal agents [4].

Excitation of a molecule by photon causes a redistribution of charges leading to conformational changes in the excited state. This can result in increase or decrease of the dipole moment of the excited state as compared to the ground state. The dipole moment of an electronically excited state of a molecule is an important property that provides information on the electronic and geometrical structures of the molecule in the short-lived state. Knowledge of the excited state dipole moment of electronically excited molecules is quite useful in designing nonlinear optical materials [5]. A number of techniques e.g. electronic polarization of fluorescence, electricdichroism and microwave conductivity [6-8] were available for estimation of excited-state dipole moment, but their use is limited because they are considered equipment sensitive and studies have been related to very simple molecules. As the solvatochromic method does not use any external field, it is experimentally much simpler and widely accepted. The solvatochromic method is based on the shift of absorption

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ORIGINAL ARTICLE

Study of Photophysical Properties on Newly Synthesized Coumarin Derivatives

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Abstract Herein, we have studied the photophysical properties for three newly synthesized coumarin derivatives; 4-((2,6-dibromo-4-methylphenoxy)methyl)-2H-benzo[h] chromen-2-one (DMB), 4-((3,4-dihydro-6,7-dimethoxyisoquinolin-1-yl)methyl)-6-methyl-2H-chromen-2-one (DIM) and 4-((p-tolyloxy)methyl)-6-methoxy-2H-chromen-2-one (TMC). The absorption and emission spectra for above said molecules were recorded in different solvents at room temperature in order to calculate their ground and excited state dipole moments. The ground (μ_{q}) and excited state dipole (μ_{a}) moments of these coumarin derivatives were calculated using Lippert's, Bakshiev's and Kawski-Chamma-Viallet's equations by the solvatochromic shift method, which involves a variation of Stokes shift with the solvent dielectric constant and refractive index. Ground state dipole moments (μ_{q}) were also calculated from the Guggenheim method using the dielectric constant and refractive index of the solute molecule. The value of ground state dipole moment obtained from these two methods is well correlated. Further, it is notified that the excited state dipole moment is larger than the ground state dipole moment for all three solute molecules. It inferred that the excited state for above said molecules is more polar than the ground state. The present investigations may shine in the design of nonlinear optical materials.

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² P. G. Department of Studies in Chemistry, K. L. E. Society's P. C. Jabin Science College, Hubli 580031, Karnataka, India **Keywords** Coumarin · Dipole moment · Electronic absorption spectra · Fluorescence spectra · Guggenheim method · Solvatochromic shift method

Introduction

Coumarin derivatives and analogues are well-known for their photochemical and photophysical properties as well as for their interesting second-order nonlinearities [1-6]. In addition, the coumarin unit is known to undergo a reversible photo-induced cyclodimerization by irradiation at λ > 300 nm that leads to stable cyclobutane based dimers, whereas the reverse photocleavage reaction occurs at shorter wavelengths ($\lambda < 280$ nm) [7–9]. Coumarin-derived Cu (II)selective fluorescent sensor and studied the fluorescence quenching mechanism by femtosecond time-resolved fluorescence (TRF) spectroscopy and quantum calculations [10]. Coumarin derivatives studied to their widespread industrial use as dye lasers [11]. In recent years, there has also been a drive to synthesize coumarin-based organic dyes for use in high-efficiency dye-sensitized solar cells (DSCs) [12, 13]. Coumarin and its derivatives have attracted significant interest in a wide range of pharmaceutical research areas such as anti-inflammatory, hepatoprotective, antiviral, anticarcinogenic and anticoagulant activities [14-17] and they have various applications in food constituents, stabilizers and clinical use [18].

Knowledge of the excited state charge distribution and the dipole moments of the molecules are important in designing the nonlinear optical materials [19, 20] and understanding the photochemical processes. Methods available for the determination of dipole moments can be classified as either external or internal. External methods includes electric dichroism [21], Stark splitting of rotational levels [22]



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ORIGINAL ARTICLE



Analysis of Fluorescence Quenching for Newly Synthesized Biologically Active 3(2H)-pyridazinone Derivative by Aniline

Vani R. Desai¹ · Shirajahammad M. Hunagund¹ · Mahantesha Basanagouda² · Jagadish S. Kadadevarmath¹ · Ashok H. Sidarai¹

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Abstract Herein, we have studied the analysis of fluorescence quenching for newly synthesized biologically active 3(2H)-pyridazinone derivative 5-(5-bromo-2-hydroxy-phenyl)-2-phenyl-2H-pyridazin-3-one [BHP] by various concentrations of aniline using UV-Visible spectroscopy, fluorescence spectroscopy and time-correlated single photon counting technique in five different solvents namely, methanol, ethanol, propan-2-ol, dimethylsulfoxide and ethyl acetate at room temperature. The fluorescence intensity of BHP molecule decrease with increasing in the aniline concentration and it is studied using the Stern-Volmer relation. The obtained Stern-Volmer plots were found to be linear in all the five solvents. The various parameters responsible for the fluorescence quenching such as quenching rate parameters (k_a) , diffusion rate parameter (k_d) and the probability of quenching per encounter (p) were experimentally calculated in all five solvents. An activation energy of quenching (E_a) was calculated using the values of activation energy of diffusion (E_d) and p. It was found that the values of E_a are greater than E_d in all five solvents studied. Further, it is inferred that the fluorescence quenching reactions in BHP molecule are more significantly affected by activation energy processes.

Keywords 3(2H)-pyridazinone · Activation energy · Fluorescence quenching · Material diffusion · Stern-Volmer relation

Introduction

The 3(2H)-pyridazinones are the pyridazine derivatives which contain two adjacent nitrogen atoms at the one and two positions in a six-membered ring and a carbonyl group at the three position and they have different functionalities in their structure [1, 2]. A substantial number of pyridazinones derivatives are reported to possess antimicrobial, antitubercular, analgesic, anti-inflammatory, cyclooxygenase inhibitor, antidiabetic, antihypertensive, antiplatelet, anticancer, antifungal, antidepressant-anxiolytic, anticonvulsant, bronchodilatory (asthma), anti-allergic, antifeedant, inhibition of linolenic acid, activity for neurological disorders and many other properties [3]. Some of the major pyridazinone derivatives which have appeared in the market are indolidan, bemoradan, pimobendan, levosimendan as antihypertensive, minaprine as an antidepressant, emorfazone as antiinflammatory and azanrinone as a cardiotonic [3].

Recently, spectroscopic and quantum chemical investigations on 3(2H)-pyridazinone derivatives such as levosimendan (IUPAC name: 2-[[4-[(4R)-4-methyl-6-oxo-4,5-dihydro-1Hpyridazin-3-yl]phenyl]hydrazinylidene]propanedinitrile) and bromopyrazone (IUPAC name: 1-phenyl-4-amino-5bromopyridazon-(6)) compounds have been reported in the literature [4, 5]. In addition, the detailed structural, conformational, spectroscopic, electronic and nonlinear optical properties of the 3(2H)-pyridazinone derivatives namely flufenpyr (IUPAC name: {2-chloro- 4fluoro-5-[5-methyl-6-oxo-4-(trifluoromethyl)-1(6H)pyridazin-1-yl] phenoxy}acetic acid)) used in agriculture as a herbicide and amipizone (IUPAC name: 6-(p-(2chloropropionylamino)phenyl)-5-methyl-4,5-dihydropyridazin-3- one)) designed to be antithrombotics and an inhibitor for platelet aggregations and the cardiovascular system) compounds estimated at the B3LYP (Becke's three-parameter

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Study of Fluorescence Quenching on Novel Coumarin Derivatives by Aniline in Different Solvents

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Abstract The steady-state fluorescence quenching of novel coumarin derivatives; 4-(2, 6-dibromo-4-methyl-phenoxymethyl)-benzo[h]chromen-2-one [DMB] and 6-methoxy-4-p-tolyoxymethyl-chromen-2-one [TMC] has been studied in toluene, benzene, dioxane, acetonitrile and tetrahydrofuran [THF] using aniline as a quencher at room temperature with a view to understanding the role of diffusion in the quenching mechanism. The probability of quenching per encounter (p) is calculated in all the solvents. Further, an activation energy for quenching (E_a) was estimated using the values of p and the literature values of activation energy for diffusion (E_d). The magnitudes of these parameters indicate that the fluorescence quenching of these molecules by aniline is not solely due to the material diffusion but there is also a contribution of an activation energy.

Keywords Activation energy · Coumarin derivative · Fluorescence quenching · Material diffusion · Stern–Volmer plot

1 Introduction

The fluorescence quenching of organic molecules in solvents by various quenchers such carbon tetrachloride, aniline, oxygen, halide ions and titanium dioxide nanoparticles has been a subject of continued investigation for the last two decades [1-5]. One of the well-known experimental techniques used to study the role of fluorescence quenching is to determine the quenching rate parameters using the Stern–Volmer [S-V] equation:

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Spectroscopic studies on newly synthesized 5-(2-hydroxy-5methoxy-phenyl)-2-phenyl-2H-pyridazin-3-one molecule

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Highlights

- HMPP molecule undergoes solvatochromism and fluorescence quenching.
- Excited state dipole moment is greater than the ground state dipole moment.
- Effect of hydrogen bonding is more as compared to solvent polarizability.
- The fluorescence quenching of HMPP molecule follows the linear S-V relation.
- Influence of activation energy process is more as compared to material diffusion.

Abstract

Spectroscopic studies on newly synthesized biologically active pyridazin-3(2H)-one derivative 5-(2-hydroxy-5-methoxy-phenyl)-2-phenyl-2H-pyridazin-3-one (HMPP) molecule have been studied at room temperature in various solvents of different polarities. Theoretically, the ground



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Journal of Molecular Liquids Volume 233, May 2017, Pages 166-172

Spectroscopic interactions of titanium dioxide nanoparticles with pharmacologically active 3(2*H*)-pyridazinone derivative

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Highlights

- HMP molecule undergoes fluorescence quenching by TiO₂ NPs.
- The fluorescence quenching of HMP molecule follows the linear S-V relation.
- The nature of fluorescence quenching is purely dynamic.
- Energy transfer from HMP molecule to TiO₂ NPs.
- Investigation is useful for sensitizing the TiO₂ NPs for solar energy conversion.

Abstract

Herein, we report the spectroscopic interactions of titanium dioxide (TiO₂) <u>nanoparticles</u> (NPs) with pharmacologically active 3(2*H*)-pyridazinone derivative, viz., 5-(2-Hydroxy-4-methyl-phenyl)-2-phenyl-2H-pyridazin-3-one [HMP] in an ethanol solvent using UV–Visible <u>spectrophotometer</u>, fluorescence spectrophotometer and time-correlated single photon counting technique at room temperature. The observed values of absorption, <u>fluorescence intensity</u> and <u>fluorescence lifetime</u> of HMP molecule decrease with increasing in the TiO₂ NPs concentration. From the linear Stern-Volmer (S-V) plot in steady state and transient state which indicates the

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Electrochemical Sensor Based on Reduced Graphene Oxide Nanoribbons for the Determination of Baicalein in Urine Samples

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Abstract

Electrochemically reduced graphene oxide nanoribbons (ErGONRs) have been prepared, characterized and utilized for sensing of a flavone, baicalein (BAI) by adsorptive stripping differential pulse voltammetric (AdSDPV) and square wave voltammetric (SWV) methods. BAI showed redox peaks ($E_{pa} = 0.582$ V and $E_{pc} = 0.557$ V) and an irreversible oxidation peak at 1.402 V on ErGONRs/GCE in phosphate buffer of pH 3. A 50-fold enhanced electrochemical response was observed at ErGONRs/GCE for BAI when compared to that noticed at bare GCE. The parameters concerning the electrochemical behavior of BAI were carefully optimized. Under optimized conditions, SWV and AdSDPV methods showed linearity in the range of 10 nM–87.4 μ M and 0.4 μ M–50 μ M, respectively. Applicability of the proposed electrode was demonstrated by determining BAI in urine samples

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Journal of Electroanalytical Chemistry Volume 797, 15 July 2017, Pages 89-96

A facile one-pot hydrothermal synthesis of tin sulfide-decorated reduced graphene oxide nanoribbons and its sensing application for a flavanone naringenin

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Highlights

- Hetero nanostructure, SnS₂ decorated reduced graphene oxide nanoribbons (SnS₂-rGONRs) was prepared.
- Selective and sensitive electrochemical sensor was proposed based on SnS₂-rGONRs for naringenin.
- Analytical and binding applications of the proposed sensor were explored for naringenin.

Abstract

New <u>electrode materials</u> have been synthesized extensively with the aim of enhancing sensitivity and selectivity besides decreasing the overpotential of <u>electrode reactions</u>. Present work describes the design of a new one-pot hydrothermal route for the preparation of highly electroactive <u>nanocomposite</u>, SnS₂ decorated reduced <u>graphene oxide nanoribbons</u> (designated as SnS₂rGONRs) for analytical and binding applications of a <u>flavanone</u>, <u>naringenin</u> (NAR). Electrode



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Full Paper

Electrochemical Oxidation and Thermodynamic Parameters for an Anti-viral Drug Valacyclovir

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Abstract- The electro-oxidation of valacyclovir has been studied at a glassy carbon electrode in phosphate buffer media by using cyclic voltammetric technique. Effects of anodic peak potential (E_{pa}), anodic peak current (i_{pa}), pH and heterogeneous rate constant (k_o) have been discussed, single irreversible voltammogram was observed. The effects of scan rate, pH, concentration and temperature were evaluated. The electrode processes were shown to be diffusion controlled and irreversible involving adsorption effects. The electro-oxidation product of valacyclovir has been identified by MALDI2-((2-amine-6,8-dioxo-7,8-dihydro-3H-purin9(6H)-yl)methoxy)ethyl2-amino-3-methylbutanoate), involving 2-electron and 2porton oxidation. Thermodynamic parameters such as activation energy $E_a=27.51$ kJmol⁻¹, enthalpy $\Delta H^{\#}=25.03$ kJmol⁻¹, entropy $\Delta S^{\#}=-284.8$ JK⁻¹mol⁻¹, Gibbs free energy $\Delta G^{\#}=109.9$ kJmol⁻¹ and Arrhenius factor, logA=-2.08 and analytical parameters linearity range 5.0×10^{-3} to 7.5×10^{-5} M, LOD=1.44 μ M, LOQ=4.83 μ M and RSD=5.26% were calculated and presented.

Keywords- Valacyclovir, Voltammetric techniques, Electrochemical studies, Oxidation thermodynamic parameters



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Research Article

ISSN 2277-7105

COMPUTATIONAL INVESTIGATION AND FACILE SYNTHESIS OF BIOLOGICALLY ACTIVE NEW CLASS OF N-SUBSTITUTED CYCLIC IMIDES OF COUMARIN HYBRIDS AS POTENT ANTI-MICROBIAL AND ANTI-CANCER AGENTS

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ABSTRACT

A series of novel N-substituted cyclic imides of coumarin hybrids (2a-2h) have been synthesized and screened for antibacterial and antifungal activities. All the newly synthesized compounds were evaluated for antibacterial activity against one Gram-positive (*Staphylococcus aureus*) and one Gram-negative (*Escherichia coli*) bacteria and antifungal activity against pathogenic strains of *Candida albicans* and *Aspergillus flavus* by Agar-well Diffusion Method. The title compounds (2a), (2d) and (2f) showed potent antibacterial activity against pathogenic strains used in the study. Compounds (2a) and (2f) showed potent antifungal activity against *A. flavus* and *C. albicans* pathogenic strains. The *in vitro* cytotoxicity was evaluated against Hela (cervical cancer) cell line by using MTT colorimetric assay. The

compound (2d) ($\mathbf{R} = 6$ -OCH₃) was found to be potent anticancer among the series. Furthermore, Molecular docking study performed for all the synthesized compounds with *S*. *Aureus* gyrase complex with Ciprofloxacin and DNA (PDB ID : 2XCT) and results were obtained, the compounds (2c), (2f), (2g) and (2h) have higher C score values than





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<u>Research Article</u> ISSN 2394-3211 EJPMR

DISCOVERY OF NEW DRUGS AND COMPUTATIONAL STUDIES OF COUMARIN-CARPROFEN SCAFFOLDS AS A NOVEL CLASS OF ANTI-TUBERCULAR, ANTI-INFLAMMATORY AND ANTI-BACTERIAL AGENTS

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ABSTRACT

Carprofen and coumarins are biologically promising potent heterocyclic compounds as they posses very good antitubercular, antimicrobial, anti-inflammatory and anticancer activities. In the present study, the condensation of substituted 4-bromomethyl coumarin and carprofen in the presence of anhydrous potassium carbonate gives exclusively coumarim-carprofen hybrids (3a-3i). Anti-tubercular assays against *M. tuberculosis* (H37Rv) coupled with in silico molecular docking studies indicated that dimethyl substituents (**3a**), (**3f**) and (**3g**) showed promising activity with higher C-score values. The synthesized compounds were also screened for *in-vitro* antimicrobial and anti-inflammatory. However, the compounds of (**3c**) and (**3f**) exhibit excellent *in-vitro* activity against *M.tuberculosis* (H₃₇Rv). These results suggested that the as synthesized compounds of (**3c**) and (**3f**) own promising lead for subsequent investigation in search of new anti-tubercular agents. Accordingly, the *in-vitro* antiinflammatory activity revealed that compounds of (**3a**), (**3b**), (**3c**) and (**3i**) exhibited highest prominent antiinflammatory activity. Compounds (**3a**), (**3b**), (**3f**) and (**3i**) have shown excellent antibacterial activity.

KEYWORDS: Coumarin-carprofen, Anti-tubercular, Molecular docking, Anti-inflammatory and Antibacterial.

INTRODUCTION

Despite tremendous progress in understanding tuberculosis disease, there remains the challenge to develop agents for its therapy with fewer side effects. Most of the approved drugs have maximum amount of side effect. Tuberculosis (TB) is an infectious disease mainly caused by Mycobacterium tuberculosis and characterized by tubercle lesions in the lungs.^[1] It is a leading cause of death worldwide, TB is one of the global health emergency because of the increase in secondary infections and/or co-infection in immunecompromised patients [such as those infected with human immunodeficiency virus (HIV)] and most worrying is the emergence of resistant strains of M. tuberculosis [multidrug-resistant (MDR) and extensively drug resistant (XDR) TB strains].^[2] The WHO has estimated that every year about eight million new cases of tuberculosis occur and up to three million individuals die due to this disease (one person dies every 10 s).^[3] It is also estimated that between 2002 and 2020, approximately a billion people will be newly infected,

more than 150 million people will get sick and 36 million will die of TB.^[4] Therefore, the development of new and more efficacious drugs against *Mycobacterium tuberculosis* is urgently needed. This made the researchers to design the drug which can exhibit less amount or zero amount of side effect.

Coumarin has become an essential biomolecule in the area of drug discovery, since incorporation of coumarin group into potent heterocyclic moieties, results in significant enhancement in efficacy of a drug. Further, coumarin has acquired the special significance in the medicinal chemistry arena, which is a class of compound widely available in the natural products, exhibits remarkable arrays of biological properties, like antimicrobial, anti-inflammatory, anti-oxidant effects, anticoagulant, anti-tumor, anti-viral, as well as enzyme inhibitory actions. Most of the anti-tuberculosis drug available in the market has the coumarin nucleas, namely novobiocin and coumarin-4-acetic acid benzylidene hydrazide. In view of their extensive application of plant



Studies on Electrical and Magnetic Properties of Mg-Substituted Nickel Ferrites

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The semiconducting polycrystalline ferrite materials with the general formula $Ni_{1-x}Mg_xFe_2O_4$ were synthesized by using the solid state reaction method. X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectrographs, and atomic force microscopy techniques were utilized to study the structural parameters. XRD confirms the formation of single phase cubic spinel structure of the ferrites. The crystallite sizes of ferrites determined using the Debye-Scherer formula ranges from 0.963 μ m to 1.069 μ m. The cation distribution of ferrite shows that Mg^{2+} ions occupy a tetrahedral site (A-site) and the Ni²⁺ ion occupy an octahedral site (B-site) whereas Fe^{3+} ions occupies an octahedral as well as a tetrahedral site. The study of elastic parameters such as the longitudinal modulus, rigidity modulus, Young's modulus, bulk modulus, and Debye temperature were estimated using the FTIR technique. The decrease of direct current (DC) resistivity with increase in temperature indicates the semiconducting nature of ferrites. The dielectric constant as well as loss tangent decreases with increase in frequency, and at still higher frequencies, they are almost constant. This shows usual dielectric dispersion behavior attributed to the Maxwell-Wagner type of interfacial polarization and is in accordance with Koop's phenomenological theory. The linear increase of alternating current conductivity with increase of frequency shows the small polaron hopping type of conduction mechanism in all the ferrites. The magnetic properties such as saturation magnetization (M_s) , magnetic moment, coercivity, remnant magnetization (M_r) , and the ratio of M_r/M_s was estimated using the M–H loop.

Key words: Powder x-ray diffraction (XRD), atomic force microscopy (AFM), Fourier transform infrared (FTIR) spectrograph, electrical resistivity, Debye temperature, Tauc plot, vibrating sample magnetometer (VSM) and magnetic moment

INTRODUCTION

Cubic spinel structured ferrites have potential applications in the field of magnetic and electronic technology; they also have a wide range of applications in drug delivery systems and in medical diagnosis.¹ Ferrites having high electrical resistivities, high saturation magnetization, and low dielectric losses are useful in microwave devices, computer memories, and magnetic recording devices. Ferrites are good magnetic material with more stability; thus they are used in transformer cores, high quality filters, radio wave circuits ,and

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Measurement of Coster-Kronig vacancy transfer factor of some lanthanides using monoenergetic X-ray photons

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Highlights

- Coster-Kronig vacancy transfer factors of some lanthanides are determined.
- Indus-2 synchrotron radiation is used to measure vacancy transfer factor values.
- The measured values are not influenced by chemical environment.

Abstract

Using monoenergetic X-ray photons from Indus-2 <u>synchrotron</u> Centre, the Coster-Kronig vacancy factor(κ) for L₃ subshell X-rays of some <u>lanthanide</u> elements such as Gd, Tb, Ho and compounds such as Pr₂O₃, Pr₂(CO₃)₃·8H₂O, Nd₂O₃, Sm₂O₃, Sm₂(CO₃)₃.2.85H₂O, Sm₂(SO₄)₃·8H₂O, Gd₂(CO₃)₃, Tb₂O₃, Dy₂(SO₄)₃, Ho₂O₃ and HoF₃ have been determined experimentally. By measuring L_{α} X-ray production cross-section, the L₃ subshell fluorescence yield and theoretical values of the L₃ subshell <u>photoionization</u> cross-section and level widths, the κ values have been determined. Comparison of the measured experimental κ values with theoretical values indicates that the influence of the chemical environment on κ values in the selected lanthanide targets is not noticeable.

Research Article

Novel High Strength Economical Shielding Materials

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Abstract

In the present study, gamma-ray shielding performance was investigated using mass attenuation coefficients and exposure buildup factors for tourmaline, datolite, galena, amethyst and hormirad. The mass attenuation coefficients were also calculated using GEANT4 simulation toolkit, compared with XCOM results, a good agreement between XCOM and GEANT4 results was observed. The exposure buildup factors were calculated using GP fitting method for photon energy 0.015 to 15 MeV up to 40 mfp. The hormirad is superior shielding material among than tourmaline, datolite and amethyst whereas galena is the best shielding materials in low photon energy except near to 100 keV. The investigation would be very useful for shielding application of these materials.

Keywords: Novel shielding, galena, XCOM, GEANT4, gamma-ray

Yeni Yüksek Mukavemetli Ekonomik Zırhlama Malzemeleri

Öz

Bu çalışmada, kütle zayıflatma katsayısı ve ekpojur buildup faktörleri kullanılarak tourmaline, datolite, galena, amethyst ve hormirad için gama ışını zırhlaması incelenmiştir. Kütle zayıflama katsayıları GEANT4 simülasyon kodu kullanılarak hesaplandığında, ve XCOM sonuçları ile karşılaştırıldığında, XCOM ve GEANT4 sonuçları arasında iyi bir uyum gözlenmiştir. Ekpojur buildup faktörleri, 0.015 ila 15 MeV arasında 40 mfp'ye kadar olan foton enerjisi için GP fittiing yöntemi kullanılarak hesaplanmıştır. Hormirad; turmalin, datolit ve ametist malzemeleri arasında üstün zırhlama malzemesiyken, galena 100 keV'e yakın düşük foton enerjisi seviyeleri haricinde en iyi koruma malzemesidir. Bu çalışma; ilgili malzemelerin zırhlama uygulamalarında faydalı bir çalışma olabilir.

Keywords: Yeni zırhlam, galena, XCOM, GEANT4, gamma ışını

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RESEARCH ARTICLE

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Design, synthesis and pharmacological analysis of 5-[4'-(substituted-methyl)[1,1'-biphenyl]-2-yl]-1H-tetrazoles

Atulkumar Kamble¹ · Ravindra Kamble¹ · Suneel Dodamani² · Sunil Jalalpure^{2,3} · Vijaykumar Rasal^{2,3} · Mahadev Kumbar¹ · Shriniyas Joshi⁴ · Sheshagiri Dixit⁴

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Abstract In the present paper 5-[4'-([4-[(4-aryloxy)methyl]-1H-1,2,3-triazol-1-yl]methyl)[1,1'-biphenyl]-2-yl]-1H-4etrazoles (5a-g) and [2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl-substituted-1-carbodithioates (11h-q) have been designed and synthesized. These compounds were subjected to docking (against AT₁ receptor protein enzyme in complex with Lisinopril), in vitro angiotensin converting enzyme inhibition, anti-proliferative, anti-inflammatory screening (through egg albumin denaturation inhibition and red blood cell membrane stabilization assay) and finally anti-fungal activity analyses. Some of the compounds have shown significant pharmacological properties.

Keywords Biphenyl - Tetrazole - Triazole - DTC -ACE inhibition - Anti-proliferative activity -Anti-inflammatory activity - Antifungal activity

Electronic supplementary material The online version of this article (doi:10.1007/s12272-017-0887-0) contains supplementary material, which is available to authorized users.

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Introduction

It has been proved that cardiovascular diseases are lifelong condition, and patients with high blood pressure need to take medicine on a regular basis. Given the advancements in society worldwide, hypertension presents a challenge not only to the people in western countries but also to the entire world. Angiotensin II receptor antagonists inhibit angiotensin converting enzyme (ACE) and influence the renin-angiotensin system which plays an important role in the regulation of cardiovascular homeostasis by acting on both the vascular resistance and the blood volume (Vallotton 1987). ACE II is produced in vivo from angiotensin I by ACE (Cockcroft et al. 1993). ACE is not a selective enzyme as it possesses important peptides such as bradykinin among its substrates and substance P (an undecapeptide composed of a chain of 11 amino acid residues). Human and animal tissues mainly have two types of ACE II receptor subtypes which have been characterized as AT₁ and AT₂ (De et al. 2000). The AT, receptor subtype belongs to the G proteincoupled receptor super family and has seven hydrophobic trans-membrane domains forming R-helices in the lipid bi-layer of the cell membrane. Majority of the effects of ACE II on the cardiovascular, renal and central nervous system (CNS) are blocked by AT₁ (Timmermans 1992). The AT₂ receptor is involved in fetal growth, adult tissue repair and remodeling, especially in the cardiovascular system (Heymes and Levy 1998).

A large number of patents and publications on ACE II antagonists have come across in the last several years. These antagonists are selective for the type 1 ACE II (AT₁) receptor which affects the blood pressure. Compounds such as Losartan (DuP-753, 1) (Carini et al. 1991; Duncia et al. 1992), IC1 D8731 (Bradbury et al. 1992) and L-159,093

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Research Article

Synthesis, Photophysical and Computational Study of Novel Coumarin-based Organic Dyes

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First published: 06 November 2017 https://doi.org/10.1111/php.12852 Citations: 6

Abstract

A series of novel coumarin pyrazoline moieties combined with tetrazoles, 3-(1-phenyl-4-(1Htetrazol-5-yl)-1H-pyrazol-3-yl)-2H-chromen-2-one, 6-chloro-3-(1-phenyl-4-(1H-tetrazol-5-yl)-1Hpyrazol-3-yl)-2H-chromen-2-one, 6-bromo-3-(1-phenyl-4-(1H-tetrazol-5-yl)-1H-pyrazol-3-yl)-2Hchromen-2-one and 6-bromo-3-(1-(4-bromophenyl)-4-(1H-tetrazol-5-yl)-1H pyrazol-3-yl)-2Hchromen-2-one7(a-d), were designed and synthesized. Single crystal X-ray diffraction and their interactions were studied by Hirshfeld surface analysis. Thermal stabilities and electrochemical properties of these compounds were examined from differential scanning calorimetry (DSC), thermogravimetric (TGA) and cyclic voltammetric (CV) studies. Their spectroscopic properties were analyzed in various alcohols and general solvents by UV–Vis absorption, fluorescence and time-resolved spectroscopy. In addition, the ground and excited state electronic properties were investigated using density functional theory (DFT). The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and energy band gap (E_g) values have revealed the effect of substitution of halogens. The substitution has equally affected the ground and excited states of 7(a-d) compounds. The solvatochromism on absorption, fluorescence spectra and fluorescence lifetimes of these compounds was investigated. All these results showed the chromen-2-one of pyrazoline tetrazole derivatives could play an important role in photonic and electronic devices.

Citing Literature

Supporting Information

Filename

Description

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Journal of Molecular Structure Volume 1149, 5 December 2017, Pages 357-366

[Dichlorido (2-(2-(1H-benzo[*d*]thiazol-2-yl)hydrazono)propan-1ol) Cu(II)]: Crystal structure, Hirshfeld surface analysis and correlation of its ESI-MS behavior with [Dichlorido 3-(hydroxyimino)-2-butanone-2-(1H-benzo[*d*]thiazol-2yl)hydrazone Cu(II)]

Vinayak Kamat ª, Karthik Kumara ^b, Krishna Naik ª, Avinash Kotian ª, Priya Netalkar ^c, Naveen Shivalingegowda ^d, Krishnappagowda Lokanath Neratur ^b, Vidyanand Revankar ª ペ ⊠

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Highlights

- Two benzothiazole based Cu(II) coordination complexes are synthesized.
- X-ray structure, intermolecular interactions and Hirshfeld surface analysis of one of the complex is explored.
- Various cationic/anionic fragments or adducts formed during electrospray ionization are identified.

Abstract



Journal of Inorganic Biochemistry Volume 177, December 2017, Pages 127-137

Synthesis, structural characterization and biological properties of phosphorescent iridium(III) complexes

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Highlights

- Two phosphorescent cyclometalated iridium(III) complexes were synthesized.
- Complexes have solvent dependent photo-physical properties.
- Complexes have low toxicity and have no DNA cleavage activity.
- These complexes condense originally circular plasmid DNA into particulate structures.
- These complexes are non-toxic and specifically stain the nucleus of the cells.

Abstract

Two phosphorescent cyclometalated iridium(III)-triptycenyl-1,10-phenanthroline complexes [Ir(ppy)₂(tpt-phen)]⁺ (1) and [Ir(bhq)₂(tpt-phen)]⁺ (2) {ppy = 2-phenylpyridine, bhq = Benzo[*h*]quinoline, tpt-phen = triptycenyl-1,10-phenanthroline} have been synthesized and structurally characterized. The structure of complex **2** has been studied by single crystal X-ray



Polyhedron Volume 127, 8 May 2017, Pages 225-237

Transition metal complexes of 2-(2-(1H-benzo[d]imidazol-2yl)hydrazono)propan-1-ol: Synthesis, characterization, crystal structures and anti-tuberculosis assay with docking studies

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Abstract

Transition metal coordination complexes of Co(II), Ni(II), Cu(II) and Zn(II) with a newly designed ligand, 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol have been synthesized and characterized using various spectro-analytical techniques. The molecular structures of Co(II), Cu(II) and Zn(II) complexes are determined by single-crystal <u>X-ray diffraction method</u>. The metal to ligand <u>stoichiometry</u> has been found to be 1:2 in the case of Cobalt(II), Nickel(II) and Zinc(II) whereas 1:1 in the case of Copper(II) complex. The newly synthesized ligand and complexes have been assessed for their growth inhibiting potencies against H37Rv strain of <u>Mycobacterium</u> <u>tuberculosis</u>. The copper and cobalt complexes have emerged to be potent *in vitro* growth inhibitors of H37Rv. All the complexes are inhibiting the growth of other tested common <u>microbial flora</u> to a significantly lesser extent, making them selective towards H37Rv in the preliminary analysis. The consensus scores obtained by the docking studies of the molecules to the target protein enoyl <u>acyl carrier protein</u> reductase of *M. tuberculosis* H37Rv are in good agreement with the obtained MIC values.

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[Dichlorido (2-(2-(1H-benzo[*d*]thiazol-2-yl)hydrazono)propan-1-ol) Cu(II)]: Crystal structure, Hirshfeld surface analysis and correlation of its ESI-MS behavior with [Dichlorido 3-(hydroxyimino)-2-butanone-2-(1H-benzo[*d*]thiazol-2-yl)hydrazone Cu(II)]



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ABSTRACT

In the present work, Cu(II) complexes of 2-(2-benzo[*d*]thiazol-2-yl)hydrazono)propan-1-ol (L¹) and 3-(hydroxyimino)-2-butanone-2-(1*H*-benzo[*d*]thiazol-2-yl)hydrazone (L²) are synthesized and characterized by various spectro-analytical techniques. The structure of Cu(II) complex of L¹ i.e., [CuL¹Cl₂], is unambiguously determined by single crystal X-ray diffraction method. While similar efforts were unsuccessful in the case of Cu(II) complex of L² i.e., [CuL²Cl₂]. Hence, to avail the structural facts, various cationic/anionic fragments or adducts formed during positive/negative mode electrospray ionization (ESI) of CuL¹Cl₂ and CuL²Cl₂ have been identified with the help of their charge, monoisotopic masses and isotopic distributions. The similarity in the ESI behavior of two complexes has inferred their structural resemblance, which is further supported by DFT optimized structures, EPR spectral studies and analytical measurements. The EPR spectral behavior ($g_{||} > g_{\perp} > 2.02$) of the complexes are attributed to an axial symmetry with the $d_{x^2-y^2}$ ground state having square pyramidal Cu(II) ion. CuL¹Cl₂ has crystallized in monoclinic crystal system in *P*2₁/*c* space group. The molecular complex has ring-metal (*Cg*-Me) interactions of the type Cg····>Cu, which contributes to the crystal packing. The Cl···H (30.6%) interactions have the major contribution among all intermolecular contacts and have played a vital role in the stabilization of the molecular structure, which is extended to 3D network through C–H···*Cg* and *Cg*-*Cg* interactions.

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1. Introduction

Polydentate heterocyclic ligands containing both sulfur and nitrogen atoms possess versatile coordination ability toward various transition metal ions. Hence, polyfunctional benzothiazole-based derivatives assume an exceptional importance in the construction of metal complexes of different types [1]. Due to this fact, a wide variety of copper (II) complexes derived from benzothiazole core have been reported in the literature [2-4].

X-ray crystallography remains the method of choice for definitive determination of the structure of a new coordination complex, despite the tremendous advances in spectroscopic methods for structure elucidation [5]. Hence, X-ray crystallography is often touted as the ultimate technique for substance characterization. While this is often true, limitations in growing the single crystals suitable for diffraction need to be recognized.

Recent developments of new soft ionization methods have made possible the application of mass spectrometry in various fields of analytical chemistry. Electrospray Ionization (ESI) is one such soft ionization method, that keeps any weakly bound ligands

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Efficient DNA condensation by ruthenium(ii) polypyridyl complexes containing triptycenyl functionalized 1,10-phenanthroline - New



at room temperature. The DNA interactions and DNA condensation properties of these complexes were investigated by absorption and emission spectroscopy, electrophoretic mobility assay, and atomic force microscopy. Their DNA cleavage inactivity and low toxicity of the complexes satisfy the requirements of a good non-viral gene delivery vector.



Electro, Physical & Theoretical Chemistry

Synthesis and Optoelectronic Exploration of Highly Conjugated 1,3,4-Oxadiazole Containing Donor- π -Acceptor Chromophores

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A series of novel highly conjugated Donor- π -Acceptor (D- π -A) chromophores 3(a-g) are designed and synthesized through the Wittig Reaction. These molecules contain an aryl/heteroaryl groups as an electron donor (D) and electron transporting oxadiazole as acceptor (A). The structural integrity of the compounds was characterized by ¹H NMR, ¹³C NMR and GC-MS analysis. The photophysical properties have been studied in detail using UV-Vis absorption, fluorescence spectroscopy and time-resolved fluorescence measurements. These synthesized compounds emit intense blue-green-yellow fluorescence with reasonably good quantum yields. In addition, steady-state absorption and fluorescence measurements were carried out in

Introduction

The increasing need for cost effective, flexible, eco-friendly and sustainable lighting systems has certainly pushed the research in the field of organic electronics like organic light emitting diodes (OLEDs),^[1-6] field effect transistors,^[7-11] lasers,^[12-16] photo-detectors,^[17-21] sensors,^[22-25] and organic photovoltaic (OPV) devices.^[26-30] Charge-transfer (CT) materials composed of an organic donor-acceptor groups exhibit an interesting property of electric conductivity in optoelectronic devices (e.g., OLEDs and solar cells).^[31-33] Organic light emitting diodes (OLEDs) have been investigated intensively in the recent past for their potential applications in display and lighting technology because of their unique advantages such as high low power,

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solvents of varying polarities to understand the intramolecular charge-transfer (ICT) characters of these compounds. The solvent dependency of the large Stokes shifts and high dipole moment of excited state also supported the charge-transfer character of the excited state. The combined experimental Cyclic Voltammetry (CV) and theoretical methods (DFT) were performed to investigate structure-property relationship and ICT property of these compounds. The computed values were found to be in good agreement with the experimental results. The results demonstrated that the novel D- π -A chromophores could play important role in organic optoelectronics.

faster response, high contrast, paper like thickness & flexibility.^[34,35] Due to their increased lifetimes and high efficiency^{[36-^{37]}of organic light emitting diodes (OLED) lead to new applications for general lighting like large-area or flexible surface-emitting light sources.}

The most appealing strategy in the field of organic electronics is incorporation of electron-deficient group as acceptor (A) and electron-donating group as donor (D). The D- π -A fluorescent dyes with electron-donating/accepting groups linked by a π -conjugated bridge are useful in dye-sensitized solar cells (DSSCs),organic light emitting diodes (OLEDs) and fluorescence sensors etc. D- π -A systems exhibit strong absorption and emission properties originating from the intramolecular charge transfer (ICT) from the donor to acceptor moiety. One of the notable structural features of D- π -A system is that the electron density of the HOMO is localized over the π conjugated system close to the donor part and that of the LUMO is localized over the acceptor part.^[38-43] Oxadiazoles act as an excellent electron-transporting/hole-blocking material in OLEDs due to their electron deficient nature. Indeed, oxadiazole units preferably restrict π -conjugation to afford materials with deeply lying HOMOs such that the triplet energies (ETs) are high.^[44-47] An intramolecular charge-transfer (ICT) compound is one of the most important molecular materials, which is functionalized by electron-donating (D) and electron-accepting (A) groups through a π -conjugated linkage. Extended π conjugation by introducing unsaturated group results in the bathochromic shift of both absorption and emission wavelengths of the molecules.^[48]

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SPECTROCHIMICA

Effect of quencher and temperature on fluorescence intensity of laser dyes: DETC and C504T



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ABSTRACT

Fluorescence quenching of 7- Diethylamino-3-thenoylcoumarin (DETC) and 2,3,6,7-tetrahydro-1,1,7,7-tetramethyl11-oxo-1H,5H,11H- [1]benzopyrano[6,7,8-*ij*]quinolizine-10-carboxylic acid, ethyl ester (C504T) by aniline(AN), dimethylaniline (DMA) and diethylaniline (DEA) was investigated in toluene by steady state and transient methods. The quenching parameters like frequency of encounter (k_d), probability of quenching per encounter (p), quenching rate parameters (k_q) and activation energy of quenching (E_a) were determined experimentally. The k_q values determined by steady state and time-resolved methods for the both dyes were found to be same, indicating the dynamic nature of interaction. Magnitudes of p and E_a suggested that the quenching reaction is predominantly controlled by material diffusion. The quenching mechanism is rationalized in terms of electron transfer (ET) from donors (aromatic amines) to the acceptors (coumarin derivatives) confirmed by correlating k_q with free energy changes (ΔG°). Further, an effect of temperature on fluorescence intensity was carried out in toluene and methanol solvents. Fluorescence intensity of both the dyes decreases with increase in temperature. Temperature quenching in case of C504T is due to intersystem crossing S₁ \rightarrow T₂, whereas for DETC, quenching is due to intersystem crossing S₁ \rightarrow T₂ and ICT \rightarrow TICT transition.

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1. Introduction

Fluorescence quenching is a process of relaxation without emission of a photon. During the relaxation, there are wide variety of quenching mechanisms occur including complex formation, molecular rearrangements, intersystem crossing, singlet-to-triplet excitation and intermolecular charge transfer both at ground state and excited state [1,2]. Fluorescence quenching of organic molecules in solutions by different quenchers such as chloroalkanes, aromatic amines, halides etc., have been the subject of interest to understand the nature of bimolecular reactions taking place under the steady state and transient conditions [3–7].

Substituted coumarin derivatives with efficient fluorescing ability have numerous photonic applications in science and technology as charge transfer complexes, solar energy concentrators, colorants, laser dyes in the blue-green range [8–10]. Fluorescence quenching of coumarin derivatives by aromatic amines/haloalkanes, with non-overlapping spectra of donor emission and acceptor absorption has been studied

* Corresponding author. *E-mail address*: sureshkumarhm@rediffmail.com (S.K. H.M.). using Stern–Volmer (S–V) equation by many researchers [11–14]. It is inferred that the quenching is due to electron transfer (ET) between donor and acceptor. ET is one of the most fundamental quenching reactions. Though ET reaction between donors and acceptors with both of them in the ground state is not encouraging, photo excitation of either of them often makes the ET process to occur with reasonable rates [15–19]. The study on ET between coumarin derivatives and amines gives us the significant information that ET rates in homogeneous solvents is faster than in any viscous solvents. It is because of that, in homogeneous medium the donors and acceptors are free to move and they can effectively diffuse together [20–22]. The dynamics of photoinduced electron transfer depends on temperature as well as nature of the medium [23].

Also the effect of temperature on the fluorescence intensity of many organic compounds has been discussed in the literature for coumarin [24–30], indole [31], anthracene [32,33] and rhodamine [34]. The change in temperature drives about a change in the probabilities of the radiative and non-radiative transitions. It is not only important to know the temperature dependence of the organic compounds but also it is equally important to understand the mechanism underlying these processes. In this paper, we present the effect of quenchers (aniline,



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EFFECT OF HYDROGEN BONDING ON FLUORESCENCE QUENCHING OF QUINOLIN-8-OL - ANALYSIS USING NEGATIVE STERN-VOLMER PLOTS

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ABSTRACT

Photophysics of fluorescent organic compounds give a better knowledge of the excited state properties which in turn will help in the design of newer molecules and understanding their performance in specific applications. Here we present the fluorescence quenching study of a Quinolin-8-ol (QO) in toluene and butanol solvents by steady state fluorescence measurements. Anilineis the quencher. Negative deviation in the Stern – Volmer (S-V) plots has been observed with moderate quencher concentration. The downward curvature in the S-V plot is interpreted in terms of existence of different conformers of the solute in the ground state. The formation of intermolecular and intra molecular hydrogen bonding is found to be responsible for the conformational changes in the ground state of the solute. Quenching data is analyzed by modified Stern-Volmer equation or Lehrer equation.

KEYWORDS: *Quinolin-8-ol (QO), fluorescence quenching, modified Stern–Volmer (Lehrer) equations and hydrogen bonding.*



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RESEARCH ARTICLE



Determination of trace elements in normal and malignant breast tissues of different age group using total reflection X-ray fluorescence spectrometer

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Nagappa M. Badiger, Department of Physics, Karnatak University, Dharwad 580003, India. Email: nbadiger@gmail.com The trace elements in normal and malignant breast tissues of different age groups have been determined using total reflection X-ray fluorescence (TXRF) spectrometry. The low Z elements are detected using a vacuum chamber of low Z-high Z (WOBISTRAX) TXRF spectrometer and medium and high Z elements using Ital structures TX-2000 TXRF spectrometers. The trace elements such as Al, P, S, Cl, K, Ca, Ti, Fe, Cu, Zn, Br, Sr, and Y have been detected in normal and malignant breast tissues in the age group 31–40, 41–50, 51–60, and 61–70 years. It is found that the concentration of trace elements such as Al and Ti, Cu and Zn, Ti and Br, and Al and Y are higher in normal breast tissues than in the malignant breast tissues in the samples of age group 31–40, 41–50, 51–60, and 61–70 years, respectively. It is very important to note that the trace element Pb is not observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 31–40, 41–50, and 51–60, but it has been observed in the samples of age group 61–70 years.

- Trace elements in normal and malignant tissues measured using TXRF spectrometers.
- Tissues of different age group have been selected to ascertain the role of trace elements.
- Trace elements P, S, Cl, K, Ca, Fe, and Sr are found to be higher in malignant tissues.
- Trace element Pb is found to be higher in malignant tissues in the age group 61–70.

1 | INTRODUCTION

Breast cancer is a common tumor in women and about 2% of breast cancer concern men. It is the second most frequent cause of cancer deaths after the lung cancer. Study of trace elements in normal and cancer breast

tissues has been evolved as one of the powerful diagnostic tools for the breast cancer. Trace elements are the micronutrients that are part of our daily diets. Although the concentration of trace elements is low, they are very important in many different biological processes, such as function of structural nutrients, normal healing (is the



Fabrication and characterization of targets of oxidizing materials for heavy ion nuclear reaction experiments

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ABSTRACT: Fabrication of targets of materials which get readily oxidized poses lot of challenges in heavy ion nuclear reaction experiments. Targets of oxidizing elements, viz. Li, Ca, Pb, Nd, Gd, Sm, Ba, Ce, Pr, Bi, Er and Eu have been frequently fabricated in target development laboratory at Inter-University Accelerator Centre (IUAC) in the form of free standing films and foils with backing support. In some cases, foils of these elements are sandwiched between two protective foils to avoid oxidation while exposed to air. Role of sandwiching (encapsulation) in minimizing the oxidation of target surface and its effect in preservation of expensive isotopic targets for longer duration is reported in the present investigations. The level of contamination from parting agents in sandwiched targets is also reported in this paper.

KEYWORDS: Accelerator Applications; Manufacturing; Overall mechanics design (support structures and materials, vibration analysis etc); Targets (spallation source targets, radioisotope production, neutrino and muon sources)



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Effect of Heat Treatment on Radiation Shielding Properties of Concretes

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ABSTRACT

Background: Heat energy produced in nuclear reactors and nuclear fuel cycle facilities interactions modifies the physical properties of the shielding materials containing water content. Therefore, in the present paper, effect of the heat on shielding effectiveness of the concretes is investigated for gamma and neutron. The mass attenuation coefficients, effective atomic numbers, fast neutron removal cross-section and exposure buildup factors.

Materials and Methods: The mass attenuation coefficients, effective atomic numbers, fast neutron removal cross-section and exposure buildup factors of ordinary and heavy concretes were investigated using NIST data of XCOM program and Geometric Progression method.

Results and Discussion: The improvement in shielding effectiveness for photon and reduction in fast neutron for ordinary concrete was observed. The change in the neutron shielding effectiveness was insignificant.

Conclusion: The present investigation on interaction of gamma and neutron radiation would be very useful for assessment of shielding efficiency of the concrete used in high temperature applications such as reactors.

Keywords: Concrete, Heat treatment, Neutron removal cross section, Gamma, Shielding

Introduction

Wide varieties of radiation shielding materials are being used in nuclear technology for exposure control of occupational radiation workers. The shielding materials are being chosen based on the requirements, application, feasibility, type of radiation, cost, availability, etc. Concrete is one of the most suitable shielding materials in view of cost effective, easily available, easy fabrication of different densities for stopping both the gamma and neutron. The concrete has combination of low- as well as high atomic number elements (H, C, O, S, Ca, Fe) to reduce gamma as well as neutron radiations, which is the most necessary for a nuclear facility. The aggregates increase the density of concrete which results in improvement of shielding efficiency [1-3]. The density is mass of constituent elements per unit volume i. e. increase in density signifies large number of target atom for interaction with incoming radiation.

The concrete is being used for biological shielding of the reactor core and other applications for exposure control. Thermal energy is transferred to the concrete from directly from reactor core as well as radiation interacting with it. Exposure of the concrete

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Organic & Supramolecular Chemistry

Microwave-Expedited Green Synthesis, Photophysical, Computational Studies of Coumarin-3-yl-thiazol-3-yl-1,2,4-triazolin-3-ones and Their Anticancer Activity

Saba Kauser J. Shaikh,^[a] Madivalagouda S. Sannaikar,^[b] Mahadev N. Kumbar,^[a] Praveen K. Bayannavar,^[a] Ravindra R. Kamble,^{*[a]} Sanjeev R. Inamdar,^{*[b]} and Shrinivas D. Joshi^[C]

Mild and efficient synthesis of 5-methyl-4-[(2Z)-4-(2-oxo-2*H*-chromen-3-yl)-2-(4-arylimino)thiazol-3(2*H*)-yl]-2-(4-aryl)-2*H*-1,2,4-triazol-3(4*H*)-ones **7(h**-s) has been developed using microwave assisted multicomponent route. The molecular structures of these novel compounds were characterized and the photo-physical and thermal properties were investigated elaborately using absorption, fluorescence, fluorescence decay lifetimes and thermo gravimetric analysis. Solvatochromism was studied as a function of polarity of the solvents. The ground and excited states of electronic geometric optimizations were computed using density functional theory (DFT and TD-DFT).

The orientation of atomic orbitals and their energies were supported by HOMO-LUMO calculations. Electrostatic potential (ESP) maps indicated the electron density predicting the reactive sites. Compounds **7(h-s)** were docked into the epidermal growth factor receptor (EGFR) tyrosine kinase domain which formed a stable complex with good C-score values. The title compounds were evaluated for their anticancer activity against A549, MDA-MBA-231, HeLa and K562 cancer cell lines which showed sensitivity against most of the tested compounds.

Introduction

The growing relevance of diversity oriented synthesis (DOS) has become benign for building the novel molecules. This shows that the synthesis of structurally diverse collection of complex molecules and small molecules in an accomplished manner.^[11] Further, this leads us to speculate the new generation for the development of multicomponent reactions (MCR). A multicomponent strategy is an efficient tool in modern organic synthesis especially for heterocycle.^[2] This approach is engaging with an outlook that products are formed in a single step and the diversity is due to varying the reacting components.^[3] MCRs portray mild conditions, speed, efficiency, easy execution, atom economy and environmental amiability. The MCRs, in spite of being convergent reactions, essay considerable process time reduction and better yields, compared to the classical ap-

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proaches which are linear or divergent.^[4,5] One of the nonconventional energy sources trending in the present synthetic route is the use of microwave irradiation. There are many cases wherein microwave irradiation offers considerable improvements in chemical yield and constitutes a very simple and extremely rapid method to access a diverse range of heterocyclic motifs.^[6–9] Microwave-assisted organic synthesis (MAOS) has been demonstrated to be effective at increasing the rate of MCR procedures.^[10,11] The present work basically employs microwave-assisted MCRs.

Coumarins are a class of 1,2-benzopyrone family which are widely available as natural and synthetic scaffolds. The special framework of lactone ring with the conjugated system enables it to interact with various enzymes and receptors in organisms.^[12] Thus coumarin has intrigued substantial interest in pharmacological activities like anti-inflammatory,^[13,14] antioxidant,^[15] anticoagulant,^[16] antituberculosis,^[17] antinociceptive,^[18] antimicrobial,^[19,20] antidepressant,^[21] cyclooxygenase inhibition^[22] and anticholinesterase activities.^[23] Among all these versatile biological activities, coumarins are notably accounted for their anticancer activities.^[24-26] There are innumerable pathways wherein coumarin triggers the cancer such as cell cycle arrest, angiogenesis inhibition, kinase inhibition, telomerase inhibition, antimitotic activity, monocarboxylate transporters inhibition, carbonic anhydrase inhibition, aromatase inhibition and sulfatase inhibition.[27-29] Daphnetin, one of the coumarin derivative was found to inhibit protein kinase specifically EGF receptor including cAMP dependent protein kinase (PKA) and


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Chemical Data Collections Volumes 17–18, December 2018, Pages 251-262

Crystal structure and Hirshfeld surface analysis of bis (2-(2-(1Hbenzo[*d*]imidazol-2-yl)hydrazono)propan-1-ol) nickel(II) chloride

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Abstract

The present work describes the crystal structure and Hirshfeld surface analysis of a transition metal coordination complex, bis (2-(2-(1H-benzo[*d*]imidazol-2-yl)hydrazono)propan-1-ol) nickel(II) chloride.Recrystallization of the title complex from aqueous methanol has crystallized the complex in monoclinic crystal system with $P2_1/c$ space group. The asymmetric unit of the complex has two monomeric distorted octahedral coordination entities, along with four chloride anions and seven water molecules as crystallization solvent. The ring puckering analysis, intramolecular hydrogen and halogen bonding interactions and the C—H… π and π – π interactions of individual intermolecular interactions and the importance of the C—H… π and π – π interactions in the crystal packing.

Graphical abstract

ORTEP projection of asymmetric unit of the title complex.

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32



Synthesis, crystal structure and biological properties of a cis-dichloridobis(diimine)copper(II) complex V. Kumbar

S. S. Bhat[®], V. K. Revankar, V. Kumbar[®], K. Bhat and [®] https://orcid.org/0000-0001-6261-1665

Other articles by this author

The mechanisms of interaction of inorganic complexes with design and development of new metal-based drug molecule have encouraged the design and development of new metal cancer drugs having reduced side effects. The complex cis-[1,10]phenanthroline- $\kappa^2 N^1, N^{10}$)copper(II), $[CuCl_2(C_{12}H_6N_{45} Mandal's NGH Institute of Dental Sciences &$ The complex crystallizes in the monoclinic space group C_2/c Research Centre, RS No. 47A/2, Bauxite was studied by absorption spectroscopy. The anticancer act Road, Belgaum, Karnataka 590 010, India Carcinoma (A549) cell line was investigated by MTT assay. platin and induces an apoptotic mode of cell death.

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Keywords: anticancer activity; copper; diimine; cytotoxicity; crystal structure.

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Chemical Data Collections Volumes 17–18, December 2018, Pages 251-262

Crystal structure and Hirshfeld surface analysis of bis (2-(2-(1H-benzo[*d*]imidazol-2-yl)hydrazono)propan-1-ol) nickel(II) chloride

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https://doi.org/10.1016/j.cdc.2018.09.004

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Abstract

The present work describes the crystal structure and Hirshfeld surface analysis of a transition metal coordination complex, bis (2-(2-(1H-benzo[*d*]imidazol-2-yl)hydrazono)propan-1-ol) nickel(II) chloride.Recrystallization of the title complex from aqueous methanol has crystallized the complex in monoclinic crystal system with $P2_1/c$ space group. The asymmetric unit of the complex has two monomeric distorted octahedral coordination entities, along with four chloride anions and seven water molecules as crystallization solvent. The ring puckering analysis, intramolecular hydrogen and halogen bonding interactions and the C—H···π and π - π interactions of the complex are explored. Further, the Hirshfeld surface analysis carried out to reveal the nature and contributions of individual intermolecular interactions and the importance of the C—H···π and π - π interactions in the crystal packing.

Graphical abstract

ORTEP projection of asymmetric unit of the title complex.





Journal of Molecular Structure Volume 1156, 15 March 2018, Pages 115-126

p-halo N4-phenyl substituted thiosemicarbazones: Crystal structure, supramolecular architecture, characterization and bioassay of their Co(III) and Ni(II) complexes

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Highlights

- Crystal structures of three p-halo N4-phenyl substituted thiosemicarbazones are explored.
- Supramolecular assemblies and Hirshfeld surfaces of these thiosemicarbazone ligands are studied.
- A series of cobalt(III) and nickel(II) complexes are synthesized and characterized.
- In vitro antimicrobial activities are presented for the synthesized compounds.

Abstract

In the present work, three potential <u>metal ion</u> chelating ligands, p-halo N4-phenyl substituted thiosemicarbazones are synthesized and characterized. The molecular structure of all (E)-4-(4-halophenyl)-1-(3-hydroxyiminobutan-2-ylidene) thiosemicarbazones (halo = F/Cl/Br) are





Journal of Photochemistry and Photobiology A: Chemistry Volume 351, 15 January 2018, Pages 225-230

Short note

Synthesis, characterization and photophysical studies of zinc(II) complexes derived from a hydralazine hydrazone

Sunil M. Patil ª, Ramesh S. Vadavi ^b, Umashri Kendur ª, Geeta H. Chimmalagi ª, G.H. Pujar ^c, Suresh D. Kulkarni ^d, M. Nethaji ^e, Sharanappa Nembenna ^f, S.R. Inamdar ^c, Kalagouda B. Gudasi ª ペ ⊠

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Highlights

- Two new zinc complexes with different geometry are synthesized using the zinc salts and a <u>hydrazone</u> ligand.
- Photophysical properties in solution phase and solid phase are carried out to have a comparative study.
- <u>Fluorescence quenching</u> in solid phase is accounted for the presence of hydrogen bonding and <u>π</u> – stacking interactions.

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Short note

Synthesis, characterization and photophysical studies of zinc(II) complexes derived from a hydralazine hydrazone



Sunil M. Patil^a, Ramesh S. Vadavi^b, Umashri Kendur^a, Geeta H. Chimmalagi^a, G.H. Pujar^c, <mark>Suresh D. Kulkarni^d, M. Nethaji^e, Sharanappa Nembenna^f,</mark> S.R. Inamdar^c, Kalagouda B. Gudasi^{a,*}

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Keywords: Mononuclear zinc(II) complexes Photophysical properties Quenching Non-covalent interactions Computational studies

1. Introduction

ABSTRACT

In the present study, we report two novel mononuclear zinc(II) complexes (1 and 2) obtained by reacting (*E*)-1-(phenyl(pyridin-2-yl)methylene)-2-(phthalazin-1-yl)hydrazine (L) with ZnCl₂ and Zn(NO₃)₂·6H₂O respectively. Photophysical properties of the compounds were studied in both solution and solid phase. The fluorescence absolute quantum yield of the complexes in solution varies in the order 1 (0.01) < 2 (0.030), on the other hand in the solid state it varies in the order 2(0.034) < 1(0.69). Quenching of fluorescence intensity of 2 in the solid-state has been attributed to intense and extensive non-covalent interactions present in the crystal structure. Theoretical calculations, density functional theory (DFT) and time- dependent density functional theory (TD-DFT) were also performed to support the experimental findings.

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Metal-coordinated organic compounds with luminescent properties have received much attention as potential electroluminescent components [1,2]. The first discovery of a bright and stable emissive material, tris-(8-hydroxyquinolinato)aluminum(III) has lead to an extensive investigation of luminescent materials based on coordination compounds [3]. Fluorescent metal complexes have many advantages such as the combination of emitting and electron transferring holes, higher environmental stability, and a better extent of diversity that is achievable through tuning of electronic properties by virtue of structural and metal-center variability [4]. Photophysical properties of luminescent complexes of earth-abundant, biologically important, essential and cheaper metals such as zinc(II) are gaining much importance in recent years as an alternative to luminescent platinum group metal complexes [5,6]. In the recent past, much attention is given to the study of a variety of non-covalent interactions [7-10]. It is now well

https://doi.org/10.1016/j.jphotochem.2017.10.024 1010-6030/© 2017 Elsevier B.V. All rights reserved. documented that non-covalent interactions like hydrogen bonding and π – stacking interactions form the backbone of the molecular aggregates [11–13]. These interactions can significantly influence the structural motif and consequently several photophysical properties of the systems [14–16]. Several reports have established that the photoluminescence properties of organic compounds are not only associated with the composition of the materials, but also depend on the non-covalent interactions [17]. The hydrogen bonding interactions and interaction between fluorophores, found in the X-ray crystal structures have been proven to be an effective means to explain the solid-state emission quenching and red-shift [18,19]. Very recently a couple of papers have reported the relationship between luminescence property and supramolecular structures of coordination compounds of zinc and cadmium [20,21].

Interest in the hydralazine hydrazones is increasing because of their ligational aspects and applications of their metal associates in various fields [22–24]. Hydralazine hydrazones are used as chemosensors for first-row transition metal ions but their solid state photophysical properties are not yet studied [25,26]. In the present work, we have synthesized a hydralazine hydrazone (Scheme 1) by the condensation of hydralazine hydrochloride with

^{*} Corresponding author. E-mail address: drkbgudasi@kud.ac.in (K.B. Gudasi).

3/1/22, 9:36 PM Dual photoluminescence and charge transport in an alkoxy biphenyl benzoate ferroelectric liquid crystalline-graphene oxide compo... ROYAL SOCIETY OF **CHEMISTRY** Q Q 9 \equiv Þ Log in / register Issue 20, 2018 Previous Next NJC From the iournal: New Journal of Chemistry Dual photoluminescence and charge transport in an alkoxy biphenyl benzoate ferroelectric liquid crystalline-graphene oxide composite † Check for updates Dharmendra Pratap Singh, 🛄 *ab Benoit Duponchel, b Yahia Boussoualem, b Kaushlendra Agrahari, c Rajiv Manohar, c Veeresh Kumar,^d Renu Pasricha, ‡^d Gonibasappa H. Pujar,^e Sanjeev R. Inamdar,^e Redouane Douali^a and Abdelylah Daoudi^b Author affiliations Corresponding authors Unité de Dynamique et Structure des Matériaux Moléculaires (UDSMM), Université du Littoral Côte d'Opale, 62228 Calais, France E-mail: Dharmendra.singh@univ-littoral.fr Fax: +33 21 46 36 42 Tel: +33 21 46 57 81 b Unité de Dynamique et Structure des Matériaux Moléculaires (UDSMM), Université du Littoral Côte d'Opale, 59140 Dunkerque, France С Liquid Crystal Research Lab, Department of Physics, University of Lucknow, Lucknow 226007, India c Electron and Ion Microscopy Division, CSIR-National Physical Laboratory, New Delhi 110012, India

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Abstract

An optimized concentration of graphene oxide (GO) has been dispersed in a ferroelectric liquid crystalline (FLC) material namely 4'-(octyloxy)-[1,1'-biphenyl]-4-yl 4-(heptan-2-yloxy)benzoate, to prepare a FLC–GO composite. Temperature dependent photoluminescence (PL) measurements for the FLC–GO composite were conducted between 30–100 °C. We observed a superlinear increase in the PL with increasing temperature. The time resolved luminescence study exhibits a bi-exponential decay time with a shorter life time for the FLC–GO composite and confirms the surface energy transfer from GO to FLC. Charge transport and current-voltage (*I–V*) characteristics for the FLC–GO composite have been investigated at ambient conditions by using current sensing atomic force microscopy. For the FLC–GO composite, critical diode like

FULL PAPER



WILEY Applied Organometallic Chemistry

Mononuclear Co(III), Ni(II) and Cu(II) complexes of tridentate di-*tert*-butylphenylhydrazone: Synthesis, characterization, X-ray crystal structures, Hirshfeld surface analysis, molecular docking and *in vivo* anti-inflammatory activity

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Funding information UGC, UPE-FAR-I Program, Grant/Award Number: 14-3/2012 A new hydrazone (LH_2) derived from the condensation of 2-(4-fluorobenzamido) benzohydrazide with 3,5-di-tert-butyl-2-hydroxybenzaldehyde was used to synthesize Co(III), Ni(II) and Cu(II) complexes. These were characterized using various physicochemical, thermal, spectroscopic and single-crystal X-ray diffraction techniques. All the complexes crystallize in a monoclinic crystal system with $P2_1/n$ space group and Z = 4. Structural studies of $[Co(L)(LH)] \cdot H_2O$ indicate the presence of both amido and imidol tautomeric forms of the ligand, resulting in a distorted octahedral geometry around the Co(III) ion. On the other hand, in the [Ni(L)(DMF)] and $[Cu(L)(H_2O)]$ complexes, the ligand coordinates to the metal through imidol form resulting in distorted square planar geometry, in which the fourth position is occupied by the oxygen of coordinated DMF in [Ni(L)(DMF)] and by a water molecule in [Cu(L)(H₂O)]. Hirshfeld surface calculations were performed to explore hydrogen bonding and C—H $\cdots\pi$ interactions. Molecular docking studies were carried out to study the interaction between the synthesized compounds and proteins (cyclooxygenase-2 and 5-lipoxygenase). The complexes along with the parent ligand were screened for their in vivo anti-inflammatory activity, using the carrageenan-induced rat paw oedema method. The complexes show significant anti-inflammatory potencies.

KEYWORDS

anti-inflammatory activity, Hirshfeld surface analysis, molecular docking, transition metal complexes, X-ray diffraction study

1 | INTRODUCTION

Over the past several decades, inflammation has been renowned as a devastating burden and the prime basis of various inflammatory-related diseases. The metabolites of arachidonic acid (AA) such as prostaglandins and leukotrienes (generated by cyclooxygenase (COX) and 5-lipoxygenase (5-LOX) enzymatic pathways, respectively) have been associated as mediators in an assortment of diseases, including asthma, inflammation



ScienceDirect

Journal of Molecular Liquids Volume 273, January 2019, Pages 83-87

Influence of concentrations of TiO₂ nanoparticles on spectroscopic properties of a novel HMPP molecule

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Highlights

- A novel 3(2H)-pyridazinone derivative shows fluorescence quenching by TiO₂ NPs.
- S-V plots were found to be linear.
- There exists a strong interaction between investigated molecule with TiO₂ NPs.
- Fluorescence quenching is purely dynamic.

J Cite

• One binding site exists in the investigated molecule for TiO₂ NPs.

Abstract

The influence of concentrations of titanium dioxide (TiO₂) <u>nanoparticles</u> (NPs) on spectroscopic properties of a novel 3(2*H*)-pyridazinone derivative; 5-(2-hydroxy-5-methoxy-phenyl)-2-phenyl-2H-pyridazin-3-one (HMPP) molecule in ethanol as a solvent has been investigated at room temperature. The increase in TiO₂ NPs concentration causes a decrease in the values of absorption, <u>fluorescence intensity</u> and <u>fluorescence lifetime</u> of HMPP molecule. The association constant k_a of HMPP molecule with TiO₂ NPs in the ground state is estimated using the Benesi– Hildebrand relation. A linear Stern–Volmer (S-V) plot is obtained in steady state and transient Influence of concentrations of TiO2 nanoparticles on spectroscopic properties of a novel HMPP molecule - ScienceDirect

state studies. In addition, we have estimated the <u>binding constant</u> and number of binding sites. Results reveal that there is a strong interaction between investigated molecule with TiO_2 NPs, <u>fluorescence quenching</u> in the said system is purely dynamic and also there exist one binding site in HMPP molecule for TiO_2 NPs.

Graphical abstract



Keywords

Pyridazin-3(2*H*)-one; Benesi–Hildebrand relation; Stern-Volmer relation; Fluorescence quenching; TiO₂ NPs

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Microwave assisted synthesis of coumarin-purine derivatives: An approach to *in vitro* anti-oxidant, DNA cleavage, crystal structure, DFT studies and Hirshfeld surface analysis

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Abstract

An easy and efficient microwave-assisted protocol has been developed for the synthesis of coumarin-purine hybrids (**3a-3j**). The newly constructed 1,3dimethyl-7-((substituted)-2-oxo-2*H*-chromen-4-yl)methyl)-1*H*-purine-2,6(3*H*,7*H*)dione derivatives were evaluated for their *in vitro* antioxidant activity by DPPH free radical-scavenging ability assay and DNA cleavage by using calf thymus. The compound **3i**, shows the most excellent DPPH scavenging activity with a –OH substitution at C7 of coumarin ring. In addition, the structure of compound **3f**, has been elucidated using single crystal X-ray diffraction technique. Theoretical calculations (DFT) were carried out using Gaussian09 program package and B3LYP correlation function. Full geometry optimization were carried out using 6-311G++(d, p) basis set and the frontier orbital energy were presented. Hirshfeld surface analysis was used for the intermolecular interactions in the crystal structure. The experimental result of the compound **3f** has been compared





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Synthesis of novel coumarin derivatives bearing dithiocarbamate moiety: An approach to microwave, molecular docking, Hirshfeld surface analysis, DFT studies and potent antimicrobial agents

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Highlights

- A series of novel Coumarin-dithiocarbamate derivatives were prepared.
- The structures of compounds **3a** & **3e** were confirmed by X-ray hirshfeld and DFT studies.
- Compound **3i** shows significant anti-microbial activity.
- Molecular docking studies have shown good binding interactions and are in agreement with *in vitro* results.

Abstract

Bacterial and fungal infections are the major effects to cause the numerous disorders in health. To overcome such disorders there will be needed to carry out the studies to find potent antimicrobial agents from many years. The titled compounds containing coumarinContents lists available at ScienceDirect



Journal of Industrial and Engineering Chemistry

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Polyelectrolyte complex membranes made of chitosan—PSSAMA for pervaporation separation of industrially important azeotropic mixtures



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Keywords: Chitosan Polyelectrolyte complex Azeotropic mixtures Pervaporation Selectivity Activation energy

ABSTRACT

Chitosan-based polyelectrolyte complex membranes (PECMs) were developed by incorporating polystyrene sulfonic acid-co-maleic acid (PSSAMA) in the chitosan membrane matrix as a pervaporation membrane by employing a solution technique. Fourier transform infrared (FTIR) spectroscopy, wideangle X-ray diffraction (WAXD), thermogravimetry analysis (TGA), differential scanning calorimetry (DSC), and scanning electron microscopy (SEM) were used to characterize the membranes. PECMs were tested for their potentiality to separate various azeotropic mixtures; water/ter-butanol, water/ isopropanol, water/n-propanol and water/1, 4 dioxane at their azeotropic point. The PECMs containing 9 mass% of PSSAMA manifest highest separation selectivity of 5352 with a flux of 4.145×10^{-2} kg/m² h for the azeotropic mixture of water/ter-butanol at 30 °C. To confirm their stability at the higher temperature, the PECMs were assessed for pervaporation (PV) separation at 40, 50 and 60 °C. For all PECMs total flux and flux of water appeared to be coinciding each other, signifying that PECMs could be used successfully to break the azeotropic point of various azeotropic mixtures. The Arrhenius activation parameters were determined by diffusion and permeation values. The activation energy values procured for water permeation (E_{pW}) were considerably lower than ter-butanol permeation (E_{pTBOH}). The heat of sorption (ΔHs) values obtained for PECMs were negative, showing that Langmuir's mode of sorption is dominant. © 2019 The Korean Society of Industrial and Engineering Chemistry. Published by Elsevier B.V. All rights reserved.

Introduction

During the last half-century, different types of separation processes have been developed and new processes are continually emerging from academic, industrial, and government laboratories. One of the most well-known membrane separation techniques that act as the core and key point of current membrane research is pervaporation (PV) [1–3]. PV is a membrane separation technology that is advantageous over the traditional distillation processes due to its energy-saving characteristic and the capability to proficiently separate the azeotropic mixtures with close boiling liquid mixtures, dehydrate organic solvents and concentrate aqueous solutions [4,5].

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Today, the main application of PV in the membrane separation technology is the dehydration of aqueous-organic mixtures. Among the many aqueous-organic mixtures, the dehydration of alcohols (ter-butanol, n-propanol, isopropanol) and 1,4 dioxane have gained greater attention because of the increase cost and their importance in different industries. Alcohols (ter-butanol, *n*-propanol, isopropanol) and 1,4 dioxane are most important solvents used on a large scale in the chemical industries [6,7]. PV dehydration performance predominately depends on the manufacture of appropriate membranes with high permeability, good selectivity and adequate mechanical strength [8]. One of the superior candidates for dehydration of organics is polymeric materials with minimal cost, and significantly improved processability [9,10]. Hydrophilic polymers such as poly (vinyl alcohol) (PVA), poly (acryli cacid) (PAA), hydroxyl ethyl cellulose (HEC), sodium alginate (SA) and chitosan (CHS) [11-15] showed strong affinity towards water. A much-favored membrane material among them is chitosan due to its good film-forming properties,

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INVESTIGATION ON GAMMA INTERACTION WITH WATER, CONCRETE, CO-FREE STEEL, PB AND UO2

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Abstract

Shielding materials used in nuclear reactors have to fulfil the requirements regarding their structure, shielding properties, cooling properties, etc. In present analysis, we have investigated radiation interaction parameters with water, concrete, Co-free steel, Pb and UO₂. Gamma ray interaction parameters viz. mass attenuation coefficients, effective atomic numbers and effective electron density have been calculated for energy range 1 keV to 100 GeV. Using these parameters, gamma ray shielding effectiveness was discussed. The investigation would be very useful in shielding performance assessment of materials in nuclear reactors.

Keywords: Shielding, Reactor, Uranium, Water, Co-free steel

Introduction

The gamma ray shielding efficiency is characterized by attenuation of photons in a material. The attenuation of gamma ray is described by linear attenuation coefficient (μ) or mass attenuation coefficient (μ/ρ) of the material for particular photon energy. Higher the values of attenuation coefficients, better is shielding efficiency. In addition to mass attenuation coefficient, effective atomic number (Z_{eff}) and effective electron density (N_{eff}) are other parameters expressing the shielding efficiency. Various studies on interaction of photon with materials are available in the scientific community [1-4].

Gamma radiation is often involved in investigation from nuclear technology, medical applications and industry. High efficient shielding materials are required to maintain low ambient radiation level and improve the level of radiation protection. The shielding materials for gamma ray radiation should be high atomic number elements, compounds or mixture. Various types of radiation shielding materials have been investigated for suitability and are in use in nuclear industries [5-11].

Interaction of photon with a material is dependent mainly on partial photon interaction process such as photoelectric effect, Compton scattering and pair production. These partial interaction processes are dependent on photon energy and atomic number. For a compound or mixture, the partial photon interaction processes depend upon atomic numbers of all the elements. The effect of atomic number will be investigated at different energies.

The objective of present study was to evaluate the shielding efficiencies of water, concrete, Co-free steel, Pb and UO_2 by using mass attenuation coefficients, effective atomic numbers and effective electron densities for photon

energy ranging 1 keV to 100 GeV, their variation with energy being also discussed.

Theoretical basis of investigation

Concrete, steel lead and water are commonly used materials for construction of nuclear reactor containment, biological shielding and cooling fluid. These materials are also selected due their properties of providing shielding against radiations. Natural Uranium (UO₂) is used as a fuel material for power production in nuclear reactors. In present study, investigation on gamma ray interaction with water, concrete, Co-free steel [12], Pb and UO₂ is considered, in order to evaluate shielding effectiveness.

The photon intensity through a medium follows the attenuation law $I = I_0 e^{-\mu t}$, where I and I_0 are transmitted and initial photon densities, μ is linear attenuation coefficient and t is the thickness of medium.

Mass attenuation coefficients

The mass attenuation coefficient of a compound or mixture is calculated using the mixture rule [13], $\mu_m = (\mu / \rho) = \sum_{i}^{n} w_i (\mu / \rho)_i$, where w_i is the proportion by weight and $(\mu / \rho)_i$ is mass attenuation coefficient of *i-th* element. Proportion by weight is given by the relation $w_i = n_i A_i / \sum_{j=1}^{n} n_j A_j$ with the condition $\sum_{i=1}^{n} w_i = 1$, where A_i is

the atomic weight of *i*-th element, n_i is the number of formula units in a compound or composite materials, n_j and A_j are the atomic density and the atomic weight of the *j*-th element. The μ/ρ value of individual element are according to National Institute of Standard Technology and were found using WinXcom program [14].

ORIGINAL PAPER

DETERMINATION OF RELATIVISTIC ELECTRON INTERACTION PARAMETERS OF HUMAN TISSUES UNDER DIFFERENT PATHO PHYSICAL CONDITIONS

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Abstract. We determined experimentally the electron interaction parameters like stopping cross section, mass stopping power and effective atomic number of normal and cancerous - solid and fluid tissues by taking their composition from ICRU-44. The mass stopping power is determined using ¹³⁷Cs and ²⁰⁷Bi internal conversion electrons and Si (Li) detector coupled to an 8K multichannel analyzer as the spectrometer to record the incident and transmitted spectra. The effective atomic numbers of these tissue samples for the relativistic electron interactions are determined by substituting the measured mass stopping power in the semi empirical relation between the mass stopping power and atomic number obtained by plotting the mass stopping power of organic elements against their atomic number. Our experimental results are compared with the theoretical values computed using direct method and found to agree within ±3%. The effective atomic number of the tissues for both electron and photon interactions are observed to be more under cancerous conditions than the normal, paving a way for unambiguous diagnosis of cancer.

Keywords: Relativistic electrons, Interaction Parameters, Mass Stopping Power, Effective atomic number, Effective atomic number for electron interaction.

1. INTRODUCTION

Physical effect of any radiation is the ionization of the matter to release electrons. It is these electrons which interacts with the matter to damage it chemical nature and hence its biological functions. Thus it is necessary to study the electron interaction with matter to understand the radiobiological damages produced in radiotherapy and nuclear medicine.

Hence the measurement of electron interaction parameters (EIP) like Mass Stopping Power (MSP), Energy Loss Straggling, Stopping Cross Section (SCS), Effective atomic Number (Z_{eff}) and Effective electron density became more essential for the medical applications of radiation.

The base of radiotherapy namely radiation dosimeter totally depends on the accurate value of stopping power of electrons in matter. SCS has several applications in radiobiology, medical physics and electron transport modelling.

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Research paper Study the effect of crystal structure on radiative vacancy transfer probabilities from L_3 to M_i , N_i and O_i subshells

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Highlights

- For the first time, effect of crystal structure on L X-rays intensity ratios and radiative vacancy transfer probabilities from L₃ to M_i, N_i and O_i subshells have been measured for Bi and its compounds, Pb and its compounds and Hg compounds using <u>synchrotron radiation</u>.
- We intentionally selected compounds having same oxidation state, chemical bonding with differ in the crystal structure.
- Effect of crystal structure is observed for radiative vacancy transfer probabilities from L_3 to M_i , N_i and O_i subshells.

Abstract

The L X-ray intensity ratios $(I_{L\alpha}/I_{Ll}, I_{L\alpha}/I_{L\beta}, I_{L\alpha}/I_{L\gamma})$ and radiative vacancy transfer probabilities η_{L3-Xi} (X=M, N, O i=1, 4, 5) have been measured for Hg compounds, Pb and its compounds, Bi and its compounds using synchrotron radiation. The L X-ray photons emitted from the elements and compounds are detected with silicon drift detector. The measured intensity ratios and η_{L3-Xi} (X=M, N, O i=1, 4, 5) have been compared with theoretical and other experimental values.

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Synthesis, X-ray characterization, DFT studies and Hirshfeld surface analysis of new organic single crystal: 2-(4-Methoxyphenyl)-4-{[2'-(1*H*-tetrazol-5-yl)biphenyl-4-yl] methyl}-2,4-dihydro-3*H*-1,2,4-triazol-3-one (MTBT)



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ABSTRACT

In this paper, we report the synthesis of a biphenyl molecule containing tetrazole and triazolone moieties (MTBT) and confirmed its structure by elemental analyses, FT-IR, ¹H & ¹³C NMR, GC-MS in addition to single crystal X-ray diffraction study. The molecular geometry, vibrational frequencies and gauge-invariant atomic orbital (GIAO) ¹H and ¹³C NMR chemical shift values of the reporting molecule have been calculated in the ground state using density functional theory (DFT) with the 6-311G(d,p) basis set. The Crystal structure is primarily stabilized through intramolecular C–H···O and C–H···N hydrogen bonds and N–H···O intermolecular hydrogen bonds. Crystal structure analysis was supported with the Hirshfeld surface analysis and fingerprint plots enabled the identification of the significant intermolecular arises from hyper conjugative interactions and charge delocalization. The electronic properties, such as MEP, HOMO-LUMO energies have been analyzed by DFT. The MEP provides the visual representation of the chemically active sites and comparative reactivity of atoms. A large HOMO-LUMO energy gap (3.95 eV) implies a high kinetic stability of the MTBT.

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1. Introduction

Synthesis of biphenyl molecules has grabbed the attention of synthetic organic chemists due to their wide applications in the field of medicinal chemistry and material chemistry. Biphenyls are two adjoined phenyl rings that are attached through their 1,1'-positions. Biphenyls have served as important structural analogs as their derivatives exhibit diverse pharmacological activities such as anti-hypertensive, anti-inflammatory and anti-diabetic [1–6]. In particular, biphenyls containing acidic tetrazoles are key moieties

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of the antihypertensive drugs like Losartan, Candesartan, Olmesartan etc., which are used to treat cardiovascular diseases [7]. Biphenyls are also used in the Organic Light Emitting Diodes (OLEDs) [8] and used as linkers in Dye Sensitized Solar cells [9]. Further, 1,2,4-triazole derivatives exhibit wide spectrum of pharmacological properties like anti-hypertensive, anti-microbial, anti-viral, anticancer [10–13], etc.

The advanced quantum chemical theoretical techniques play an important role in understanding the structure, spectra and various properties of biologically important organic molecules [14]. Recently, Density Functional Theory (DFT) has become the most popular and versatile tool for theoretical modeling, with broad application in the chemical and material sciences for the interpretation and prediction of molecular structure, spectroscopic and other molecular properties [15]. Moreover, DFT methods have proved to be exceptionally effective due to their low computational

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Original research article

Synthesis and photoluminescence properties of titanium oxide (TiO₂) nanoparticles: Effect of calcination temperature



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ARTICLE INFO

Keywords: Titanium oxide Nanoparticles Effect of calcination temperature Photoluminescence Optical properties

ABSTRACT

In the present work, we report photoluminescence properties of TiO₂ nanoparticles synthesized by chemical co-precipitation method using titanium oxysulphate and sodium hydroxide as a primary sources. The nanopowder is calcinated at different temperatures ($300 \,^\circ$ C, $400 \,^\circ$ C, $500 \,^\circ$ C and $600 \,^\circ$ C). The effect of calcination temperature on structural, morphological and optical properties of TiO₂ nanopowder is investigated through XRD, FESEM, EDX, FTIR, UV–Vis absorption and fluorescence emission spectroscopy. XRD spectra confirms the formation of TiO₂ in anatase phase and degree of crystallinity of samples increases with calcination temperature. At 600° C the phase transition from anatase to anatase-rutile mixed phase is noticed. The FESEM shows the nanophase with irregular morphology of the particles. EDX and FTIR spectra confirms the formation of TiO₂ in crystalline phase. The absorption spectra shows strong quantization up to 10 nm in contrast to earlier studies and is explained by indirect band transition rather than direct interband transition. Photoluminescence spectra exhibits the change in intensity and peak position with calcination temperature and is in accordance with indirect transition.

1. Introduction

In recent past metal oxides nanoparticles, in particular Titanium Oxide (TiO_2) nanoparticles have become a promising material due to their unique properties [1,2].TiO₂ besides having wide range of applications such as dye-sensitized solar cells [3], photocatalysis [4,5], photovoltaics [6], photo sensors [7,8], electrode materials [9], self-cleaning agent [10], pigment in paints [11], cosmetics [12], purification of water and air [13], possesses high refractive index [14], high dielectric constant [15] and highly photoactive surface as compared to other metal oxides. Because of its band gap (3.2 eV), it finds application in a solar cells as a photo catalyst. Among its three polymorphs - anatase, brookite and rutile, the anatase is suitable for photo catalysis due to its high photo stability and photo sensitivity [16]. The optical properties of metal oxide nanostructures are sensitive to structure, size and composition. The optical properties of TiO_2 is peculiar in many facets. The optical anisotropy and the controversy about the existence of size quantization puts an additional complexity on optical properties. Further, there is no consensus till today about the direct and indirect band transition in this genuine indirect band semiconductor.

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Mycogenic Selenium Nanoparticles as Potential New Generation Broad Spectrum Antifungal Molecules [†]

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- + Running title: Trichoderma SeNPs exhibits broad spectrum antifungal properties.

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Abstract: The current challenges of sustainable agricultural development augmented by global climate change have led to the exploration of new technologies like nanotechnology, which has potential in providing novel and improved solutions. Nanotools in the form of nanofertilizers and nanopesticides possess smart delivery mechanisms and controlled release capacity for active ingredients, thus minimizing excess run-off to water bodies. This study aimed to establish the broad spectrum antifungal activity of mycogenic selenium nanoparticles (SeNPs) synthesized from Trichoderma *atroviride*, and characterize the bioactive nanoparticles using UV–Vis spectroscopy, dynamic light scattering (DLS), Fourier transform infrared (FT-IR), X-ray diffraction (XRD), scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS), and high-resolution transmission electron microscopy (HR-TEM). The synthesized nanoparticles displayed excellent in vitro antifungal activity against Pyricularia grisea and inhibited the infection of Colletotrichum capsici and Alternaria solani on chili and tomato leaves at concentrations of 50 and 100 ppm, respectively. The SEM-EDS analysis of the bioactive SeNPs revealed a spherical shape with sizes ranging from 60.48 nm to 123.16 nm. The nanoparticles also possessed the unique property of aggregating and binding to the zoospores of *P. infestans* at a concentration of 100 ppm, which was visualized using light microscope, atomic force microscopy, and electron microscopy. Thus, the present study highlights the practical application of SeNPs to manage plant diseases in an ecofriendly manner, due to their mycogenic synthesis and broad spectrum antifungal activity against different phytopathogens.

Keywords: Trichoderma atroviride; selenium nanoparticles; broad spectrum; antifungal agents

1. Introduction

Nanoparticles are gaining rapid momentum in plant disease management due to their large surface area to volume ratio, which allows them to establish better contact with microorganisms, thus leading to enhanced antimicrobial activity [1,2]. The synthesis of nanoparticles by fungi, also called myconanotechnology, is an emerging branch of nanotechnology that has the potential to meet the crucial needs of disease control and crop management [2–4]. The application of myco-nanostructures can effectively reduce the excessive use of agrochemicals and site targeted active ingredients [4–6]. The bio-reduction of metal oxides to their elemental form is catalyzed mainly by the extracellular





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A NOVEL AND EFFICIENT METHOD TO SYNTHESIS MICONAZOLE ANALOGUE AND ITS INTERMEDIATES

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ABSTRACT

An alternative method for the preparation of Micanozole intermediate 1-(2,4-dichlorophenyl)-2-(1H-imidazol-1yl)ethanolis described, process involves the 2,4-Dichlorocaetophenone as the key raw material from which the substituted 2-chloro-1-(2,4-dichlorophenyl)ethanone was prepared. 2-chloro-1-(2,4-dichlorophenyl)ethanone was reduced to 2-Chloro-1-(2,4-dichlorophenyl)ethanol and via S_N^2 reaction with imidazoles the 1-(2,4-dichlorophenyl)ethanol. 2-(1H-imidazol-1-yl)ethanol was obtained, further1-(2-(2,4-dichlorobenzyloxy)-2-(2,4-dichlorophenyl)ethyl0-1Himidazole was synthesized.

Keywords: Micanozole, Antifungal, Imidazoles, Fungal infections

RASAYAN J. Chem., Vol. 14, No.1, 2021

INTRODUCTION

Fungal infections on skin, mucosa and hair are due to dermatophytes, induced by pathogens collectively known as tinea, Candida albicans cause vulvovaginitis and oral candiasis. The fungal infection has greatly increased as a consequence of various factors in immune-suppressed patients.¹

Patients with incompetent immune systems have a large contribution to both increased use of antifungals and the evolution of resistant organisms.³ In this setting, more efficient formulations are an attractive alternative to the systematic treatment of fungal diseases. Miconazole is one such medication as an antifungal drug for many fungal diseases.⁴⁹

Micanozole is a synthetic lipophilic compound that was initially for topical use, also it is used orally and intravenously,¹⁰⁻¹³ it was the first patented¹⁴ in 1968 and approved for medical use in 1971, World Health Organization considers it as one among the essential medicine, the most effective and safe medicines in health system.¹⁵

Prior art on micanozole synthesis disclosed in patent¹⁴ in 1973 involves the 2,4-Dichlororo phenacyl chloride as the key starting material reacting with imidazoles to yield intermediate 2-(1-Imidazolyl) 2,4-Dichloroacetophenone further reduced to ethanol. Sodium salt of ethanol reacted with substituted benzylchloride to yield micanozole. The later patents published involve the 2,4-Dichloro-α-chloroacetophenone or 2-Chloro-1-(2,4-dichlorophenyl) ethanol as key starting material ¹⁷. One of the recent Chinese patents discloses the synthesis of micanozole by preparing the 2,4-Dichloro-a-chloroacetophenone by halogenation of 2,4-Dichloroacetophenone^{16,18}. Remaining non-commercial synthetic route^{1,19-20} involves 2-(2,4-dichlorophenyl)oxirane and 2,4-Dichlorobenzaldehyde as the starting material.2

The process or synthetic methods discussed above has shortcomings like a tedious process, side products, low yield, costly raw material. Therefore there is scope for the alternative method or to improve the process. Therefore we have developed a synthetic route starting from 2,4-dicloroacetophenone as Kew raw material.

EXPERIMENTAL

In the new method developed, the 2-chloro-1-(2,4-dichlorophenyl)ethanone(1) used as starting material for miconazole was prepared by carrying out fridalcraft acylation of m-Dichlorobenzene with chloroacetyl <u>و</u>

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Research Article

SYNTHESIS, ANTIFUNGAL AND ANTI BACTERIAL ACTIVITY OF N-(4-CHLORO-2-TRIFLUOROACTYL PHENYL) - AMINOTHIAZOLE DERIVATIVES Sujatha K^{1*}, Shilpa², Ramesh S.Gani² ¹Department of Chemistry, Karnatak Universty, Pavate Nagara Dharwad-580003 India ²Department of Chemistry, JSS, Dharwad-580003, India ³Department of Industrial Chemistry, Mangalore University, Mangalagangothri-575199, India

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DOI: 10.7897/2230-8407.1004141

ABSTRACT

In this study,1-(2-amino-5-chlorophenyl)-2,2,2-trifluoroethanone was synthesized by reacting p-chloroaniline with ethyl trifluroacetate in presence of n-butyl lithium, further reacting with ammonium thiocyanate with hydrochloric acid leads to 1-(4-chloro-2-(2,2,2-trifluroacetyl)phenyl)urea. Then reacted with ArCOCH2BT and sodium acetate gave 1-{5-chloro-2[(4-substituted-1, 3-thiazo1-2-yl) amino] phenyl)-2,2,2-trifluroethanone derivatives. The chemical structure of newly synthesized compounds has been confirmed on the basis of elemental analysis, IR, ¹H NMR and Mass spectral data. The newly synthesized compounds were screened for their antibacterial activity invitro against Gram-positive bacteria namely Escherichia coli, Staphylococcus aureus, and Gram-negative bacteria namely Pseudomonas aeruginosa, Bacillus subtilis and the fungus namely Candida albicans by disc diffusion method. Among the synthesized compounds 5b, 5f, 5g, 5h, 5j were found to have a very good antibacterial and antifungal activity.

Key words: Aminothiazole, trifluroetahnone, thiosemicarbazone, antibacterial, antifungal.

INTRODUCTION

Now days due to increase in no of multi-disease, consumption of antibiotic drugs quantity is increasing because of this reason abnormal side effects have become predominant, therefore, pathogenic bacteria¹ has developed resistance to beta lactam antibiotics. The thiazole and its derivatives are playing a very important role in medicinal chemistry. Its intermediates are used as synthetic drugs, dyes and fungicides². Due to the Therapeutic importance of heterocyclic compounds, chemists are showing more interest in the preparation of new heterocyclic compounds, in order to explore their biodynamic properties³⁴. Nitrogen and sulfur containing organic compounds show wide range of biological activity⁵. According to the literature survey 2-amino thiazole nucleus have been incorporated into a wide variety of therapeutically interesting candidates. Thiazoles Particularly are showing effective antimicrobial activity⁶⁻¹⁰. Fungal infections are caused by microscopic organism that can invade the epithelial cells in immune compromised¹¹ patients. Simple 2-aminothiazole is known as thyroid inhibitor¹². In market many 2-aminothiazole derivatives drugs such as sulfathiazole and ceftibuten encouraging us to synthesize aminothiazole derivatives 13-14 Ritonavir is an anti-HIV agent, Nizatidine is an antacid used for the treatment of gastroesophageal reflux disease, dasatinib is an antineoplastic agent and ravuconazole is an antifungal agent15. Thiazole derivatives not only show potent FabI and FabK inhibitory activity, but also have an antibacterial effect. Abafungin is the low toxic thiazole containing antimicrobial¹⁶ present in market, which unlike imidazole and triazole antifungals directly impairs the fungal cell membrane and in addition inhibits stero-2,4-methyl transformation modifying the composition of cell membrane, it also acts as antibiotic against Gram +ve 5-fluorocytosine is an antifungal used along bacteria.

with amphotericin –B specifically for serious candida infection. Cefdinir is broad spectrum cephalosporin antibiotic used for treatment of pneumonia, chronic bronchitis, sinusitis, pharyngitis, tonsillitis¹⁷, 4-Chloro-2-(trifluoroacetyl)aniline is one of the important pharmacophore found in the anti HIV Effavirenz, the fluorine containing moiety are most widely found in active pharma ingredients due its high biological activity. Due to the demand of the trend for more safe and effective antifungal agents made us to bring two different biologically active scaffolds like 2-aminothiazole and 4-Chloro-2-(trifluoroacetyl)aniline in one frame to synthesis new and novel thiazole derivative having very good antimicrobial activity.

MATERIALS AND METHODS

The general method to prepare the title compounds is outlined in scheme 1. The synthesis of 2-mercaptothiazoles was first attempted in a stepwise manner via the isolation of intermediate. Phenacyl bromides (1a-k) employed in the preparation of 2.4-disubstituted-1,3-thiazoles (5) are prepared by the reaction of various substituted acetophenones with bromine in chloroform at 0°C. However in few cases readily available phenacyl chlorides were used instead of phenacyl bromides. Further reaction of 4-Chloro-2-(trifluoroacetyl)aniline hydrochloride with ammonium thiocyanate was carried out by heating the mixture of 4-Chloro-2-(trifluoroacetyl) substituted phenyl] thiourea (4). 4-Chloro-2-(trifluoroacetyl) substituted phenyl] thiourea (4). 4-Chloro-2-(trifluoroacetyl)aniline (3) was in turn obtained by the reaction of p-chloroniline with ethyl trifluoroaceta in presence of n-butyl lithium at -70°C. The Hantz reaction of 1-[4-Chloro-2-(trifluoroacetyl)] thiourea (4) with appropriate phenacyl bromides (1a-k) in aqueous alcoholic medium employing sodium

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SYNTHETIC STUDIES ON 3-ARYLOX YETHYL-4-ARYLIDENE AMINO-5-MERCAPTO-1,2,4-TRIAZOLES AND BIOLOGICAL EVALUATION AS ANTIFUNGAL AND ANTIBACTERIAL AGENTS

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ABSTRACT

A novel series of 3-aryloxyethyl-4-arylidene amino-5-mercapio-1,2,4-triazoles were prepared from 5-(α aryloxy ethyl)-1,2,4 triazole. The structures of new compounds have been established by spectral and analytical data. The sewly synthesized compounds have been tested for their antimicrobial activity. Keywords: Triazole, Schiff's Base, Docking Study.

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INTRODUCTION

Azoles are the most widely used antifungal agents in current clinical use.¹ Due to the increased incidence of invasive fungal infections worldwide in the past two decades.²³ IFIs increased the high rate of morbidity and mortality and to diagnose, treat and prevent is the most difficult task. *Condida* spp. is the fourth most common nosocomial pathogen causing the highest crude mortality rate (40%) in USA.⁴ In patients with hematological malignancies³ apart from *Aspergillar* spp., new and emerging fungal pathogens like *Zygomyceics*, *Fasarian* spp. Or *Scedosporian* spp. have become major pathogens resulting in mortality rate is \geq 70%. Their susceptibility to a currently available antifungal is limited.

The Standard systemic antibiotic therapy is unsatisfactory in certain circumstances. More attention has to be focused on solving the problem of multidrug-resistant bacteria and the staggering costs and consequences resulting from this. The resistance developed by microorganisms for many antimicrobial agents compels to search for new synthetic antimicrobial substances.

Triazole moiety can be considered as a bioisostere of imidazole, which imparts the main functional role in the azole group of antifungal drugs (i.e., fluconazole). The biological activities of various triazole derivatives have been extensively studied. Even though triazole and imidazole are five membered ring beterocycles, triazoles contain three-ring nitrogen atoms, and imidazole has two. On comparison of triazoles with imidazoles (clotrimazole, ketoconazole, miconazole), triazoles exhibit greater target specificity, increased potency and an expanded spectrum of activity and moreover are less susceptible to metabolic degradation.⁶¹

Triazole has versatility infusing to various ring systems and possesses a broad spectrum of biological activity. Since triazole is capable of forming more hydrogen bond, which is the most essential aspect in binding biomolecular targets as well as to increase the solubility.⁸ Moreover, to have an innovative bifunctional drug, triazoles can function as attractive linker units which could connect two pharmacophores, and thus plays a vital role in constructing bioactive and functional molecules.⁹¹¹ significantly expanding the chemical space of triazole scatfolds possessing potent activities or enhancing biological activities.¹² Additionally, extensive studies have shown that the addition of alkyl chains and/or

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REVIEW



Estimation of Photophysical and Electrochemical Parameters of Bioactive Thiadiazole Derivative

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Abstract

The absorption and fluorescence spectra of synthesized 4-[5-(2,5-Dimethyl-pyrrol-1-yl)-[1, 3, 4] thiadiazol-2-ylsulfanylmethyl]-6-methoxy-chromen-2-one (DTYMC) compound were recorded in various solvents like acetone, acetonitrile, chloroform, dimethyl formamide (DMF),1,4-dioxane, ethanol, ethyl acetate, methanol, tetrahydrofuran (THF) and dimethylsulphoxide (DMSO) at room temperature in order to estimate the ground and excited state dipole moment. The ground state dipole moment (μ_g) and excited state dipole moment (μ_e) were calculated using solvatochromic shift method which involve equations proposed by Lippert, Bakshiev and Kawski-Chamma-Viallete. The results were signified that the excited state dipole moment is greater than the ground state dipole moment, which indicates the excited state is more polar than the ground state of the molecule. The bond angle between the ground state and excited state dipole moments were found to be 0⁰, The change in dipole moment ($\Delta\mu$) was calculated using microscopic solvent polarity parameter (E_T^N). Further multiple linear regression analysis of Kamlet-Taft parameter, HOMO-LUMO energy were determined by cyclic voltammetry using phosphate buffer solution.

Keywords DTYMC molecule \cdot Solvatochromic shift \cdot Cyclic voltammetry \cdot Scan rate \cdot HOMO-LUMO calculation \cdot The Kamlet-Taft multiple linear analyses

Introduction

The synthesis of triheterocyle is having coumarin, thiadiazole and pyrrole moieties in its structure called 4-[5-(2,5-dimethyl-pyrrol-1-yl)-[1,3,4]thiadiazol-2-ylsulfanylmethyl]-6-methoxy-chromen-2-one (DTYMC). Coumarin derivatives have huge applications in the field of pharmacological, biological activities, these derivatives are used in fluorescent probes for metal ions [1], polymer-ic materials of their immense performance [2], coumarin

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influenced in the structural, morphological and optical properties of the CdO films [3]. Highly efficient energy transfer can be done by coumarin 153 to the gold nanoparticles of various dimensions [4]. Highly selective turn on coumarin fluorescent probe for detecting Al³⁺in aqueous systems [5]. 1,3,4-thiadiazoles were used in pharmaceuticals, agrochemicals and material chemistry [6] and also used as high sensitive fluorescent probes for pH of medium [7]. Pyrroles are used as electropolymerization [8]. Polypyrrole used mainly because of high electrical conductivity applications in fabrication of actuators, electrochromic devices and sensors, electroactive pyrrole used in degradation of organophosphate [9]. The fused heterocyclic compounds have been used in various applications like fluorescent probes for detecting for Cu²⁺ ions in biological systems [10]. Coumarin fused coumarin has radical scavenger activity and it is able to inhibit the DNA oxidations caused by the OH, Cu²⁺ even in the absence of hydroxyl group [11].

The synthesized DTYMC molecule, has no reports available based on photophysical and electrochemical studies, most of the researches were studied recently on

Copper-Doped Nickel Zinc Nanoferrites by Solution-Combustion Synthesis Using Sucrose as a Fuel

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Abstract—Copper-doped nickel zinc nanoferrites $Ni_{0.45}Zn_{0.55-x}Cu_xFe_2O_4$ (x = 0.0, 0.1, 0.2, 0.3) were prepared by solution-combustion synthesis using sucrose as a fueland characterized by XRD, TEM, FTIR, and Raman spectra. The XRD results suggest the formation of single-phasenanoferrites with a cubic spinel structure. The FTIR spectra of synthesized nanoferrites showed two strong absorption bands (v_1 and v_2) at 569 cm⁻¹ and 422 cm⁻¹. For synthesized materials, their structural and elastic parameters were determined as a function of x. Our results may turn interesting to those engaged in combustion synthesis of substituted ferrites.

Keywords: solution-combustion synthesis, sucrose method, Cu-doped Ni–Zn nanoferrites, structural/elastic parameters

DOI: 10.3103/S1061386220040135

1. INTRODUCTION

Due to their interesting physics, nanoferrites have gained much attention in recent research [1] and found numerous applications in technology, industry, and medicine [2]. Among others, Ni-Zn ferrites are more significant due to their wide application [3] in frequency devices in view of their higher electrical resistivity and low eddy-current losses [4, 5]. The ferrites prepared by ceramic route are coarse and non-uniform [1]. To overcome these drawbacks, several methods of synthesis such as sol-gel [6, 7], co-precipitation [8, 9], reverse micelle technique [10, 11], and oxidation [12] are employed. To our knowledge, the synthesis of Ni_{0.45}Zn_{0.55-x}Cu_xFe₂O₄ nanoferrites has not been reported so far.

In this communication, we report on the structural and elastic properties of $Ni_{0.45}Zn_{0.55-x}Cu_xFe_2O_4$ nanoferrites prepared by solution-combustion synthesis (SCS) using sucrose as a fuel.

2. EXPERIMENTAL

AR grade nitrates of nickel, zinc, copper, and iron were taken in stoichiometric amounts and dissolved in double distilled water. To this solution, 10% PVA solution and sucrose solution were added to get a homogeneous mixture. This mixture was kept at 80°C on a magnetic stirrer until disappearance of NO₂ fumes and then heated on low flame until the mixture turned into a mass that burned like a live charcoal to yield ferrite powders. Synthesized nanoferrites were characterized by XRD (Rigaku IV Ultima diffractometer), FTIR spectra (Cary 660 FTIR spectrometer), Raman spectra (SEKI Technotron Model STR-300 spectrometer), and TEM (FEI model Titan G2 60 300 machine).

3. RESULTS AND DISCUSSION

3.1. XRD Analysis

Figure 1 shows the diffraction patterns of synthesized Ni_{0.45}Zn_{0.55-x}Cu_xFe₂O₄ nanoferrites with different x. The peaks were indexed by comparing with ASTM data [13]. Lattice parameter a, crystallite size D, dislocation density $1/D^2$, A-site and B-site bond lengths(A–O, B–O), site radii (r_A , r_B), micro strain ε , and X-ray density ρ were calculated as described elsewhere [14] and the results are collected in Table 1.

Lattice constants *a* are seen to grow with decreasing *x*. Because of smaller radius of Cu ion (0.70 Å) compared to that of zinc (0.82 Å), Cu²⁺ displaces Zn²⁺ and acts according to Vegard's law [13]. The crystallite size was around 14 nm. The bond lengths and site radii

Cobalt-Doped Nickel Zinc Nanoferrites by Solution-Combustion Synthesis: Structural and Elastic Parameters

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Abstract—Cobalt-doped nickel zinc nanoferrites $Ni_{0.45}Zn_{0.55-x}Co_xFe_2O_4$ (x = 0.0, 0.1, 0.2 and 0.3) with a particle size of 8–12 nm were prepared by solution-combustion synthesis (SCS) using sucrose as a fuel and characterized by XRD, FTIR, Raman, and TEM techniques. For synthesized materials, their structural and elastic parameters were determined as a function x. Our results may turn interesting to those engaged in combustion synthesis of ferrites.

Keywords: solution-combustion synthesis, sucrose as a fuel, nanoferrites, structural/elastic properties **DOI:** 10.3103/S1061386220030115

1. INTRODUCTION

Because of their small size and large surface area, Ni–Zn nanoferrites exhibit surprisingly unusual physicochemical properties that strongly differ from those of bulk materials [1–3]. Preparation of ferrites through solid-state reaction requires high calcination temperature which in turn results in aggregation of particles [3]. To date, a number of methods have been employed to synthesize nanoferrites such as mechanical alloying [4], sol–gel [3], hydrothermal-microwave [5], pulsed wire discharge [6], microemulsion [7], coprecipitation [8], hydrothermal processes [9] and aerosolization [10].

In this communication, we report on the preparation of $Ni_{0.45}Zn_{0.55-x}Co_xFe_2O_4$ nanoferrites (x = 0.0, 0.1, 0.2, 0.3) by solution-combustion synthesis (SCS) using sucrose as a fuel and their characterization.

2. EXPERIMENTAL

AR grade nickel nitrate hexahydrate $Ni(NO_3)_2 \cdot 6H_2O$, zinc nitrate hexahydrate $Zn(NO_3)_2 \cdot 6H_2O$, cobalt nitrate trihydrate $Co(NO_3)_2 \cdot 3H_2O$, and iron(III) nitrate $Fe(NO_3)_3 \cdot 9H_2O$ were taken in stoichiometric amounts and dissolved in double distilled water. To this mixture, 10% solution of polyvinyl alcohol (PVA) in double distilled water and aqueous solution of sucrose were added and stirred vigorously until homogeneity. The resultant mixture was held at 80°C

3. RESULTS AND DISCUSSIONS *3.1. XRD Results* The XRD spectra of combustion-synthesized ferss are shown in Fig. 1.The peaks were identified by papering with ASTM data [11]. The absence of any

(SEKI Technotron, Model STR-300).

used in further experiments.

rites are shown in Fig. 1. The peaks were identified by comparing with ASTM data [11]. The absence of any other peaks confirms that SCS reactions yielded single-phase nanoferrites [12]. Structural parameters—lattice parameter *a*, crystallite size *D*, dislocation density $1/D^2$, bond lengths A–O and B–O, site radii r_A and r_B , micro strain ε , and X-ray density ρ —were obtained as described elsewhere [12] and the results are collected in Table 1.

for 1.5 h in a magnetic stirrer. The solution emitted NO_2 fumes and turned dark brown. The latter was put

in a beaker and heated on a low-flame gas stove until

it turned into a mass that burnt like live charcoal.

During this process, large amounts of NO, NO₂, CO,

CO₂ gases and water vapors were released to leave a

remnant of ferrite powder. After grinding in an agate

mortar for 1 h, we obtained fine powders that were

(Rigaku IV Ultima diffractometer, $Cu-K_{\alpha}$ radiation),

TEM (FEI model: Titan G2 60 300 apparatus), FTIR

(Nicolet 6700 spectrometer), and Raman analyses

Product powders were characterized by XRD

ORIGINAL PAPER



Development of novel 3D scaffolds using BioExtruder by varying the content of hydroxyapatite and silica in PCL matrix for bone tissue engineering

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Abstract

Polycaprolactone (PCL) is considered as a most widely used biodegradable polymers in tissue engineering. But, PCL is also associated with certain limitations like, low stiffness, hydrophobic nature and limited cell affinity. These drawbacks are addressed in the present study by incorporating different wt% of silicon dioxide (SiO₂) and hydroxyapatite (HAp) in the PCL matrix. 3D scaffolds were developed using a novel BioExtruder. The physicochemical properties, thermal stability and wettability of the composite scaffolds were studied systematically. Optical and Scanning Electron Microscopic images were analysed for morphological evaluation of the scaffolds. The pore size of the developed scaffolds increased from 290 to 315 μ m with increasing SiO₂ content, as examined by scanning electron microscope. An improved compressive modulus of 68.82 MPa was observed for 15 wt% SiO₂ incorporated composite scaffold. The in-vitro degradation study of the composite scaffolds demonstrated an increase in the degradation rate for PCL/HAp scaffolds, while no significant change was observed for SiO₂ incorporated scaffolds revealed no toxic effects towards the cellular response and an increase in cell proliferation of \geq 90% was observed during 7 days of cell culture. Thus, the scaffolds were proved to be potential candidate for bone tissue engineering application, particularly the scaffold with 10 wt% SiO₂ incorporation into PCL/HAp (75/15) composite has resulted into higher cell proliferative % and improved mechanical strength.

Keywords Biodegradable · Scaffold · Bone tissue engineering · Three dimensional · Wettability · Biocompatibility

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Introduction

Bone tissue repair is one of the widely emerging areas under the field of tissue engineering and regenerative medicine. Bone has a hierarchical structure at multiple length scales which provides multiple functions such as, structural support, protection and storage of healing cells, and mineral ion homeostasis [1-3]. Under a variety of clinical situations the natural bone regeneration fails and it is necessary to undertake an interventional therapy. Bone grafting was one of the earlier methods for bone tissue repair. The grafting of bone in reconstructive surgery is based on the principle of replacing defective tissues with viable and functioning alternatives. It provides the structural stability and osteogenic behaviour to the defective site. But the method was not proved to be 100% effective because of some immunogenic responses to the foreign tissue as well as leading to some inflammatory reaction [4, 5]. To overcome this, a new approach of bone tissue engineering (BTE) has come to picture which includes the use of

Evaporation-residue-gated spin distribution measurements of the highly fissile compound nucleus 224 Th* through 16 O + 208 Pb and 18 O + 206 Pb reactions

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Measurements of cross sections of evaporation residue (ER) and spin distributions of heavy nuclei, produced via compound nuclear fusion-evaporation reactions, provide crucial information about the dynamics of nuclear fission and the survival probability of the system against fission. Such measurements help in probing the evolution of the compound system from equilibrium to the saddle and the underlying role of nuclear dissipation in hindering fission. The purpose of the present measurements is to understand the survival probability of the ²²⁴Th* compound nucleus against fission and its dependence on angular momentum. Measurements of the ER cross sections and spin distributions have been carried out for the ¹⁶O + ²⁰⁸Pb and ¹⁸O + ²⁰⁶Pb reactions which form the same ²²⁴Th* compound nucleus. The two reactions have been carried out at laboratory energies ranging from 87 MeV to 122.6 MeV and 85.7 MeV to 121.4 MeV, respectively. The measurements have been performed at Inter University Accelerator Centre, New Delhi using the Hybrid Recoil mass Analyzer in gas-filled mode, coupled with the 4π spin spectrometer of Tata Institute of Fundamental Research. The reduced ER cross sections ($\sigma_{ER}/\pi R_B^2$) for both systems are comparable at low excitation energies while at higher excitation energies the ¹⁸O + ²⁰⁶Pb system shows nearly 50% higher values. However, the ¹⁸O + ²⁰⁶Pb system shows lower mean γ ray multiplicity (and hence lower mean angular momentum) at all excitation energies which is a surprising result.

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I. INTRODUCTION

Heavy-ion-induced nuclear fusion-evaporation reaction is a well established tool to understand the nuclear dynamics at different stages of fusion-fission process and the associated time-scale. The dynamic properties of a fused compound nuclear system can be studied by measuring the evaporation spectra of neutrons, charged particles, giant dipole resonance (GDR) γ rays and evaporation residues (ERs). The evolution of the compound system from the initial equilibrium state to the scission point as a function of the deformation can be mapped by studying the different evaporation spectra. The emitted particle/radiation (charged particles, neutrons, and γ rays) also serve as clocks for the dynamically evolving system. The observed excess of pre-scission particles and GDR γ rays in comparison with standard statistical model predictions indicates hindrance to the fission process. Frobrich et al. [1] pointed out that ERs are the most sensitive and suitable probes for studying the dynamics of fusion-fission process in presaddle region. The hindrance in nuclear fission process due to nuclear viscosity increases the pre-saddle and/or pre-scission life time of compound nucleus (CN) and leads to enhanced yields of evaporation residues. Therefore, measurements of ER cross sections and spin distributions would, undoubtedly, provide the necessary information on nuclear fission and the possible role of nuclear viscosity hindering it. It is also understood that the ER production cross section is the only

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Pre-scission neutron multiplicity in the ${}^{32}S + {}^{184}W$ reaction

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The neutron energy spectra in coincidence with both the correlated fission fragments in ${}^{32}\text{S} + {}^{184}\text{W}$ reaction forming the compound nucleus ${}^{216}\text{Th}$ at an excitation energy of 71.31 MeV have been measured at various angles with respect to one of the fission fragments. Pre- and post-scission neutron multiplicities of 2.68 ± 0.48 and 3.3 ± 0.20 , respectively, have been extracted by analyzing angular correlation of the neutron energy spectra using moving source fitting procedure. The excess pre-scission neutron multiplicity in comparison to statistical model JOANNE2 code predictions have been converted into total fission delay. A comparative study of fission delay has been carried out for the ${}^{16}\text{O} + {}^{208}\text{Pb}$ reaction forming the compound nucleus ${}^{224}\text{Th}$ at similar excitation energy as in ${}^{32}\text{S} + {}^{184}\text{W}$ reaction. Both the reactions have been analyzed within the frame work of JOANNE2 code including fission delay, deformation dependent level densities, particle binding energies, and transmission coefficients. The observed fission delay for both the reactions can be quantitatively understood if different formation time predicted by dynamical model HICOL code are considered.

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I. INTRODUCTION

Heavy-ion-induced fusion-fission (HIFF) dynamics is an area of current research due to prominent signatures of entrance channel effects in fission-fragment mass distributions and particle multiplicities. A variety of experiments have been carried out in the past to explore the shell and dissipative effects in the HIFF process with various possible projectile and target combinations around the Coulomb barrier [1-8]. One of the major puzzles of HIFF reactions is the fission hindrance. The fission hindrance can be understood in terms of dissipation and fission delay time, which are responsible for the increased survival probability of the compound nucleus (CN), which in turn increases the emission of light charged particles, γ rays and neutrons from the excited CN. Extensive studies have been carried out in the past to estimate the fission delay time from pre-scission neutron, proton, α , and giant dipole resonance γ rays measurements in HIFF reactions [9-16]. The measured pre-scission neutron multiplicities were observed to be higher as compared to the statistical model predictions indicating the dynamical effect of nuclear fission. The cause for the excess emission of prescission neutrons arising from three distinct origins in FF dynamics can be qualitatively understood as follows. First, due to nuclear deexcitation an excess number of neutrons will be emitted from temperature equilibrated intermediate dinuclear system during its evolution towards the formation of CN, which is termed as formation delay (τ_{fr}). Second, as reported by Kramer [17] dissipation will delay the onset of fission event due to the occurrence of finite transition time as the equilibrium configuration diffuses over the saddle point causing an excess emission of neutrons. This delay is termed as transient delay (τ_{tr}). Third, in the postsaddle phase, dissipation causes excess emission of neutrons during the dynamical evolution of the system from saddle point to scission point (τ_{ssc}).

Since the last decade extensive measurements on neutrons in coincidence with fission fragments have been carried out for various entrance channel mass asymmetries at different excitation energies to provide an adequate explanation for excess emission of pre-scission neutrons during the presaddle to postsaddle region [1–5,11]. Wei has reported lower prescission neutron multiplicity (v_{pre}) for shell-closed (N = 126) ²¹⁶Th nucleus compared to non-shell-closed ²¹⁴Th nucleus [10]. Sandal *et al.* [11] have measured the v_{pre} for the compound nuclei ^{210,212,214,216}Rn formed in the reactions ^{16,18}O + ^{194,198}Pt in the excitation energy (E^*) range of 50–79 MeV and reported lower dissipation (β) for shell-closed ²¹²Rn isotope at the lowest $E^* = 50$ MeV.

In earlier works, fission-fragment angular distributions and the evaporation residue (ER) cross sections have been studied to understand the fusion-fission (FF) dynamics in the ${}^{32}\text{S} + {}^{184}\text{W}$ reaction. Zhang *et al.* [18] have measured the

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I

RESEARCH ARTICLE

Measurement of L subshell fluorescence yield ratios of some high Z elements by selective excitation method

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The L₁, L₂ and L₃ subshells of Hf, Ta and Re atoms have been excited selectively by using microprobe XRF beam line, Indus-2, RRCAT, India. The consequent characteristic L X-ray photons, emitted from the targets due to creations of vacancies in L subshells, are measured using silicon drift detector (X-123) spectrometer. As the energy of synchrotron radiation increases, the contribution of characteristic L X-ray intensity increases. The advantage of the increase in the intensity of the characteristic L X-ray photons with an increase in the energy of synchrotron radiation has been used to determine the L subshell fluorescence yield ratios of Hf, Ta and Re atoms by adopting the selective excitation method. The measured ratios of L subshell fluorescence yield have been compared with theoretical and other experimental values.

X-RAY

1 **INTRODUCTION**

It is well known that the intensity of characteristic X-ray photons, emitted from the target, is proportional to the square of the atomic number of the target. The X-ray fluorescence is the number of X-ray photons produced per vacancy created in the atomic shell and has wide applications in various fields.^[1] The L subshell fluorescence yield is the number of L X-ray photons produced per the number of vacancies created in the L shell. The study of L subshell fluorescence parameters has been of theoretical and experimental interest in view of the involvement of L X-ray emission, the Coster-Kronig transition and the Auger transition. Several investigators have measured the L X-ray intensity ratios, L subshell fluorescence yield and Coster-Kronig transition parameters by exciting the target with gamma radiation, charged particles and synchrotron radiation.^[2-19] Singh et al.^[4] have measured average L shell fluorescence yields for some elements in the range $56 \le Z \le 92$. Ertugrul et al.^[5] have measured average 2p subshells fluorescence yields for the elements $60 \le Z \le 90$. Kacal et al.^[6] have determined L subshell fluorescence yields (ω_1 , ω_2 , ω_3) for high

Z elements such as Er, Yb, Lu, Ta, W, Os, Pt, Au, Hg, Tl, Pb, Bi, Th and U by creating the vacancies in the L shell with 22.6 keV gamma photon using ¹⁰⁹Cd radioactive source. They suggested that the solid-state effects are to be included in theory in order to understand the observed deviations between experimental and theoretical values. Xu^[7] have measured the ratios of L subshell fluorescence yields for the elements in the atomic range $73 \le Z \le 83$ by exciting the target with 50 keV electron beam and the consequent L X-ray spectra are recorded with a curved crystal spectrometer. Sharma et al.^[8] have measured L Xray production cross sections, L subshell fluorescence yields and L subshell fluorescence yield ratios for Au, Hg and Tl. Bonzi and Badiger^[9] have measured L subshell fluorescence yields (ω_1 , ω_2 , ω_3) in the atomic range $45 \le Z \le 50$ using LNLS synchrotron radiation. Badiger and Bonzi^[10] have determined L subshell fluorescence yields for Ba, La and Pr targets using LNLS synchrotron radiation. Sogut et al.^[11] have measured L subshell fluorescence yield ratios $(\omega_2/\omega_3, \omega_1/\omega_3, \omega_1/\omega_2)$ for the elements in the range $55 \le Z \le 92$ at an excitation energy of 59.54 keV. Krishnananda et al.^[12] have determined the L subshell fluorescence yields for Gd, Tb and Ho using



Measurement of L subshell fluorescence yield ratios of some high Z elements by selective excitation method

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Correspondence N. M. Badiger, Department of Physics, Karnatak University, Dharwad-580003, India. Email: nbadiger@gmail.com The L_1 , L_2 and L_3 subshells of Hf, Ta and Re atoms have been excited selectively by using microprobe XRF beam line, Indus-2, RRCAT, India. The consequent characteristic L X-ray photons, emitted from the targets due to creations of vacancies in L subshells, are measured using silicon drift detector (X-123) spectrometer. As the energy of synchrotron radiation increases, the contribution of characteristic L X-ray intensity increases. The advantage of the increase in the intensity of the characteristic L X-ray photons with an increase in the energy of synchrotron radiation has been used to determine the L subshell fluorescence yield ratios of Hf, Ta and Re atoms by adopting the selective excitation method. The measured ratios of L subshell fluorescence yield have been compared with theoretical and other experimental values.

1 | INTRODUCTION

It is well known that the intensity of characteristic X-ray photons, emitted from the target, is proportional to the square of the atomic number of the target. The X-ray fluorescence is the number of X-ray photons produced per vacancy created in the atomic shell and has wide applications in various fields.^[1] The L subshell fluorescence yield is the number of L X-ray photons produced per the number of vacancies created in the L shell. The study of L subshell fluorescence parameters has been of theoretical and experimental interest in view of the involvement of L X-ray emission, the Coster-Kronig transition and the Auger transition. Several investigators have measured the L X-ray intensity ratios, L subshell fluorescence yield and Coster-Kronig transition parameters by exciting the target with gamma radiation, charged particles and synchrotron radiation.^[2-19] Singh et al.^[4] have measured average L shell fluorescence yields for some elements in the range $56 \le Z \le 92$. Ertugrul et al.^[5] have measured average 2p subshells fluorescence yields for the elements $60 \le Z \le 90$. Kacal et al.^[6] have determined L subshell fluorescence yields ($\omega_1, \omega_2, \omega_3$) for high

Z elements such as Er, Yb, Lu, Ta, W, Os, Pt, Au, Hg, Tl, Pb, Bi, Th and U by creating the vacancies in the L shell with 22.6 keV gamma photon using ¹⁰⁹Cd radioactive source. They suggested that the solid-state effects are to be included in theory in order to understand the observed deviations between experimental and theoretical values. Xu^[7] have measured the ratios of L subshell fluorescence yields for the elements in the atomic range $73 \le Z \le 83$ by exciting the target with 50 keV electron beam and the consequent L X-ray spectra are recorded with a curved crystal spectrometer. Sharma et al.^[8] have measured L Xray production cross sections, L subshell fluorescence yields and L subshell fluorescence yield ratios for Au, Hg and Tl. Bonzi and Badiger^[9] have measured L subshell fluorescence yields $(\omega_1, \omega_2, \omega_3)$ in the atomic range $45 \le Z \le 50$ using LNLS synchrotron radiation. Badiger and Bonzi^[10] have determined L subshell fluorescence yields for Ba, La and Pr targets using LNLS synchrotron radiation. Sogut et al.^[11] have measured L subshell fluorescence yield ratios $(\omega_2/\omega_3, \omega_1/\omega_3, \omega_1/\omega_2)$ for the elements in the range $55 \le Z \le 92$ at an excitation energy of 59.54 keV. Krishnananda et al.^[12] have determined the L subshell fluorescence yields for Gd, Tb and Ho using

ORIGINAL PAPER



Physicochemical and Biological Evaluation of Different Extracts of Edible Solanum nigrum L. Leaves Incorporated Chitosan/Poly (Vinyl Alcohol) Composite Films

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Abstract

In this work, composite films for food packaging were prepared from chitosan (CS) and polyvinyl alcohol (PVA) incorporated with extracts of edible *Solanum nigrum* L. (SN) leaves by solvent casting method. The effect of water (SW), ethanol (SE), and methanolic (SM) extracts of SN leaves on the mechanical, physical, barrier, optical, soil degradability, antimicrobial, and antioxidant properties of the films were studied. The composite films have smooth homogeneous surface morphology and showed enhanced UV blocking properties. Incorporation of SN leaves extract greatly enhances the tensile strength. The water vapor transmission rate also improved by the influence of SN extracts. The surface wettability of the composite films have an overall migration rate within the permitted limit. Besides, the SN leaves incorporated CS/PVA films showed enhanced antibacterial activity towards *Staphylococcus aureus* and *Escherichia coli* bacteria and samples did not show significant antifungal activity towards Candida albicans. All SN extracts incorporated samples showed enhanced antioxidant activity by DPPH scavenging assay. These results suggest that all three SN leaves extract induced CS/PVA composite films can be used for food packaging applications.

Keywords Chitosan · PVA · Solanum nigrum L. · Biodegradable films

Introduction

In recent years, the usage of non-biodegradable plastic is increasing very rapidly due to large applications such as packaging, automobiles, etc. [1]. These plastic materials cause serious environmental pollutions [2]. To minimize

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this problem, development of biodegradable polymer films from natural sources like Cellulose [3], Starch [4], Chitosan [5, 6], etc. are employed, but these natural polymeric films have limited strength and flexibility; therefore blending of natural polymers with other synthetic biodegradable polymers is a method to modify their properties of interest [7]. In the recent years, the actualization of a blending of natural polymers with synthetic polymers altered with the addition of different fillers which attract the preparation of synthetic biodegradable polymers having the multifaceted properties such as good water-resistant and enhanced mechanical properties [8], and good thermal stability with retaining the biodegradability [9]. Incorporation of active ingredient from plant extract into polymer matrix has received enormous interest as they contain a high concentration of phenolic components that possess strong antimicrobial and antioxidant activities. Hence the addition of natural extracts into the polymer matrix has great potential for being developed into packaging material for food and is a promising alternative for synthetic materials [10].

Chemical Data Collections 33 (2021) 100684



Data Article

UV screening, swelling and in-vitro cytotoxicity study of novel chitosan/poly (1-vinylpyrrolidone-co-vinyl acetate) blend films



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Keywords: Chitosan PVP-co-VAc UV screening Swelling Cvtotoxicity

ABSTRACT

The novel Chitosan (CS)/ Poly (1-vinylpyrrolidone-co-vinyl acetate) (PVP-co-VAc) blend films (CSP) were prepared by solvent casting method. The film properties were studied by FT-IR spectroscopy, UV—visible spectroscopy, Thermal analysis, and Water contact angle. The light transmittance and UV screening rate of CSP films remarkably increased (85.22%) than CS film. The CSP blend films attained high thermal stability as well as glass transition temperature (Tg) than CS. The surface roughness and hydrophilicity of the CSP films significantly enhanced by the influence of PVP-co-VAc that leads to increase in the swelling property of the CSP films about \approx 91% than CS film. In addition, in-vitro cytotoxicity of the CSP films showed cell viability (%) > 90% against human embryonic kidney cell line. These results suggest that the prepared CSP blend films have the potential to be implemented in the field of UV screening barriers, drug delivery and wound dressing material.

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Smart biodegradable films based on chitosan/methylcellulose containing Phyllanthus reticulatus anthocyanin for monitoring the freshness of fish fillet

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ARTICLE INFO

Keywords: Chitosan Methylcellulose Phyllanthus reticulatus Anthocyanin Smart packaging

ABSTRACT

The current work aims to prepare biologically active and pH responsive smart films based on Chitosan (CS)/ Methylcellulose (MC) matrix integrated with Phyllanthus reticulatus (PR) ripen fruit anthocyanin. The prepared smart films (CMPR) were fabricated through a cost-effective solvent casting technique. The existences of secondary interactions were confirmed by the FT-IR analysis. The smooth SEM images revealed the miscibility and compatibility of the CS/MC matrix with PR anthocyanin. The incorporation of PR anthocyanin significantly blocked the UV light transmission of the CS/MC films while slight decrease in the transparency was observed. The water solubility, moisture retention capacity, and water vapor transmission rate were significantly enhanced with an increase in the FR anthocyanin content. Additionally, the prepared CMPR smart films showed pink color in acidic pH while yellowish in basic pH solution and further exhibited strong antioxidant activity as well as antibacterial activity against the common foodborne pathogens such as S. aureus, P. aeruginosa, and E. coli. The CMFR smart film also displayed potential result for monitoring the fish fillet freshness at room temperature. The results proclaim that the prepared CMPR smart films could be utilized for quality assurance as well as shelf life extension of the marine food products.

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Chitosan/pullulan based films incorporated with clove essential oil loaded chitosan-ZnO hybrid nanoparticles for active food packaging

Tilak Gasti^a, Shruti Dixit^b, Vishram D. Hiremani^a, Ravindra B. Chougale^{a,*}, Saraswati P. Masti^c, Shyam Kumar Vootla^b, Bhagyavana S. Mudigoudra^d

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ARTICLE INFO

Keywords: Chitosan Pullulan Chitosan-ZnO nanoparticles Clove oil Active packaging

ABSTRACT

Herein, we developed clove essential oil (CEO) loaded Chitosan-ZnO hybrid nanoparticles (CS-ZnO@CEO (CZC NPs)) integrated chitosan/pullulan (CS/PL) nanocomposite films. SEM images revealed a homogenous distribution of CZC NPs with minimum aggregation in nanocomposite films. The incorporation of CZC NPs led to enhanced tensile strength (-39.82%), film hydrophobicity (-35.36%), UV light blocking ability, water vapor barrier (~84.64%), and oxygen barrier (~57.66%) compared to the bare CS/PL film and overall migration limit of CPCZC films were found below the permitted limit of 1000 µg/dm². Besides, incorporation of CZC NPs into the CS/PL films enhanced antioxidant activity and showed strong antibacterial activity against P. aeruginosa, S. aureus, and E. coli. Also, the CPCZC films displayed potential to extend the shelf-life of chicken meat by up to 5 days when stored at 8 ± 2 °C. These results suggest that the prepared CPCZC films acquire the ideal prerequisites for potential active packaging materials.
ORIGINAL PAPER



Fabrication and Study of Poly (vinyl alcohol) Film Functionalized with *Basella alba* Stem Extract

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Abstract

In this study eco-friendly composite films were prepared based on poly(vinyl alcohol) (PVA) containing different content of *Basella alba* stem extract (BA) (1.5 mL, 2.5 mL and 3.5 mL) by cost effective solvent casting technique. The physicochemical properties of the prepared films were investigated using different instrumental techniques. The molecular interaction between PVA and BA was confirmed by FTIR studies. The incorporation of BA at higher content leads to more strengthen and less flexible bio-composite films which was determined by mechanical test. DSC studies confirmed the miscibility of BA with PVA matrix. TGA studies revealed increased thermal stability of PVA/BA composite films in contrast with pristine PVA. The morphological studies disclosed that a uniform distribution of BA at lower content in the bio-composite film. The X-ray Diffraction study illustrated that, increased BA content reduces the semicrystalline structure of PVA. Moreover, Moisture Content, Water Solubility, Water Contact Angle and Water Vapor Transmission Rate results indicated that, bio-composite films had high surface hydrophilicity. Additionally, PVA/BA films exhibited low transparency value compared to control film and improved UV barrier property. Soil degradation rate of PVA/BA films increased as the BA content increased signifying the films are biodegradable in nature. Furthermore, doping of BA into PVA enhanced antibacterial potential of the bio-composite film towards *Staphylococcus aureus* and *Escherichia coli*. These results suggest that PVA/BA composite films can be utilized as promising material for green packaging application.

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Preparation and physicochemical assessment of bioactive films based on chitosan and starchy powder of white turmeric rhizomes (*Curcuma Zedoaria*) for green packaging applications

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ARTICLEINFO

Keywords: Mcchanical Thermal Biodegradable Oil resistant Autimicrobial

ABSTRACT

In the current study, the bioactive films of chitosan/white turmeric (CH/WT) were prepared by employing solvent casting technique and analyzed their physicochemical and biological properties for active packaging applications. The successful inclusion of white turmeric into the chitosan matrix is confirmed by Fourier Transform Infrared Spectroscopy. Due to the presence of hydrogen bonding interaction, the active films exhibited good tensile properties, smooth surface morphology, miscibility, water resistance and UV barrier properties. The incorporation of white turmeric reduced the water vapour transmission rate and oxygen permeability (p < 0.05) in contrast with pristine film. The prepared blend films revealed soil degradation rate more than 60% within 15 days. Furthermore, the blend films exhibited lesser water solubility, moisture content and swelling index after addition of white turmeric to chitosan (p < 0.05). The prepared films revealed extensive antimicrobial activity against gram positive and gram negative bacteria. The antioxidant activity and total phenolic content were improved upon the incorporation of white turmeric. Moreover, the oil absorption rate of the blend films was decreased by 46% in comparison with pristine film. Overall, white turmeric incorporated chitosan films were employed as a green packaging material to extend the shell life of the foodstuff.

ORIGINAL PAPER



Dominant nature of 7-hydroxy 4-methyl coumarin dye on thermal, fluorescence and antimicrobial properties of PVA/OMS blend films

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Abstract

This article focused on the fabrication of 7-hydroxy 4- methyl coumarin (7H4MC) dye doped Polyvinyl alcohol/Oxidized Maize Starch (PVA/OMS) blend films by employing user friendly solvent casting technique. The thermal stability, crystallanity, surface morphology and optical properties of the films were investigated by using Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Atomic Force Microscopy (AFM), Fluorescence (FL) and Ultraviolet–Visible (UV–Vis) Spectroscopy respectively. The TGA and DSC results illustrate that the blend films are thermally stable and miscible over the entire composition. The XRD analysis confirmed the semi crystalline nature of all the obtained films with the intense peak at $2\theta = 19$. 49°. The AFM topographic images had shown a smoother and homogeneous surface at the higher weight percentage of 7H4MC of blend films. The UV–Visible spectra display the absorption peaks at 325 nm for control PVA/OMS and two peaks at 329 nm, 370 nm arises after doping of 7H4MC in PS blend associated with π - π * electronic transition may be due to the charge transfer (CT) groups. The optical band gap is reduced on the addition of 7H4MC dye in the control blend. The fluorescence spectra revealed that the fabricated films exhibited good blue light emission under ultraviolet light and shows maximum fluorescence emission at 442 nm for 0.008 wt. % of 7H4MC. Moreover PSC blend films exhibited superior antimicrobial properties as compare to control blend film. Hence, the obtained outcomes are suggested that the PVA/OMS (PSC) blend films are appropriate materials for optical and biological application.

Keywords Thermal · Fluorescence · Optical and Antimicrobial

Introduction

Currently the organic dye induced polymer composites has emergent attention, owing to its multifunctional properties and applications in the field of the optical devices [1]. The speedy expansion in the functionalities of organic materials

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is helpful in the variety of organic electronic devices like light emitting diodes, sensors and field effect transistors [2]. The organic materials can absorb the light energy and transfers it into thermal, optical and electrical energy which leads to attractive applications in the field of storage devices and luminescence materials [3, 4]. Moreover, the addition of organic or fluorescent dyes in a polymeric matrix leads to the invention of large-area devices and also improves the efficiency of polymer composites [2]. This is mainly depending on the type of polymer, nature of the dye and the way in which the polymer interacts with the doped dye [5]. The fluorescent dye doped polymer is expected as candidates having strong absorption and emission bands in the visible spectral region this is due to the hydrophobic nature and high surface energy of the dye molecules which has a great deal of consideration for both industrial and specialized analysts. The polymer composites with light emitting behaviour have an extensive history in research, which has been approved for fluorescence properties [6, 7].

ORIGINAL RESEARCH



Polysaccharide-based blend films as a promising material for food packaging applications: physicochemical properties

Vishram D. Hiremani¹ · Tilak Gasti¹ · Saraswati P. Masti² · Ravindra B. Malabadi³ · Ravindra B. Chougale¹

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Abstract

To achieve eco-friendly polysaccharide-based blend films, the different weight percentages of chitosan (CH) and oxidized maize starch (OMS) were mixed and the blend films were fabricated by employing the solution casting method. The interaction between the components of the blend films were confirmed by Fourier transform infrared spectroscopy. The presence of hydrogen bonding interaction enhanced the elongation of the blend films from $3.430 \pm 0.75\%$ to $43.26 \pm 1.21\%$. The results from the differential scanning calorimetry exhibited a single glass transition temperature for all the films, depicting that the components of the blend films were reduced after the inclusion of the OMS into CH. A decrease in the transmittance percentage of the blend films compared to neat CH film was observed, which helps to reduce oxidative deterioration in packed food products caused by UV radiation. The transparency of the films decreased at lower weight percentage of OMS and showed higher transparency as the amount of OMS increased in the blend matrix. The XRD results revealed that the prepared films are amorphous in nature. All the prepared films exhibited a smooth and homogeneous surface morphology which was confirmed by the SEM analysis. The moisture content, water absorption capacity, water solubility and soil degradation of the blend films decreased in contrast with pristine CH film. Hence, the prepared films have the potential to be used for food packaging applications.

Graphical Abstract



Keywords Mechanical properties · Biodegradable · Miscibility · Barrier · Water resistant

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Introduction

The main intention of food packaging material is to sustain the quality of the food products throughout the transportation and storage, as well as also to extend the shelf life of

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ORIGINAL PAPER



ZnO NPs Doped PVA/*Spathodea campanulata* Thin Films for Food Packaging

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Abstract

The present study aims to investigate the influence of Zinc Oxide nanoparticles (ZnO NPs) on the physicochemical properties of poly(vinyl alcohol)/*Spathodea campanulata* bud fluid (PSC) matrix. The FITR study assured the physical interaction between ZnO NPs and the PSC matrix. Tensile strength was enhanced by 18% with the incorporation of ZnO NPs into the PSC matrix. The DSC measurements depicted an increased glass transition temperature than PSC matrix at lower content of ZnO NPs. The thermal stability of nanocomposite films was remarkably improved (about 50 °C). The XRD results depicted the homogeneous distribution of ZnO NPs in the PSC matrix. The morphology studies revealed the homogeneity due to good dispersion of ZnO NPs. The water contact angle findings shown the nanocomposite films was improved by 56%. The bionanocomposite films exhibited good antibacterial activity and excellent preservation capacity and could be a potent alternative to the nonbiodegradable packaging material.

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ORIGINAL PAPER



Exploration of Multifunctional Properties of *Piper betel* Leaves Extract Incorporated Polyvinyl Alcohol-Oxidized Maize Starch Blend Films for Active Packaging Applications

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Abstract

This study explains the development of eco-friendly polyvinyl alcohol (PVA)/oxidized maize starch (OMS)/Betel leaves extract (BLE) blend films by employing a cost effective technique. The influence of BLE on structural, Thermal, Mechanical, Morphological, Optical, Antibacterial and Antioxidant properties of the PVA/OMS blend were investigated successfully by applying various characterization techniques. The hydrogen bonding interaction among the components of the blend films led to enhance thermal stability, miscibility, mechanical properties, smooth surface morphology and UV blocking properties of the blend films. The addition of BLE enormously improved the antibacterial and antioxidant properties of the PVA/ OMS blend films. Moreover, the obtained films were hydrophilic, water soluble and biodegradable in nature. With regard to barrier properties the water vapour transmission rate and oxygen permeability of the blend films were enhanced after doping of BLE. These experimental outcomes suggest that the BLE containing PVA/OMS films can be used for the expansion of active packaging materials.

Authors and Affiliations

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Journal of Molecular Structure Volume 1224, 15 January 2021, 129055

Hydroxyacetone derived N4-methyl substituted thiosemicarbazone: Syntheses, crystal structures and spectroscopic characterization of later first-row transition metal complexes

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Highlights

- Crystal structures of Co(II) and Ni(II) complexes of ligand, 1-(1-hydroxypropan-2-ylidene)-N4-methylthiosemicarbazone are explored.
- Later first row transition metal complexes are synthesized and characterized.
- In vitro antitubercular activities are presented for the synthesized compounds.

Abstract

The present work reports the syntheses, crystal structures and spectroscopic characterization of later first-row transition metal complexes of hydroxyacetone derived N4-methyl substituted thiosemicarbazone. The molecular structures of Co(II) and Ni(II) complexes are determined by single crystal X-ray diffraction method. The crystal structures reveal that the Co(II) and Ni(II)



ScienceDirect

Chemical Data Collections Volume 26, April 2020, 100359

Data Article

Highly sensitive and selective colorimetric probe for detection of Cu²⁺ in aqueous medium based on rhodamine B

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Received 12 November 2019, Revised 20 February 2020, Accepted 27 February 2020, Available online 9 March 2020, Version of Record 19 March 2020.

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Highlights

- A colorimetric sensor selective for Cu²⁺ in the aqueous medium is developed.
- The sensor shows color change from colorless to pink for Cu²⁺.
- The detection limit of probe towards Cu^{2+} was 4.59×10^{-7} M.
- The DFT and TDDFT studies support the spirolactam ring opening of the sensor on the addition of Cu²⁺.

Abstract

A colorimetric probe L based on rhodamine was designed and synthesized. It exhibits very high sensitivity and selectivity towards Cu²⁺ in an aqueous medium with a color change from colorless to pink. The competitive experiments of probe L showed excellent colorimetric selectivity for Cu²⁺ over other metal ions. The recognizing behavior of L has been investigated both experimentally and computationally. The mechanism of L for sensing Cu²⁺ has been demonstrated by IR, ESI-MS, density functional theory calculation and time-dependent density functional theory calculations.

ROYAL SOCIETY Q Q 9 \equiv Þ Log in / register Previous Issue 40, 2020 Next NJC From the iournal: New Journal of Chemistry Synthesis, structural characterization and biological properties of cyclometalated iridium(III) complexes containing [1,2,5]-thiadiazolo-[3,4-f]-[1,10]-phenanthroline * Check for updates Satish S. Bhat, 🔟 * a Naveen S., 🔟 bc Vidyanand K. Revankar, * a N. K. Lokanath, d Rahul V. Pinjari, 🔟 e Vijay Kumbar f and Kishore Bhat f Author affiliations (-)Corresponding authors Department of Chemistry, Karnatak University, Dharwad-580003, Karnataka, India E-mail: <u>bhatsatish111@gmail.com</u>, <u>vkrevankar@rediffmail.com</u> b Department of Physics, Faculty of Engineering & Technology, Jain (Deemed-to-be University), Bangalore 562112, India С Center for Emerging Technologies, Faculty of Engineering & Technology, Jain (Deemed-to-be University), Bangalore 562112, India c Department of Studies in Physics, University of Mysore, Manasagangotri, Mysuru 570006, Karnataka, India е School of Chemical Science, Swami Ramanand Teerth, Marathwada University, Nanded, Maharashtra, India f Maratha Mandal's Central Research Laboratory, Marathamandal Dental College and Research Centre, Belgaum, Karnataka, India Abstract Two cationic iridium(III) complexes, $[Ir(ppy)_2((tdzp))]^+$ (1) and $[Ir(bhq)_2((tdzp))]^+$ (2) {ppy = 2phenylpyridine, bhq = benzo[h]quinoline, tdzp = [1,2,5]-thiadiazolo-[3,4-f]-[1,10]-phenanthroline}, have been synthesized and structurally characterized. The molecular structures of the iridium complexes have

Synthesis, structural characterization and biological properties of cyclometalated iridium(iii) complexes containing [1,2,5]-thiadiazol..

3/2/22, 1:41 AM

been confirmed by single-crystal X-ray structure determination. Extensive hydrogen bonding between lattice water molecules, solvated methanol, and chloride anions is observed in the crystal structure of complex 1, which leads to the formation of 1D polymeric cyclic hybrid water-chloride-methanol clusters. The complexes show different photophysical properties in different solvents. The experimental photophysical properties of the synthesized iridium(III) complexes match well with the theoretically calculated results obtained by density functional theory (DFT) and time-dependent density functional theory (TD-DFT) studies. The HOMO of complexes 1 and 2 is restricted on the indium and cyclometalated aromatic https://pubs.rsc.org/en/content/articlelanding/2020/nj/d0nj03421e/unauth

ROYAL SOCIETY OF CHEMISTRY Q Q 9 ਸ਼ੁ Log in / register Issue 35, 2021 Previous Next NJC From the journal: New Journal of Chemistry Synthesis, structural characterization, protein binding, DNA cleavage and anticancer activity of fluorophore labelled copper(II) complexes based on 1,8-naphthalimide conjugates † Check for updates Sabiha A. Shaikh , a Satish S. Bhat , ២ a Pooja L. Hegde , Vidyanand K Revankar , ២ * Anup Kate , Deepti Kirtani , Anupa A. Kumbhar,^b Vijay Kumbar^c and Kishore Bhat^c Author affiliations (-)Corresponding authors Department of Chemistry, Karnatak University, Dharwad-580003, Karnataka, India E-mail: vkrevankar@rediffmail.com

Synthesis, structural characterization, protein binding, DNA cleavage and anticancer activity of fluorophore labelled copper(ii) comp...

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Abstract

3/2/22, 1:36 AM

The two novel fluorophore labelled copper(II) complexes [Cu(L)₂(DMF)Cl₂] (1) and [Cu(phen)(L)Cl₂] (2) (where L = *N*-(3-pyridyl)-1,8-naphthalimide, phen = 1,10-phenanthroline, DMF = dimethylformamide) were synthesized and structurally characterized by single-crystal X-ray structure determination. Complexes 1 and 2 were highly fluorescent in aqueous as well as organic solvents. The complexes efficiently cleave DNA, which was investigated by agarose gel electrophoresis. The interactions of the complexes with BSA (bovine serum albumin) were investigated by fluorescence spectroscopy. The anticancer activity of 1 and 2 in comparison with cisplatin was studied by MTT (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide) assay towards MDA-MB-231 (epithelial human breast cancer cell line) and A549 (adenocarcinomic human alveolar basal epithelial cell line) cell lines. Both the copper complexes have better anticancer activity than cisplatin towards the MDA-MB-231 and A549 cell lines. Complex **2** has nine times higher anticancer activity than cisplatin towards the A549 cell line. The mode of cell death induced by the complexes was investigated by DAPI staining and flow cytometry. The cellular uptake of the complexes was investigated by fluorescence microscopy. The complexes induce an apoptotic mode of cell death.





Journal of Luminescence Volume 226, October 2020, 117509

Full Length Article Photoluminescence modulation in the graphene oxide dispersed 4-n-octyl-4'-cyanobiphenyl molecular system

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PDF

Highlights

- GO nanoflakes lower the weakly first-order N-Iso transition temperature.
- A blue shift in the absorption band of the 8CB is noticed due to GO dispersion.
- GO causes photoluminescence modulation due to electron-phonon interaction.
- The optical properties were found to be nonlinear as a function of GO concentration.

Abstract

Herein, we investigate the mechanism of photoluminescence modulation (PLM) in the 4-n-octyl-4'-cyanobiphenyl liquid crystal (8CB LC) in the presence of various doping concentrations (0.02 to 0.4 wt%) of 2D-GO (two-dimensional graphene oxide) nanoflakes. The role of intermolecular



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Phase Contraction, fluorescence quenching and formation of topological defects in chiral smectic C matrix by Cd_{0.15}Zn_{0.85}S/ZnS core/shell quantum dots dispersion: Faster electro-optic response for gadget displays

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ABSTRACT

Cd_{0.15}Zn_{0.85}S/ZnS core/shell quantum dots (CSQDs) of size 7.54 \pm 0.99 nm in diameter were prepared via gram-scale one-pot synthesis method and dispersed in a ferroelectric liquid crystalline (FLC) material into two different concentrations. Spectroscopic, electro-optical (E-O) and morphological characterisations of aforementioned composites have been carried out. CSQDs cause a significant contraction in the width of chiral smectic C (SmC*) mesophase that has also been theoretically verified. Diffusion–controlled processes are responsible for the fluorescence quenching in the FLC/CSQDs composites which has been explained by using the Stern–Volmer quenching equation. The mesomorphic investigation has revealed that helical deformation takes place in the FLC/CSQDs composites, due to which the temperature-dependent gradual growth of ferroelectric domains is noticed. The perturbed helical geometry evinces a new structure-property correlation having a molecular switching time of 135 μ s that is 51% faster response as compared to the pristine system. Resultant spontaneous polarisation in the matrix of FLC/CSQDs composites is diminished because of the induced homeotropic and flexoelectric contributions. The faster E-O response and optical imaging are the fascinating features of the FLC/CSQDs composites that can probably be utilised in gadget displays.



ARTICLE HISTORY

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KEYWORDS

Ferroelectric liquid crystal; quantum dots; electrooptical response; fluorescence quenching; dsc; polarised optical microscopy

1. Introduction

Nowadays, the inclusion of nanoparticles in condensed mesophase is comparatively an easy prospective for the experimentalists to tune the physical and chemical properties [1–4]. Recently, several research articles have been reported on the quantum dot dispersed liquid crystalline system describing their superior applications

in low operating LC devices [5], holographic displays [6], memory devices [7], plasmonic devices [8], and colloids [9]. Chiral smectic C mesophase is ferroelectric and commonly termed as ferroelectric liquid crystals (FLCs). This phase has technical superiority for various promising applications like two electro-optical mode grating [10], optical memory devices [11], light CrossMark

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PAPER

Structural and optical properties of zirconium oxide (ZrO₂) nanoparticles: effect of calcination temperature

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Keywords: optical properties, fluorescence emission, life time measurement, zirconium oxide

Abstract

In this article, we report the structural and optical properties of zirconium oxide (ZrO_2) nanoparticles synthesized via chemical co-precipitation method. The effect of calcination temperature on structural and optical properties of ZrO_2 nanoparticles is investigated through XRD, FESEM, EDX, FTIR, UV– Vis absorption, fluorescence emission and life time measurements. XRD spectrum reveals the tetragonal phase at calcination temperature 600 °C and crystallinity of samples increases with calcination temperature. At 800 °C the phase transition from tetragonal to tetragonal-monoclinic mixed phase is noticed. The FESEM images show the particles are of irregular shape and highly agglomerated. FTIR spectra also confirm the formation of ZrO_2 in crystalline phase. From UV–vis absorption spectra it is found a strong quantization and varying band gap with calcination temperature. The change in emission wavelength and intensity with phase change is observed form fluorescence emission spectra. At higher calcination temperature emission intensity is decreased which may be due to the phase change and the formation of surface defects. The life time measurements also reveal the different trap states and life time with calcination temperature.

1. Introduction

Wide band gap metal oxide nanoparticles have attracted scientific attention due to their wide range applications. Zirconium oxide (ZrO_2) also known as zirconia with its excellent chemical and physical properties have applications such as fuel cells [1], gas sensors [2], optoelectronics [3], catalyst [4], and corrosion resistant material [5]. With band gap > 5 eV, ZrO_2 is an important luminescent material with good optical transparency [6] and a potential candidate for photocatalytic applications due to its high surface area and presence of large number of oxygen vacancies [7]. It comes in three crystal phases namely tetragonal, monoclinic and cubic. The existence of these polymorphs depend on the synthesis process, particle size, calcination temperature and defects. There are contrasting reports on the existence of the phases with calcination temperature. Although monoclinic ZrO_2 is believed to be more stable at room temperature than the other two polymorphs but the tetragonal phase can also be stabilized at room temperature depending on the synthesis process [8]. In literature there exist various methods of synthesis of ZrO_2 nanostructures like sol-gel [9], hydrothermal [10], combustion [11], and co-precipitation [12, 13].

Calcination temperature not only modifies the morphology and size of nanoparticles but also create the defects and thus generating new energy levels. Further, the calcination temperature modifies the phase of the materials and it affects the optical and structural properties. Photoluminescence is sensitive to structure, chemical composition and defects is an important property to study in ZrO₂. The photocatalytic activity of ZrO₂ and other metal oxide semiconductor have been well studied [14–17]. Ilkhechi and group have reported the

Photoluminescence Properties of Zirconium Oxide (ZrO₂) Nanoparticles

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ABSTRACT

In the present article, we report the structural and optical properties of zirconium oxide (ZrO_2) nanoparticles, synthesized via chemical co-precipitation method. The effect of calcination temperature on structural and optical properties of ZrO_2 nanoparticles is analyzed through XRD, FESEM, EDX, FTIR, UV–Vis absorption and fluorescence emission spectroscopy. XRD spectra reveals the tetragonal phase at calcination temperature $600^{\circ}C$ and crystallinity of samples increases with calcination temperature. At $800^{\circ}C$ phase transition from tetragonal to tetragonal-monoclinic mixed phase is noticed. The FESEM images shows that the particles are of irregular shape and highly agglomerated. From Uv-Vis absorption spectra it is found a strong quantization and varying band gap with calcination temperature. At higher calcination temperature emission intensity is decreased which may be due to phase change and the formation of surface defects such as oxygen vacancies and interstitials.

Keywords: Zirconium Oxide, Optical Properties, Fluorescence Emission Spectroscopy, Calcination Temperature.

INTRODUCTION

Wide band gap metal oxide nanoparticles have attracted scientific attention due to their wide range of applications. Zirconium oxide nanoparticles also called zirconia with excellent chemical and physical properties has wide spread applications such as fuel cells[1], gas sensors[2],optoelectronics material[3], catalyst,and corrosion resistant material [3,4] with band gap > 5 eV. Zirconia comes in to three crystal phases namely tetragonal, monoclinic and cubic. The existence of these polymorphs depends on the synthesis process, particle size and the calcination temperature. There are contrasting reports on the existence of the phases with calcination temperature. The phase formation of ZrO_2 basically depends on the synthesis methods and size of the particles. In literature there exist several synthesis methods of ZrO₂ nanostructures like sol-gel, hydrothermal, combustion, and co-precipitation [4-6]. Due to calcination not only the crystal and stoichiometric composition can change but also it affects the optical and structural properties. Photoluminescence is sensitive to structure, chemical composition and defects is an important property to study in ZrO_2 . Recently the optical properties of ZrO_2 have gained tremendous interest from both theoretical and experimental investigations. There are many contrasting reports of broad PL emission ranging from 480 nm to 300 nm. Due to defects and excess vacancies the PL band position of ZrO₂ depends on excitation wavelength ranging from 340nm to 240 nm[7]. Cong et al[8] have shown that the PL intensity of nano-ZrO₂ decreases with increase in calcinations temperature because of oxygen vacancies as well as phase transformation. Further, they have noticed that PL intensity depends on the excitation wavelength clearly pointing the different trap levels due to defects. Joy et al[9] have studied effect of annealing temperature on photoluminescence properties of ZrO₂ thin films and shown how λ_{ex} changes with coating. In the present work, we report the effect of calcination temperature on structural and optical properties of ZrO_2

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ORIGINAL PAPER



Synthesis and photoluminescence properties of polycarbazole/tin oxide (PCz/SnO₂) polymer nanocomposites

N. C. Horti, et al. [full author details at the end of the article]

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Abstract

In this article, polycarbazole/tin oxide polymer nanocomposites were synthesized by an in-situ chemical polymerization of carbazole monomers using anhydrous iron (III) chloride as an oxidizing agent. The influence of SnO_2 filler concentration on structural properties is investigated through X-ray diffraction, field emission electron scanning microscopy, energy-dispersive X-ray and Fourier transform infra-red spectroscopy. The optical studies were performed using UV–Vis absorption and fluorescence emission spectroscopy. X-ray diffraction spectrum reveals the formation of pure polycarbazole and incorporation of tin oxide nanoparticles into the polycarbazole matrix. EDX and FTIR spectra also confirm the formation of polymer nanocomposites. The change in morphological and nodular nature with the change in the weight percentage of SnO_2 is noticed from FESEM. UV–Vis absorption spectra reveal the red shift of π — π * transition of polycarbazole due to the incorporation of tin oxide into the polymer chain. From photoluminescence spectra, we have observed that fluorescence emission intensity and wavelength varies with different weight percentage of SnO_2 nanoparticles.

Graphic abstract

Pictorial representation of synthesis of PCz/SnO2 polymer nanocomposites



Keywords Polycarbazole \cdot SnO₂ \cdot Nanocomposites \cdot Optical properties \cdot Photoluminescence

Förster resonance energy transfer studies between Bovine Serum Albumin and Stilbene 420 dye

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Abstract

In the present work, we report evidence for efficient Förster resonance energy transfer (FRET) between Bovine Serum Albumin (BSA) and Stilbene 420 (S420) dye based on both steady-state time-resolved and (TR) fluorescence spectroscopic This study measurements.



predominantly shows that decrease in the Photoluminescence (PL) intensity of BSA and enhancement PL intensity of S420 dye provides the information about efficient energy transfer (ET) between the two fluorophore. This is a signature that, BSA acts as a proficient donor and S420 dye as an excellent acceptor in FRET mechanism. The Spectral overlap integral (J(λ)), Forster distance (R₀), intermolecular distances (r), and energy transfer efficiency (E) are obtained experimentally from FRET theory. The ET efficiency of up to 36% has observed in this FRET system from TR measurements. The Stern-Volmer plot suggests that the quenching mechanism is dynamic and bimolecular quenching rate constants (k_q) shows this interaction is not diffusion-controlled process.

Keywords: BSA; Stilbene 420; FRET; Spectral overlap; Forster distance; Stern-Volmer. Article history: Received: 6 July 2020; Revised: 8 August 2020; Accepted: 9 August 2020

1. Introduction

Förster/fluorescence resonance energy transfer (FRET) is a process in which an excited state donor chromophore can transfer energy to a proximal acceptor chromophore (typically less than 10 nm) through a long-range nonradiative dipole-dipole coupling [1-4]. It has been extensively and intensively studied as a powerful analytical technique to interrogate changes in molecular conformation, association and the assembly or disassembly of biomolecular machinery [2]. The interest has been growing quickly amongst researchers in the field of FRET sensors, which are used to quantify molecular dynamics in protein-protein interactions, protein-DNA interactions, and protein conformational changes [2, 5]. The advantage of the FRET



Applied Organometallic Chemistry / Volume 34, Issue 4 / e5567

FULL PAPER

Biosynthesis and characterization of *Dillenia indica*-mediated silver nanoparticles and their biological activity

Sreenivasa Nayak, Meghashyama P. Bhat, A.C. Udayashankar, T.R. Lakshmeesha, Nagaraja Geetha, Sudisha Jogaiah 🔀

First published: 06 February 2020 https://doi.org/10.1002/aoc.5567 Citations: 13

Abstract

Dillenia indica L. is a traditional medicinal plant well known for its ability to cure various human diseases. In the current study, silver nanoparticles have been synthesized by simple and eco-friendly method using Dillenia indica extract. The green synthesized nanoparticles were characterized by Fourier transform infrared (FTIR), UV–visible spectroscopy, Atomic force microscopy (AFM), High-resolution transmission electron microscopy (HR-TEM), Zeta Potential and Size Distribution. UV–visible and FTIR spectra, AFM, HR-TEM and Zeta Potential readings and size distribution conformed that the synthesized silver particles were in the size of nano. The green synthesized silver nanoparticles were subjected for antibacterial activity against Gram-positive bacteria Enterococcus faecalis and Gram-negative bacteria Escherichia coli by agar well diffusion method. The synthesized AgNPs exhibited significant inhibition of 27 and 16 mm against the test bacteria at 0.25 mg/ml. Further the antibacterial activity was confirmed by live and dead cell assay by fluorescence microscopy and morphological changes of bacteria were studied by Scanning electron microscope (SEM). The study recommends that the synthesized silver nanoparticles using Dillenia indica extract have potential application in inhibition of bacteria owing to their potent antibacterial activity.

Citing Literature

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Dominant nature of 7-hydroxy 4-methyl coumarin dye on thermal, fluorescence and antimicrobial properties of PVA/OMS blend films

Vishram D. Hiremani¹ · Mallikarjun H. Anandalli² · Tilak Gasti¹ · Shruti Dixit³ · Praveen K. Bayannavar¹ · Saraswati P. Masti⁴ · R. F. Bhajantri² · Shyam Kumar Vootla³ · Bhagyavana. S. Mudigoudra⁵ · Ravindra B. Chougale¹

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Abstract

This article focused on the fabrication of 7-hydroxy 4- methyl coumarin (7H4MC) dye doped Polyvinyl alcohol/Oxidized Maize Starch (PVA/OMS) blend films by employing user friendly solvent casting technique. The thermal stability, crystallanity, surface morphology and optical properties of the films were investigated by using Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC), X-ray Diffraction (XRD), Atomic Force Microscopy (AFM), Fluorescence (FL) and Ultraviolet–Visible (UV–Vis) Spectroscopy respectively. The TGA and DSC results illustrate that the blend films are thermally stable and miscible over the entire composition. The XRD analysis confirmed the semi crystalline nature of all the obtained films with the intense peak at $2\theta = 19$. 49° . The AFM topographic images had shown a smoother and homogeneous surface at the higher weight percentage of 7H4MC of blend films. The UV–Visible spectra display the absorption peaks at 325 nm for control PVA/OMS and two peaks at 329 nm, 370 nm arises after doping of 7H4MC in PS blend associated with π - π * electronic transition may be due to the charge transfer (CT) groups. The optical band gap is reduced on the addition of 7H4MC dye in the control blend. The fluorescence spectra revealed that the fabricated films exhibited good blue light emission under ultraviolet light and shows maximum fluorescence emission at 442 nm for 0.008 wt. % of 7H4MC. Moreover PSC blend films exhibited superior antimicrobial properties as compare to control blend film. Hence, the obtained outcomes are suggested that the PVA/OMS (PSC) blend films are appropriate materials for optical and biological application.

Keywords Thermal · Fluorescence · Optical and Antimicrobial

Introduction

Currently the organic dye induced polymer composites has emergent attention, owing to its multifunctional properties and applications in the field of the optical devices [1]. The speedy expansion in the functionalities of organic materials

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is helpful in the variety of organic electronic devices like light emitting diodes, sensors and field effect transistors [2]. The organic materials can absorb the light energy and transfers it into thermal, optical and electrical energy which leads to attractive applications in the field of storage devices and luminescence materials [3, 4]. Moreover, the addition of organic or fluorescent dyes in a polymeric matrix leads to the invention of large-area devices and also improves the efficiency of polymer composites [2]. This is mainly depending on the type of polymer, nature of the dye and the way in which the polymer interacts with the doped dye [5]. The fluorescent dye doped polymer is expected as candidates having strong absorption and emission bands in the visible spectral region this is due to the hydrophobic nature and high surface energy of the dye molecules which has a great deal of consideration for both industrial and specialized analysts. The polymer composites with light emitting behaviour have an extensive history in research, which has been approved for fluorescence properties [6, 7].

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Influence of magnesium doping on structural and elastic parameters of Nickel Zinc nanoferrites



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HIGHLIGHTS

G R A P H I C A L A B S T R A C T

- The Ni–Zn nano-ferrites with magnesium substitution were successfully prepared by Sucrose method.
- XRD investigations confirmed single phase cubic structure having Fd3m space group.
- The TEM images confirm nano scale nature and almost spherical shape of ferrite.
- FTIR spectra confirmed presence of M O bond.

ARTICLE INFO

Keywords: Nanoferrite Cell parameter Bond length Moduli of elasticity Debye temperature



ABSTRACT

The Ni_{0.45} Zn_{0.55-x}Mg_xFe₂O₄ (x = 0.0, 0.1, 0.2 and 0.3) nanoferrites were synthesized by the sucrose method. The prepared nanoferrites were characterized by XRD, TEM, FTIR and Raman techniques. The XRD studies verified the cubic spinel-type structure of the samples. The lattice constant, particle size, bond lengths, X-ray density were determined. The lattice constant decreased as Magnesium content increased. The SAED image shows a ring pattern that establishes polycrystalline state of ferrites. The TEM image reveals a spherical shape of nanoferrite particles. The elastic parameters were calculated for obtained nanoferrites using FTIR data. The moduli of elasticity and Debye temperature decreased with increase in Magnesium content. Five first order Raman active modes were revealed by Raman Spectroscopy.

1. Introduction

The synthesis of magnetic nanomaterials is of immense interest because of their novel mesoscopic properties. Each nanoparticle is considered as a single magnetic domain due to its large surface area which changes few of their properties [1]. Ferrites are ferromagnetic materials and they are oxides of different metals along with iron [2]. The spinel nanoferrites have novel magnetic, optical and photoelectric properties. Ferrites are used in data storage materials, catalysts, antenna bodies, humidity sensors, drug delivery processes, converters, inductors [3–10] and microwave devices [11,12]. These materials have high magnetization and permeability [13]. The preparation of spinel

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Target-to-substrate distance influenced linear and nonlinear optical properties of *a*-plane oriented ZnO:AI thin films

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ABSTRACT

This manuscript deals with the investigation of the impact of target-to-substrate distance on the linear and nonlinear optical properties of a-plane oriented aluminum-doped ZnO (ZnO:Al) thin films synthesized by the pulsed laser deposition (PLD) technique. X-ray diffraction studies proclaim an increment in the crystallinity with a decrement in target-to-substrate distance from 6 to 3 cm, attributed to increased thickness, decrease in stress, and defect levels in the thin films. A relaxation in the stress induces a decrease in the energy gap (3.47–3.37 eV) with a reduction in target-substrate distance from 6 to 3 cm is observed from UV-visible spectroscopic analysis. Spectroscopic ellipsometry confirms an increment in the refractive index and extinction coefficient with a decrease in target-to-substrate distance. From the Photoluminescence spectrum, the presence of low defect levels in the ZnO:Al thin films prepared at a shorter target-to-substrate distance is observed. The induced absorption (RSA) and selfdefocusing process of ZnO:Al thin films are revealed by open aperture and closed aperture Z-scan measurements at 532 nm wavelength. The optical limiting behavior of all the thin films strongly suggests their applicability in optical power limiting. Thus, the present study emphasizes the optimization of the target-to-substrate distance to tailor the structural, linear, and nonlinear optical properties of the a-plane oriented ZnO:Al thin films.

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Radiation Physics and Chemistry

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Physico-chemical properties of PVA-Nile blue ($C_{20}H_{20}ClN_3O$) polymer composite structures for γ -ray protection: A comparative γ -ray irradiation studies

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ARTICLE INFO

Keywords: Nile blue Polyvinyl alcohol Irradiation Chain scission Crosslinking y-ray protective materials.

ABSTRACT

Nile blue (NB, (C20H20ClN3O)) dye/polyvinyl alcohol (PVA) polymer composite films were developed by solvent casting technique, and were further exposed to high energy γ-ray (25-125 kGy) radiation. The influence of dye content and y-ray radiation on the optical-spectral behaviour, structural, thermal and mechanical properties of the PVA-NB composite films was discussed. Modifications of the chemical structure of the host matrix - PVA polymer upon dye intercalation and subsequent radiation exposure on these composite structures was confirmed by FTIR analysis. The UV-Vis studies showed a decrease in both band gap (E_g) and Urbach energies (E_u) on the increase of dye concentration while the band gap decreased and the Urbach energy was found to increase on γ-irradiation (25-125) kGy. These variations could be due to an increase of crystallinity on dye content loading and contrarily to an increase of amorphous nature upon radiation exposure which is supported by XRD results. Further, the thermal behaviour of the pre and post irradiated composite films were studied using DSC. Consequently, these observed modifications in the physico-chemical properties of the pre and post gamma irradiated PVA-(C20H20ClN3O) polymer composite structures impact the mechanical properties. The mechanical studies have revealed an increase in tensile strength and Young's modulus parameters (maximum of 94.688 MPa and 2185.7 MPa for 1 wt%) upon dye content inclusion. However, these parameters decreased (46.396 MPa and 357.76 MPa for 125 kGy) upon radiation-matter interaction. Interestingly, these films could withstand a gamma radiation upto 75 kGy. Therefore, clearly, these observations suggest that the developed polymer composite films are better candidates for the y-ray protective kits such as gloves, layers/shields in a variety of industries.

1. Introduction

Naturally, in the environment, radiations of varying degree cause and induce many physico-chemical changes in the materials that encounter round the clock. They affect these materials to the extent that depends on type of radiation, radiation dose level, time of exposure, material properties and the environmental conditions etc. Generally, when high energetic radiation (i.e., X-rays, γ -rays, neutrons, electrons etc.,) interact with the polymeric materials causes chain scission, that leads to a reduction in molecular weight, inter/intra-molecular crosslinking, that causes an increase in molecular weight, emission of atoms, molecules and molecular fragments, free radical formation, and the production of reactive oxygen species (ROS) which eventually leads to degradation, color change, brittleness, and hardness etc. Owing to these structural changes, there might be some fine tuning in the optical, thermal, mechanical, dielectric and conductivity properties of the radiation exposed composite materials.

In order to probe the unique properties, many scientists have been studying the irradiation effects on the doped polymer composite materials. As a radiation shielding material, lead suffers from toxicity, heaviness; lot of organic dye molecules have been utilized in this direction to improve the radiation shielding materials in composition with

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Indigenously Designed and Fabricated Mechanical Milling set-up to Synthesis Nanoparticles: A Cost-effective Method

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In recent days, the area of nanomaterial synthesis has been very attractive due to the distinguished physicochemical properties which can be modified with a different nanostructure and morphology. In this present investigation, a simple and unique approach on fabrication and testing of homemade ball milling has been developed for laboratory use. In the set-up, the gears have been used to provide positive drive over the container by meshing teeth with driver and driving shaft. Just by changing the position of gears horizontally, the different sized container can be mounted for the same set-up based on the requirement. Container was made of stainless-steel metal; it was then threaded on both sides to suit the stainless-steel caps using a lath system and made easy for cleaning container. Reduction of size of the Fe₂O₃ particles was achieved in short period of time. The particle size of pure and ball milled samples from scanning electron microscope was 227-36 nm. Whereas, the particle analyzer measurement shows that particle size ranges from 230-22 nm.

Keywords: Ball milling, Nanoparticles, Cost-effective, Gears, Zeta potential.

1 Introduction

Mechanochemistry has been well established for the mineral extraction in material science and chemistry. This process involves the nature of reaction and frequency of solids caused by the incorporation of mechanical energy with the samples such as grinding using a mortar and pestle. The traditional system of metals extraction from minerals were initiated long ago during the early stage of evolution of chemistry1-3 that involves some practices of mechanical character ameliorating the approachability of the fine powder. The typical speed of traditional ball milling was 30 - 150 rotations per minute (RPM). However, the limited chemical reactions were successfully carried out by grinding due to its low grinding strength and speed. Generally, one can expect fine and better quantity milling in lesser time. To overcome this limitation associated ball-milling, a planetary mill (mixer mill) has been developed.⁴ Further, the planetary milling accounts for up to 30% of power consumption in mineral operations. Planetary milling has smaller chamber balls and limited capacity.

Various processes take place during mechanochemical procedure such as the reduction of particle size,^{2,5} the generation of new surfaces,^{6,7} point defects and dislocations⁸ in the crystalline structure and polymorphic transformations.^{2,9} The equipment used for characteristically mechanical activation includes the retschmill,⁹ tumbling mill,⁹ stirring (attritor) ball mill,⁸⁻¹⁰ vibration mill,⁹ pin mill,^{8,9} rolling mill,^{8,9} and planetary ball mill.^{9,11} Recent innovative procedures in mechanochemistry are more ecofriendly and have many advantages over the traditional ones.¹² Ball milling process is an original strategy to modify materials at the nanometer scale.¹³ Particle size reduction, increase of specific surface area, crystalline structure decomposition and bond breakage have been identified as the main process during ball milling process.⁹

A variety of nanoparticles were fabricated by topdown approaches like mechanical milling, etching, laser ablation, sputtering and electro-explosion.¹⁴ This top-down technique has been used as a simplest way to synthesis a variety of nanomaterials such as metal oxides,¹⁵⁻¹⁷ carbon materials,^{15,18} zeolites,^{15,19} and metal organic frame works.¹⁵ Ball-milling is a wellestablished method for obtaining fine particles with high surface area from bulk materials.²⁰ Grinding method or ball milling is used to grind the

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FULL PAPER

WELPSA: A natural catalyst of alkali and alkaline earth metals for the facile synthesis of tetrahydrobenzo[b]pyrans and pyrano[2,3-d]pyrimidinones as inhibitors of SARS-CoV-2

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Aravind R. Nesaragi¹ | Ravindra R. Kamble¹ | Swati R. Hoolageri¹ Ahmedraza Mavazzan¹ | Suresh F. Madar¹ | Ashish Anand²

> Since 2019, the infection of SARS-CoV-2 has been spreading worldwide and caused potentially lethal health problems. In view of this, the present study explores the most commodious and environmentally benign synthetic protocol for the synthesis of tetrahydrobenzo[b]pyran and pyrano[2,3-d] pyrimidinones as SARS-CoV-2 inhibitors via three-component cycloaddition of aromatic aldehyde, malononitrile, and dimedone/barbituric acid in water. Lemon peel from juice factory waste, namely, lemon (Cltrus limon), sweet lemon (C. limetta), and Kaffir lime or Citron (C. hystrix), effectually utilized to obtain WELPSA, WESLPSA, and WEKLPSA, respectively, for the synthesis of title compounds. The catalyst was characterized by scanning electron microscope (SEM) and energy-dispersive x-ray spectroscopy (EDX). The concentration of sodium, potassium, calcium, and magnesium in the catalyst (WELPSA) was determined using atomic absorption spectrometry (AAS). The current approach manifests numerous notable advantages that include ease of preparation, handling and benignity of the catalyst, low cost, green reaction conditions, facile workup, excellent yields (93%-97%) with extreme purity, and recyclability of the catalyst. Compounds were docked on the crystal structure of SARS-CoV-2 (PDB: 6M3M). The consensus score obtained in the range 2.47-4.63 suggests that docking study was optimistic indicating the summary of all forces of interaction between ligands and the protein.

KEYWORDS

atomic absorption spectrometry, Covid-19, pyrano[2,3-d]pyrimidinones, tetrahydrobenzo [b]pyrans, WELPSA

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Bioorganic & Medicinal Chemistry Letters

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Green synthesis of therapeutically active 1,3,4-oxadiazoles as antioxidants, selective COX-2 inhibitors and their in silico studies



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ARTICLEINFO

Keynerde Antioxidam COX-2 inhibitory Coumarin Micronosa Molecular docking Mercapio benzoazole 1,3,4-Duadiousle

ABSTRACT

A modest, competent and green synthetic procedure for novel cournarinyi-1,3,4-oxadiazoly1-2mercaptobenzosazoles 8i-t has been reported. Analysis of the docked (PDB ID: SIKR; A-Chain) poses of the compounds illustrated that they adopt identical conformations to the extremely selective COX-2 inhibitor. The biological outcomes as well as computational study suggested that the compounds originated to have elevated resentblance towards COX-2 enzyme than COX-1. The compounds 8i, 8l, 8g, 8r, 8s and 8t emerged as most potent and selective COX-2 inhibitors in contrast with Melenamic acid. The selectivity index of 81, 8n and 8r was respectively found to be 33.95, 20.25 and 24.98 which manifested their high selectivity against COX-2. Interestingly, the compounds which were active as COX-2 inhibitors were also active as antioxidant agents.

Inflammation is a multifarious occurrence concerning humoral and cellular reactions through innumerable inflammatory mediators.1 A great deal of attentiveness has been attracted by Cyclooxygenase (COX) enzymes as significant targets for drug pioneering due to their crucial role in prostaglandin biosynthesis. Inhibition of COX enzymes is a promising approach for the pharmacological intervention in inflammation. Non-steroidal anti-inflammatory drugs (NSAIDs) are the most recurrently stipulated clinical tools due to their superior antiinflammatory, analgesic and antipyretic effects which employ through the inhibition of COX-I and COX-2 however, COX-1 is inhibited more vigorously than COX-2. NSAIDs are predominantly used for diminishing pain and inflammation in osteoarthritis, rheumatoid arthritis and arthritis of systemic lupus erythematosus, psoriasis and other seronegative spondyloarthropathies.2 Nevertheless, their therapeutic benefit is habitually limited by troublesome side effects at the gastrointestinal level (mucosal damage, bleeding). Profound investigation divulged that inhibition of COX-2 is associated with anti-inflammatory and analgesic properties, whereas COX-1 executes a significant role in physiological homeostasis. Subsequently, a new genre of selective COX-2 inhibitors

(coxibs) had been evolved,² While, the selective COX-2 inhibitors have not exhibited any gastrointestinal side effects, they endure from the drawbacks of cardiovascular complications that preceded to the withdrawal of Rofecoxib (Vioxx) and Valdecoatb (Bextra) from the market in 2004 and 2005, respectively.

Heterocycles encompassing five-membered oxadiazole nucleus procure a miscellany of useful biological consequences such as anti-edema, antioxidant and anti-inflammatory activities. 1.3.4-Oxadiazoles exhibit anti-inflammatory activity by virtue of dual mechanism i.e., their enzyme inhibiting properties for both cyclooxygenase and 5-lipourverses to bring down gastric uleer formation." During the last decade 686 patent applications concerning to drug discovery program have been filed on oxadiazole scaffold.7 For the treatment of cancer and cystic fibrosis the valuable privileges of the oxadiazole scaffold such as Zibotentan and Ataluren respectively are enduring clinical trials with respect to the drug discovery.¹⁰ In recent years there has been a massive analysis on the diverse set of oxadiazoles among which several such scaffolds were found to possess an extensive spectrum of pharmacological activities.

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Synthesis of metal free organic dyes: Experimental and theoretical approach to sensitize one-dimensional cadmium sulphide nanowires for solar cell application

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CdS namework

ABSTRACT

Synthesis of metal-free organic dyes PDR and PDP based on the phenothiazine core and have been attempted through solution chemistry approach and anchored on to one dimensional cadmiam valobade nanosetres (CdS NWh) to be used as light harvesters in eye sensitized solar cell (DSSC) device application Simple and cost effective solution claemintry approach leads to enable CdS NWs interconnected date network. Synthesized dyes have been immitigated through optical and electrochemical studies in addition to theoretical calculations using density functional theory (DPT). Dye anchored CdS films cover wider light absorption than have GrB in the wisible part of solar spectrum. The complete device configuration has been assembled as PTO/CdS compact/CdS MWs/Organic dye/electrolyte/Wattman electrode, POB and POP sensitized Cd5 NWs yield 0.24 and 0.28% efficiency which are 2.38 and 2.77 times as compared to hare CdS NWs (0.100) with yun lister of standard conditions of illuminations. Extended exactly of financy enforcement is well supported with the obtained couple, and convoluted well with the absorption studies The present work successfully demonstrates the use of soviel synthesized organic dyes as light harvesters. © 2021 Elsevier S.V. All rights reserved.

1. Introduction

The increasing global energy sequirement made inferior by burning the fossil fuels resulting in accetic environmental issues. Hence, there is prevailing need to avoid the use of nonrenewable energy resources and relevant search for the renewable one. Among the several promising renewable energy sources, solar energy is the one that could contribute for the development of such a society. Monover, DSSE has well focused owing to its prospective for efficient energy conversion, easy processing and low cost [1-5]. In DSSCs, sunlight is absorbed by molecular dyes responsible for generation of electron-hole after photoescitation those which are anchored on the high surface area large energy gas semiconducting weatheright Hill

A lot of investigations have been accomplished extensively on the constituents of DSSCs, including photoanode, semitizing dye, redex electrolytes and counter electrodes in order to improve the

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photovoltaic device performance [7-10]. Amongst these, sensitiz ers play vital role which significantly influence the efficiency and the stability of DSSC. Metal-free organic dyes are very attractive amongst various types of sensitizers due to their facile synthetic methodologies, low production cost and their high melar extinc-tion coefficients [11-14]. Metal-free organic derivatives such as phenothiazine, triphenylamine, coumarin, indoline and carbozole based dyes have shown promising power conversion efficiency (PCE) approaching 10% in DSSCs [15-19]. Among these various metal-free organic derivatives, 10ff-phenothiazine have shown very promising results in DSSCs due to their low cost, easily tupeable structures and low environmental pollution [20]

Phenothiazine is a renowned organic molecule containing electron-rich nitrogen and sulphur hetero-atoms. Due to the electron rich behaviour, it enables noble electron donating cauability through charge transfer that occurs during illumination and thus responsible for photo-excited electron transition. Furthermore, it demonstrates a small and reversible oxidation potential for the establishment of a steady radical cation [21-22]. Apart from its electron rich behaviour, its non-planar geometry, favourable thermal and electrochemical strength along with excellent hole

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SCXRD, DFT and molecular docking based structural analyses towards novel 3-piperazin-1-yl-benzo[*d*]isothiazole and 3-piperidin-4-yl-benzo[*d*]isoxazoles appended to quinoline as pharmacological agents

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Highlights

- Novel <u>quinoline</u> containing 3-piperazin-1-yl-benzo[d]isothiazole and 3-piperidin-4yl-benzo[d]isoxazoles were synthesized.
- The <u>single crystal</u> XRD, <u>DFT studies</u> and *in silico* <u>pharmacokinetic</u> and toxicity parameters were done.
- *In vitro* <u>antimicrobial activity</u> was analysed and correlated with energy difference in <u>Frontier Molecular Orbitals</u>.
- Antimicrobial activity observed from *in vitro* assays and DFT studies were validated by Docking studies.



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Bioorganic Chemistry Volume 112, July 2021, 104962

8-Hydroxyquinoline derived p-halo N4-phenyl substituted thiosemicarbazones: Crystal structures, spectral characterization and *in vitro* cytotoxic studies of their Co(III), Ni(II) and Cu(II) complexes

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Highlights

- Crystal structures of the 8-hydroxyquinoline <u>thiosemicarbazone</u> ligandsare explored.
- Transition metal complexes [Co(III), Ni(II) & Cu(II)] are synthesized and characterized.
- *In vitro* cytotoxicity studies are presented for the synthesized compounds.
- The <u>fluorescence microscopy</u> images of the cell are portrayed for the compounds.

Abstract



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Full Paper

Fluorophore Tagged Mixed Ligand Copper(II) Complexes: Synthesis, Structural Characterization, Protein Binding, DNA Cleavage and Anticancer Activity

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First published: 01 December 2021 https://doi.org/10.1002/slct.202103314

Abstract

Fluorophore tagged copper(II) complexes incorporating 1,8-naphthalimide based ligands have been synthesized and structurally characterized. Copper complexes have enhanced plasmid DNA photocleavage activity. The cytotoxicity of copper complexes is much higher than that of cis-platin against A549 and MCF-7 cell lines. The fluorescence microscopy study indicates cellular uptake and localization of the complexes. The complexes induce an apoptotic mode of cell death.



Abstract

Two fluorophore tagged copper(II) complexes $[Cu(phen)(L)(ClO_4)_2]$ (**1**) and $[Cu(bpy)(L)(H_2O) (ClO_4)](ClO_4)$ (**2**), (where L=2-amino-1*H*-benzo[de]isoquinoline-1,3-(2*H*)dione (**L**), phen=1,10-phenanthroline and bpy=2,2'-bipyridine) have been synthesized and structurally characterized. Structures of the copper complexes **1** and **2** were confirmed by single-crystal



The ligand 4-(naphthalen-1-yl)-1-((quinolin-2-yl)methylene)thiosemicarbazide (**HL**) and its cobalt(III), nickel(II) and copper(II) complexes of type $[Co^{III}L_2]Cl$ (**1**), $[Ni^{II}L_2]$ (**2**), $[Cu^{II}LCl]$ (**3**) were synthesized and structurally characterized by various spectral techniques. The structure of **2** was confirmed through single-crystal X-ray structure

determination. Complex **2** crystallized in the triclinic system with the *P*-1 space group.

HL acts as tridentate chelate with N,N,S-donor sites. The spectrochemical analysis of





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Research paper

The Co(II), Ni(II), Cu(II) and Zn(II) complexes of aroylhydrazone of quinolone core: Syntheses, characterization and evaluation of antimicrobial and antitubercular activity

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Highlights

- The Co(II), Ni(II), Cu(II) and Zn(II) complexes of aroylhydrazone of quinolone core were synthesized.
- Cobalt, nickel, copper complexes were characterized by single crystal X-ray structure determination.
- The antimicrobial and antitubercular activities of the complexes is studied.
- The antitubercular activity of copper complexes as good as the standard *Streptomycin* drug.

Abstract



Electro, Physical & Theoretical Chemistry

Design and Synthesis of D- π -A form of *p*-Nitrophenylacrylonitrile Substituted Triphenylamine Chromophores; Photophysical, Electrochemical Properties, DFT and Thermal Studies

Shivaraj Mantur,^[a] Mallikarjun K. Patil,^[b] Mahesh S. Najare,^[a] AfraQuasar A. Nadaf,^[a, c] Mohammed Yaseen,^[a] Supreet Gaonkar,^[a] Sanjeev R. Inamdar,^[b] Imtiyaz Ahmed M. Khazi,^[a] and Ravindra R. Kamble^{*[a]}

This paper reports a novel Donor- π -Acceptor type of π conjugated triphenylamine (TPA) dyes bearing a 4-nitrophenyl acrylonitrile units (abbreviated as TPA-4(a–e) which were synthesized by Knoevenagel condensation followed by palladium catalyzed Suzuki-Miyaura cross coupling reaction with good yield. These dyes contain TPA as electron donor (D) and 4-nitrophenyl acrylonitrile as electron acceptor (A) and probes were confirmed by standard spectroscopic techniques viz.,¹H, ¹³C NMR, FT-IR, GC-MS and ESI-MS. Herein, for the D- π -A pushpull structure, TPA and 4-nitrophenyl acrylonitrile are connected by vinylene bond as the π -bridge. Optical/Solvatochromic properties were studied in detail by UV-Vis absorption and fluorescence spectroscopy. The intramolecular charge transfer

1. Introduction

Clean, eco-friendly and sustainable energy/lighting sources have become one of the current interests in the field of research from both scientific and practical point of view. Thermally durable amorphous thin-film materials have been developed recently in organic light emitting diodes (OLEDs) with the aim of long-life; full-color flat panel displays and solidstate lighting sources, because of their features like low power consumption, wide viewing angles, rapid responses, and potential use in light-weight flexible devices.^[1-6] Electrondonating/hole transporting π -conjugated polycyclic aromatics, (TPA),^[7-8] such as triphenylamine carbazole,^[9–10] phenothiazine,^[9,11] anthracene,^[12] pyrene,^[13-14] etc, along with electron accepting/electron-transporting materials such as 4H-

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properties were studied using DFT model with the CAM-B3LYP function and solvatochromism by experimental method. The synthesized materials have shown moderate quantum yields. Optical bandgap values range from 2.33 to 2.39 eV and these derivatives exhibit well judged thermal stability and their 5% weight loss temperature are in the range 178–220 °C. Cyclic voltametery study of the title compounds indicated that E_{ox}^{onset} values ranging from 1.05–1.25 eV. Quantum yields (Φ) of the probes are experimentally measured in the 1, 4-dioxane and the Stokes shifts are observed to be in the range of 4882–5545 cm⁻¹. The results displayed that these novel (D–A–D) chromophores could play an important role in the organic optoelectronics.

1,2,4-triazole,^[4,15] oxadiazole,^[15–16] thienopyrazine,^[17–18] 2-(4-nitrophenyl)acetonitrile,^[19] forms D- π -A type of push pull system with a bipolar nature amid better photophysical properties for photovoltaic application. This D- π -A system helps to increase the conjugation in the fluorophore which leads to wide use of these compounds in electronics and optoelectronics, including light-emitting diodes, photovoltaic cells, thin film transistors and electrochromic cells,^[20] solid-state lasers,^[21] cellular imaging, optical data storage media, detection of microenvironmental changes, field-effect transistors (FETs),^[22] biosensors,^[23] nonlinear optical devices, [24] organic light emitting transistors (OLETs),^[25] etc. Strong absorption and emission properties were exhibited by the D- π -A system which is due to intramolecular charge transfer (ICT) from the donor to acceptor units.^[26] Now a day's along with D- π -A, D-A strategy plays important role in OLED due to the electron donor and electron acceptors forming a push pull system and facilitates injection and transport of both holes and electrons.^[27]

In inorganic materials the entire expanse of solids consists of covalent or ionic bonds where as in organic materials by weak intermolecular interactions therefore metal free π -conjugated organic materials can be readily performed on the molecular level. Hence organic molecules were preferred for photo- and electro-active materials.^[28] Among other organic molecules the most frequently used functional moieties in π conjugated materials have the triphenylamine group. This is

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Synthesis of metal free organic dyes: Experimental and theoretical approach to sensitize one-dimensional cadmium sulphide nanowires for solar cell application



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ARTICLE INFO

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Keywords: Dye sensitized solar cells CdS nanowires Metal-free organic dyes DFT calculations Solar cell fabrication

ABSTRACT

Synthesis of metal-free organic dyes PDR and PDP based on the phenothiazine core unit have been attempted through solution chemistry approach and anchored on to one dimensional cadmium sulphide nanowires (CdS NWs) to be used as light harvesters in dye sensitized solar cell (DSSC) device application. Simple and cost effective solution chemistry approach leads to enable CdS NWs interconnected nano network. Synthesized dyes have been investigated through optical and electrochemical studies in addition to theoretical calculations using density functional theory (DFT). Dye anchored CdS films cover wider light absorption than bare CdS in the visible part of solar spectrum. The complete device configuration has been assembled as FTO/CdS compact/CdS NWs/Organic dye/electrolyte/Platinum electrode. PDR and PDP sensitized CdS NWs yield 0.24 and 0.28% efficiency which are 2.36 and 2.77 times as compared to bare CdS NWs (0.10%) with sun light of standard conditions of illuminations. External quantum efficiency enhancement is well supported with the obtained results and correlated well with the absorption studies. The present work successfully demonstrates the use of novel synthesized organic dyes as light harvesters.

1. Introduction

The increasing global energy requirement made inferior by burning the fossil fuels resulting in ascetic environmental issues. Hence, there is prevailing need to avoid the use of nonrenewable energy resources and relevant search for the renewable one. Among the several promising renewable energy sources, solar energy is the one that could contribute for the development of such a society. Moreover, DSSC has well focused owing to its prospective for efficient energy conversion, easy processing and low cost [1–5]. In DSSCs, sunlight is absorbed by molecular dyes responsible for generation of electron-hole after photoexcitation those which are anchored on the high surface area large energy gas semiconducting materials [6].

A lot of investigations have been accomplished extensively on the constituents of DSSCs, including photoanode, sensitizing dye, redox electrolytes and counter electrodes in order to improve the

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photovoltaic device performance [7–10]. Amongst these, sensitizers play vital role which significantly influence the efficiency and the stability of DSSC. Metal-free organic dyes are very attractive amongst various types of sensitizers due to their facile synthetic methodologies, low production cost and their high molar extinction coefficients [11–14]. Metal-free organic derivatives such as phenothiazine, triphenylamine, coumarin, indoline and carbazole based dyes have shown promising power conversion efficiency (PCE) approaching 10% in DSSCs [15–19]. Among these various metal-free organic derivatives, 10*H*-phenothiazine have shown very promising results in DSSCs due to their low cost, easily tuneable structures and low environmental pollution [20].

Phenothiazine is a renowned organic molecule containing electron-rich nitrogen and sulphur hetero-atoms. Due to the electron rich behaviour, it enables noble electron donating capability through charge transfer that occurs during illumination and thus responsible for photo-excited electron transition. Furthermore, it demonstrates a small and reversible oxidation potential for the establishment of a steady radical cation [21–22]. Apart from its electron rich behaviour, its non-planar geometry, favourable thermal and electrochemical strength along with excellent hole

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Nanoparticle surface energy transfer (NSET) in ferroelectric liquid crystal–metallic-silver nanoparticle composites: Effect of dopant concentration on NSET parameters

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In the recent past, the resonance energy transfer studies using metallic nanoparticles has become a matter of quintessence in modern technology, which considerably extends its applications in probing specific biological and chemical processes. In the present study, metallic-silver nanoparticles of 2–4 nm (diameter) capped with hexanethiol ligand are developed and dispersed in ferroelectric liquid crystal (FLC). The morphology of nanoparticles was characterized using HR-TEM and SEM techniques. Furthermore, a systematic study of energy transfer between the host FLC material (as donors) and metallic-silver nanoparticles (as acceptors) has been explored employing steady state and time resolved fluorescence spectroscopic techniques. The nanoparticle based surface energy transfer (NSET) parameters viz., transfer efficiency, transfer rate, and proximity distance between donor and acceptor, have been determined for NSET couples (FLC material–metallic-silver nanoparticle) composites. It is observed that various NSET parameters and quenching efficiency follow a linear dependence on the concentration of metallic-silver nanoparticles in host FLC material. The nonradiative energy transfer and superquenching effect of the silver nanoparticles can be used for sensing applications that require high degree sensitivity.

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I. INTRODUCTION

Over the past decade nanoscience has gained prominence and the ever increasing growth has been contemplated in its advances in the field of nanomedicine, drug delivery, bioimaging, sensing, nanofabrication, etc. [1]. Among all the nanostructures, metallic nanoparticles are of interest in both research and technology, due to their specific properties not available in isolated molecules or bulk metals. Because of these properties nanoparticles have many important applications in catalysis, sensing, and imaging [2-5]. The localized surface plasmon resonance makes the metallic nanoparticles good scatterers and absorber of visible light [6]. Due to the surface characteristics and high stability of the metallic nanoparticles, they have been extensively employed as fluorescence quenchers. Highly efficient fluorescence quenching of the fluorescence of dyes and polymers (conjugated and nonconjugated) in the presence of metallic nanoparticles has been reported by several groups [7,8]. The dynamic quenching has been well explained by the process of Förster resonance energy transfer (FRET) between the FRET pairs (donor and acceptor). The energy transfer efficiency highly depends upon the relative distance between the FRET pair. In the case of metallic nanoparticles, energy transfer between the donoracceptor pair can be termed as nanoparticle based surface energy transfer (NSET) due to the dipole-surface type energy

transfer [9]. The efficiency of NSET is usually high over FRET. Fluorescence lifetime is a more reliable parameter to validate the possibility of energy transfer in a system, as it is largely independent of the fluorescence intensity and fluorophore concentration. Time resolved fluorescence measurements also provide significant and precise information about the molecular interactions in comparison to the steady state measurements [10].

The chemically tailored tunable optoelectronic properties, shapes, and size of metallic nanoparticles such as gold, silver, copper, etc. make them suitable to be used as dopant in liquid crystals (LCs). The incorporation of metallic nanoparticles could effectively improve the optical, electrical, and dielectric properties of the LC material [11–14]. Dispersion of a small quantity of metallic nanoparticles can efficiently influence the fluorescence properties of host liquid crystalline material [15–17]. However, in literature, changes in fluorescence intensity of host FLC material in the presences of metallic nanoparticles has not been discussed by considering FRET or NSET mechanism.

In the present article we have investigated the interaction of hexanethiol capped silver nanoparticles with ferroelectric liquid crystalline material. Absorbance and florescence properties of the FLC material in the presence of silver nanoparticles have been studied. Steady-state measurements reveal the fluorescence quenching of FLC material after the dispersion of metallic-silver nanoparticles. Time-resolved fluorescence spectroscopic techniques have been used to confirm the results obtained from the steady-state measurements.

022708-1

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Biogenic Synthesis of Iron Oxide Nanoparticles Using Moringa olifera leaf extract

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ABSTRACT

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Keywords:

Fe₃O₄; NPs; XRD; Debye-Scherer; SEM; The present study is an effort on green synthesis of iron oxide nanoparticles (NPs) by using Moringa olifera leaf extract as reducing agent. Crystalline nature, size, morphology, chemical composition



and its optical features were analysed using X-ray diffraction (XRD), Scanning electron microscope (SEM), Fourier transform infrared (FTIR) and UV-Visible absorption spectroscopic measurements, respectively. XRD spectrum manifests the cubic phase of the NPs with average size of about 24nm. SEM analysis confirms the spherical shape of NPs with agglomeration. FTIR spectrum reveals the occurrence of Fe-O vibrational bond. The NPs are optically active and can be utilized in light harvesting and biosensor applications.

1. Introduction:

Recently, research on nanoparticles (NPs) gained a wide range of interest among the scientific community due to its applications in biology, medicine, and engineering [1]. NPs exhibit unique optical, electrical and magnetic properties upon changing their size, shape and composition, respectively [1, 2]. Currently, there is a large number of NPs are extensively applied in biomedical studies in particularly antimicrobial, antioxidant, and drug delivery agents. The development in nanoscience has to lead to the production of NPs by various chemical and physical techniques. Conversely, these techniques have a negative impact on the environment and living organisms because an un-reacted chemicals are discharged in the environment [3].

The introduction of NPs in biomedicine and drug delivery has turned out to be a source of urge therefore it is also essential to develop hygienic, safe, simple and non-toxic materials through eco-friendly synthesis [4]. There are various synthesis methods are available to

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Original research article

Reaction temperature based synthesis of ZnO nanoparticles using co-precipitation method: Detailed structural and optical characterization

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ARTICLEINFO

Keywords: Nanoparticles ZnO Co-precipitation XRD SEM Fluorescence

ABSTRACT

ZnO nanoparticles (NPs) have synthesized by using the co-precipitation method at two different reaction temperatures (50 °C and 70 °C) by using zinc nitrate hexahydrate and sodium hydroxide as precursors in an aqueous medium. X-ray diffraction, SEM, EDS, and FTIR analysis confirmed the formation of good quality ZnO NPs with some minor impurities. Here, Debye-Scherrer (DS) and size-strain plot (SSP) theoretical methods have been employed to inspect the crystalline size and the intrinsic strain from the XRD peak broadening analysis and obtained average crystalline sizes were found to be 24 nm and 29 nm for the NPs prepared at 50 °C and 70 °C, respectively. Further, ZnO NPs have shown broad absorption, narrower emission spectrum and wide energy bandgap; these characteristics help in the potential applications of optoelectronic devices and biosensors e.g. solar cell and fluorescence resonance energy transfer techniques.

1. Introduction

In the past few years, the application of NPs has paid attention due to its novel and unique properties (optical, electrical, mechanical, etc.) resulted from quantum confinement effects compared with their bulk counterpart [1,2]. These properties are easily attuned by changing their shape, size and composition during the synthesis of materials at the nanoscale [3–5] and due to these factors, synthesis and analysis of NPs has gained significant importance in the recent past [1,6,7]. Among various NPs studied, ZnO gained a lot of popularity and become multifunctional material due to its exceptional properties including high chemical, thermal, photo and mechanical stability, low toxicity, a wide range of energy absorption, biocompatibility and biodegradability [8,9]. These attributes make this material for the successful utilization in solar cells, optical coatings, photocatalyst, gas sensors, and active medium in UV semiconductor lasers [9–11]. ZnO NPs additionally display the incredible ability for the improvement of optical recognition of target biological macromolecules, as ZnO NPs are biologically adaptable in normal detecting conditions [11]. Hence, this wide range of applications made the scientific community to take keen research interest in ZnO NPs.

In the current work, the co-precipitation technique has utilized to prepare ZnO NPs at two different reaction temperatures i.e., at 50 °C and 70 °C in an aqueous medium. The structural parameters like the presence of chemical bonding, average crystalline size, shape, and optical properties were determined by using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD),

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- Published: 11 February 2022

Bio-inspired silver nanoparticles from *Artocarpus lakoocha* **fruit extract and evaluation of their antibacterial activity and anticancer activity on human prostate cancer cell line**

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Abstract

The growing multi-drug resistance in human disease causing pathogens is an issue of great concern, and there is a need for broad-spectrum antibiotic to fight severe diseases. As silver is toxic to microbes like fungi, bacteria and yeast, the use of silver nanoparticles as antimicrobial agent may help control the resistant pathogenic microbes. During this study, the bio-fabrication of silver nanoparticles was done from *Artocarpus lakoocha* fruit extract and characterized using various morphological and structural analysis. The agar well diffusion technique was performed to determine the bactericidal potential of nanoparticles against human disease causing pathogenic bacteria; finally, the anticancer activity was assessed by employing 96-well plate MTT assay and flow cytometry-assisted apoptosis on human prostate adenocarcinoma (PC-3) cells. The primary indication on nanoparticles synthesis was given by colour change from slight yellow to brown; further, reaffirmed by the peak obtained at 415 nm for absorption maximum in UV–vis. analysis. Meanwhile, the smooth surface and spherical shapes were determined by AFM and SEM analyses. Similarly, poly-dispersed distribution, size range of 6.59– 25 nm and FCC crystalline nature were confirmed by TEM and XRD analyses. The silver nanoparticles displayed higher antibacterial activity by forming clear zones of inhibition and exhibited increased anticancer activity on PC-3 cells. The IC₅₀ value obtained was 30.62 µg/ml and 48.11 ± 0.7%, 24.92 ± 0.5%, and 1.19 ± 0.4% of early, late apoptosis and necrosis was observed in flow cytometry-assisted Annexin V/PI study. The


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Original article

Biogenic synthesis, characterization and antimicrobial activity of *Ixora brachypoda* (DC) leaf extract mediated silver nanoparticles

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Abstract

The present investigation was aimed at the evaluation of synthesis, characterization and antimicrobial activity of *Ixora brachypoda* DC. leaf extract mediated silver nanoparticles (AgNPs). The AgNPs were characterized by UV–Visible (UV–Vis) spectrophotometer, Fourier transform infrared spectroscopy (FTIR), Atomic force microscopy (AFM), Scanning electron microscopy (SEM) with Energy dispersive X-ray spectrometry (EDS), Transmission electron microscopy (TEM), Zeta potential and X-ray diffractometry (XRD). Finally, the antimicrobial activity of synthesized AgNPs was investigated against pathogenic microorganisms. The absorption peak, obtained at 423 nm in UV–Vis analysis, confirmed the synthesis of AgNPs and the presence of biological functional groups involved in the capping and stabilization were determined by FTIR analysis. The other characterizations revealed the details about the AgNPs as spherical, polydispersed and size ranging from 18 to 50 nm with an average diameter of 27.76 nm. The zeta potential was calculated to be -30.4 mV and the typical Bragg's planes in the metallic silver range indicated the confirmation of AgNPs formation. The *in-vitro* analysis confirmed the antimicrobial potential of I. brachypoda leaf aqueous extract synthesized AgNPs, which effectively inhibited the growth of pathogens and it can be concluded that the I. brachypoda AgNPs can be used as broad-FEEDBACK 💭 spectrum antimicrobials against multi-drug resistant microbial pathogens.