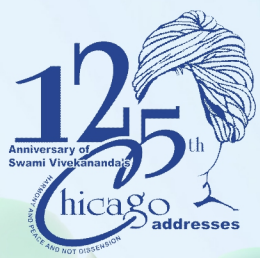
NATIONAL CONFERENCE ON

RECENT TRENDS IN CHEMISTRY - 2019 (RTC'19)

1st & 2nd, February 2019

ABSTRACTS



Celebration of 125th Anniversary of
Swami Vivekananda's Historic Speech
at the World Parliament of Religions in Chicago

In Honour of retirement of
Prof. Dr. M. Dhandapani

Editors
Dr. A. Muthusamy (Convener)
Dr. V. Mohanraj (Co-Convener)

Organised by
Post Graduate and Research Department of Chemistry
Sri Ramakrishna Mission Vidyalaya College of Arts and Science
(An Autonomous Institution affiliated to Bharathiar University
Re-accredited by NAAC with "A" Grade)
Coimbatore - 641 020
Tamil Nadu, India

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Coimbatore - 641 020
Tamil Nadu, India

Swami Nirmaleshananda
Secretary
Sri Ramakrishna Mission Vidyalaya
College of Arts and Science
Coimbatore - 641 020

Date: 28.01.2019

Message

My hearty and cheerful compliments to the Post Graduate and Research Department of Chemistry of our College for organising a National Conference on "Recent Trends in Chemistry – 2019" (RTC'19) on 01.02.2019 and 02.02.2019.

I strongly hope that this National level conference will be a curtain raiser for fresh concepts and novel speculations among the young talents of our country. The resourceful lectures by the eminent personalities will have a great knowledge explosion in Chemistry.

I congratulate the organisers of this National Conference a great success.

Swami Nirmaleshananda

(SWAMI NIRMALESHANANDA)

Dr. V. Ponnuswamy
Principal
Sri Ramakrishna Mission Vidyalaya
College of Arts and Science
Coimbatore- 641 020

Message

Academic conferences are good for networking researchers engaging research of the same field. One can discuss ideas for future co-operation and sometimes also work on ongoing projects/papers. Sometimes conferences are also good for getting new ideas and understanding what is becoming 'hot' in the current research. Besides, researchers can know about the future research trends from the invited talks and keynote addresses.One might see the conference paper also as a precursor of a follow-up publication in mind and a forum where you get valuable feed-back what needs to be improved.

With all these thoughts, the Post Graduate and Research Department of Chemistry is organizing a National Conference on **"Recent Trends in Chemistry -2019"** on 01 & 02 February 2018.

I congratulate all the Faculty Members and Research Scholars with heartful of wishes for the success of the conference.

30.1.19

Dr. V. PONNUSWAMY

Sri Ramakrishna Mission Vidyalaya
College of Arts and Science

Sri Ramakrishna Mission Vidyalaya College of Arts and Science, an autonomous institution affiliated to Bharathiar University is one of the oldest institutions of Ramakrishna Mission Vidyalaya established in the year 1964. It is one of the top institutions providing higher education known for its focus on academic excellence and social relevance. The College of Arts and Science has 13 UG and 7 PG Programmes both under aided and un-aided streams. Autonomous status was conferred in the academic year 1981-82 and ranked 39 by NIRF in 2018. The College celebrated its Golden Jubilee in 2014. It was Re-accredited by NAAC with 'A' grade in 2016. UGC sponsored DDU Kaushal Kendra of this College offer 3 B.Voc. and 2 Diploma Courses.

Department of Chemistry

The PG and Research Department of Chemistry of Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore is one of the oldest Chemistry Departments in Tamil Nadu with 11 faculty members and one DST – INSPIRE faculty member. The Department offers programmes from B.Sc. to Ph.D. Currently research is being pursued in a wide spectrum of disciplines. The Department is DST-FIST sponsored and has undertaken Research Projects from leading funding agencies such as UGC and CSIR. With rich experience of teaching and research, the department focuses on enhancing Chemistry Education with Global Perspective. The Department has produced 41 PhDs and 125 MPhils. It has the privilege of possessing more than 300 publications in reputed journals with high impact factor.

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ORGANISING COMMITTEE

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	Assistant Professor of Chemistry
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	Dr. A. Murugesh, ***Assistant Professor of Chemistry***
	Dr. E. Selvakumar, ***Assistant Professor of Chemistry***
	Dr. V. Rajapandian, ***DST-INSPIRE Faculty***
	Dr. B. Siva Senthil Kumar, ***Assistant Professor of Chemistry***

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Abstract Book	**Mr. S. Kathiravan** (Research Scholar)
Press	**Mr. S. Manigandan** (Research Scholar)
Guest Care	**Mr. S. Madhan Kumar** (Research Scholar)
	Mr. K. Singaravelan(Research Scholar)
Registration	**Ms. Haseena Sheik** (Research Scholar)
	Mr. M. Palanivelmurugan (PG Student)
Accounts	**Mr. R. Ragul** (Research Scholar)

Professor Dr. M. Dhandapani was born in 1961 in a small hamlet Eragampatty near Dharapuram, Tirupur District. During his schooldays, he was awarded 'National Scholarship for Talented Children from Rural Areas'. Following this, he was admitted in the prestigious Pudukkottai Model School, Pudukkottai where he studied from 1975 to 1977. Then, he completed his BSc (1981) in Chemistry from Chikkaiah Naicker College, Erode and MSc (1983) in Chemistry from PSG College of Arts and Science, Coimbatore, Tamil Nadu. He got his MPhil in 1985 in Analytical Chemistry from University of Madras, Chennai.

He joined UPASI Tea Research Institute, Valparai, Tamil Nadu in 1985 as an Assistant Tea technologist in Research and Development and worked up to 1988. In the same year, he became Assistant Professor in Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore, Tamil Nadu (1988-1996) and later Lecturer (SG). In 2006, he was promoted as an Associate Professor of Chemistry. He earned his PhD degree in Solid State Chemistry under the guidance of Dr. M. A. Kandhasamy, from the same Department in 2008, where he continued to be involved in research and development on metal organic non-linear optical materials. In 2010, he started guiding PhD Scholars and he shifted his interest in Supramolecular and Computational Chemistry especially in Hydrogen bonding and non-covalent interactions for optical and biological applications. He was awarded a research project by UGC in the same research area that he pursued till 2018. In the last several years, he collaborated and taught computational chemistry to many Professors and Research Scholars to enrich their knowledge on material characterization using software. He is author of more than 75 original research articles published in peer-reviewed journals and his work has been cited more than 346 times (SCI). He is also an attractive and popular speaker from fundamental to research topics. He is a reviewer in several peer reviewed SCI journals. He became the lightening lamp for more than 34 research Scholars who did MPhil and PhD under his guidance. He acted as a Resource Person/reviewer/ Member in many Academic and Research bodies. His elegant way of teaching attracted many students and kindle interest towards the Chemistry. At present, a number of his students are Scientists/ Teachers /Professors/ Professionals/ Entrepreneurs. He has taken up several responsibilities in the College. In 2000, he was founder-Coordinator of Career and Guidance Cell and fetched jobs for a good number of students. Between 2011 and 2016, he served as the Research and Faculty Enrichment Council coordinator. The Department of Chemistry, SRMVCAS is proud to honour Prof. Dr. M. Dhandapani through a National Conference on recent trends in Chemistry.

Sri Ramakrishna Mission Vidyalaya College of Arts and Science
Coimbatore 641 020
Post Graduate and Research Department of Chemistry
National Conference on Recent Trends in Chemistry (RTC'19)
Programme Day 1

Date: 01-02-2019 **Venue: GKD Auditorium**

9.00- 9.45 am	: **Registration**		
09.45 - 10.25 am	**- Inauguration**		
9.45 am	: Prayer		
9.48 am	: Lighting the KuthuVilakku	-	Dignitaries
9.53 am	: Welcome Address	-	**Dr. A. Muthusamy,** *Convener (RTC'19)*
9.58 am	: Presidential Address	-	**Dr. A. Chandramohan,** *HoD of Chemistry* Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore
10.03 am	: Benedictory address	-	**Swami Nirmaleshananda,** *Secretary* Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore
10.08 am	: **Inaugural Address**	-	**Dr .N. Sugumaran** *International Battery Consultant,* Coimbatore
10.20 am	: Vote of Thanks	-	**Dr. V. Mohanraj,** *Co-Convener (RTC'19*)
10.25 am	: **Tea break**		
10.40 am	: **Keynote address**	-	**Dr. N. Sugumaran** *International Battery Consultant* Coimbatore
11.25 am	: **Invited Talk I**	-	**Dr. R. Prabhakaran**, *Department of Chemistry* Bharathiar University, Coimbatore
12.10 pm	: **Invited Talk II**	-	**Dr. S. Muthukumar,** *Saradha Terry Products Ltd* Mettupalayam
1.00-2.00 pm - Lunch Break			
2.00 pm	: **Invited Talk III**		**Dr. P. S. Vijayanand,** *Department of Chemistry* Bannari Amman Institute of Technology Sathyamangalam, Erode
2.45 pm	: **Technical Session I: Oral Presentation**		
	Chair Person:		**Dr. R. Nandhakumar,** *Department of Chemistry* Karunya Institute of Technology& Sciences Coimbatore
3.45 pm	: **Technical Session II: Poster Presentation**		
	Chairperson:		**Dr. M. Sureshkumar,** *University of Suwon* Republic of Korea
4.40 pm	: **Tea Break**		

Sri Ramakrishna Mission Vidyalaya College of Arts and Science
Coimbatore 641 020
Post Graduate and Research Department of Chemistry
National Conference on Recent Trends in Chemistry (RTC'19)

Programme Day 2

Date: 02-02-2019 **Venue: GKD Auditorium**

9.40 am	: Welcome &Briefing the Events		**Dr. A. Muthusamy, *Convener (RTC'19)***
9.45am:	: **Technical Session III Oral Presentation**	**Chair Person:**	**Dr. N. Velumani** *Government Arts College* Coimbatore
10.45 am	: **Tea Break**		
11.00 am	: **Invited Talk – IV**	-	**Dr. S. Senthilkumaar** *Department of Chemistry* PSG College of Technology, Coimbatore
11.45 am	: **Invited Talk – V**	-	**Dr. C. Selvaraju** *National Centre for Ultrafast processes* University of Madras, Chennai
12.30 pm :	**Technical Session IV Poster Presentation**	**Chairperson:**	**Dr. Yuvaraj Haldorai** *Department of Nanoscience and Technology* Bharathiar University, Coimbatore

1.15 - 2.15 pm - Lunch Break

2.15 pm	`: **Invited Talk – VI**	-	**Dr. R. Arun Prasath** *Centre for Green Energy Technology* Pondicherry University, Puducherry

3.00 - 4.00 pm- Valedictory

3.00 pm	: Welcome Address	-	**Dr. M. Sekar**, *Department of Chemistry* Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore
3.05pm	: Presidential Address	-	**Dr. V. Ponnuswamy**, *Principal* Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore
3.10pm	: Felicitation to **Dr M. Dhandapani**		
3.25 pm	: Motivation to Students & Researchers-		**Dr. M. Dhandapani**
3.40 pm	: Award distribution	-	**Swami Nirmaleshananda** *Secretary* Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore
3.50 pm	: Feedback	-	Participants
4.00 pm	: Vote of Thanks	-	**Dr. A. Muthusamy,** *Convener (RTC'19)*
4.10 pm	: National Anthem		
4.15 pm	: High Tea		

KEYNOTE ADDRESS

Keynote Address

ENERGY STORAGE TECHNOLOGIES

(The factor which is will make India a Developed Nation)

Dr. N. Sugumaran
International Battery Consultant
Coimbatore

Government of India is planning to increase annual per capita energy consumption from 1075 units (year 2016) to 2900 units by year 2040 to alleviate poverty and make India as one of the developed nation. It necessitates generation of energy in the range of 4647 TWh. India is having limited conventional energy sources such as coal, oil and gas but blessed with renewable energy sources like solar and wind. Due to this GOI is planning to alter the energy mix ratio. The ratio of thermal energy is going to be decreased from present 76% to 52% at 2040 and renewable energy to be increased from 8% to 36%. The solar energy generated in the day time will not be consumed online and to be stored because energy is consumed mainly in the morning and evening when solar energy at nadir. Electrochemical power sources in other words Batteries are proved to be the appropriate technology for energy storage. The talk will highlight the type of batteries presently available and research progress in various types of battery.

Dr. N. Sugumaran is an eminent alumnus of SRMV CAS. He studied both undergraduate and postgraduate studies in the Department of Chemistry. He was a prestigious winner of gold medal from Bharathiar University in postgraduation. He completed his Ph.D. in electrochemistry in National fame Indian Institute of Science, Bengaluru. He has 20 years of industrial experience in the field of batteries. At present he is the consultant for various national and international battery manufacturers. His area of interests is energy storage, electric mobility and corrosion. He is a very popular speaker among battery researchers.

INVITED TALK

INVITED TALK

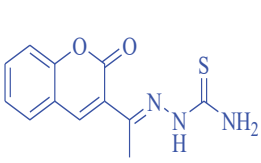
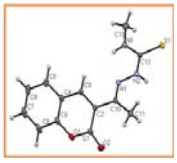
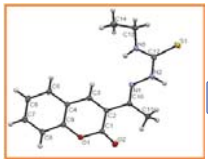
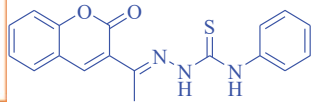
IT No.	DETAILS
01.	**DEVELOPMENT OF COUMARIN BASED METALLOCYCLES AND THEIR BIOLOGICAL PROPERTIES** **Dr. R. Prabhakaran** Department of Chemistry Bharathiar University, Coimbatore
02.	**TECHNIQUES ON TEXTILE WASTE WATER TREATMENT** **S. Muthukumar** Sharadha Terry Products Limited Mettupalayam, Coimbatore.
03.	**SYNTHESIS AND CHARACTERIZATION OF NEW NANOSTRUCTURED ELECTRO ACTIVE POLYMERS** **Dr. P. S. Vijayanand** Department of Chemistry Bannari Amman Institute of Technology Sathyamangalam, Erode.
04.	**QUENCHING OF FERROMAGNETISM OF ZnO UPON Mn DOPING** **Dr. S. SENTHILKUMAAR** PSG College of Technology Coimbatore.
05.	**SPECIFIC SOLVENT EFFECT AND HALOGEN BONDING: SOLVATOCHROMISM AND ULTRAFAST FLUORESCENCE SPECTROSCOPY OF HEMICYNANINE DYE IN CHLORINATED SOLVENTS** **Dr. C. Selvaraju** National Centre for Ultrafast Processes University of Madras, Chennai.
06.	**RENEWABLE ENERGY TECHNOLOGIES FOR SUSTAINABLE DEVELOPMENT** **Dr. R. Arun Prasath** Laboratory for Energy Materials and Sustainability Centre for Green Energy Technology Madanjeet School of Green Energy Technologies Pondicherry University.

IT-01

Development of Coumarin based Metallocycles and their Biological properties

Dr. R. Prabhakaran
Department of Chemistry
Bharathiar University
Coimbatore- 641046
E.mail:rpnchemist@gmail.com

Coumarins (1-benzopyran-2-one) are chemical compounds in the benzopyrone class of organic compounds found in many plants of the family *Orchidaceae*, *Leguminaceae*, *Rutaceae*, *Umbellifferae* and *Labiatae*. They are a part of flavonoid group of plant secondary metabolite, are a wide class of natural and synthetic compounds that showed versatile pharmacological activities. Coumarin Schiff bases derived metallocycles are expected to have enhanced activity. Some of the metallocycles prepared in our laboratory have exhibited relatively higher activity than the most widely used anti-cancer drug *cisplatin* while screening their efficacy in selective malignancies.

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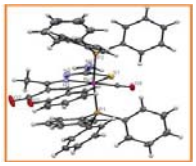
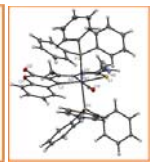
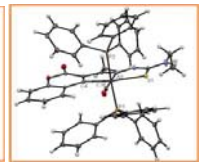
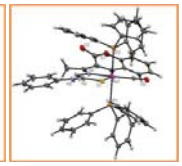
IC50:

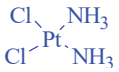
19.18±0.23 (MCF 7)	18.17±0.29 (MCF 7)	17.88±0.15 (MCF 7)	18.47±0.20 (MCF 7)
12.67±0.14 (A549)	12.11±0.19 (A549)	11.58±0.14 (A549)	13.28±0.14 (A549)

[Ru(3AC-tsc)(CO)(PPh_3)$_2$] **[Ru(3AC-mtsc)(CO)(PPh_3)$_2$]** **[Ru(3AC-etsc)(CO)(PPh_3)$_2$]** **Ru(3AC-ptsc)(CO)(PPh_3)$_2$]**

IC50:

2.97±0.11 (MCF 7)	2.94±0.09 (MCF 7)	2.29±0.11 (MCF 7)	3.08±0.08 (MCF 7)
2.89±0.11 (A549)	2.81±0.13 (A549)	2.56±0.10 (A549)	3.06±0.08 (A549)



Cisplatin
16.97±0.08
(MCF7)
15.10±0.05
(A549)

Dr. R. Prabhakaran is a prestigious alumnus of the Chemistry Department of SRMV CAS. He studied PG degree course during the period 2000-2002. He was a best outgoing student of our department in the year 2002. He acquired his Doctoral degree from Bharathiar University in the year 2006. After his Ph.D., he pursued his post-doctoral research in University of Aix-Marseille, France and Chung-Ang University, South Korea. He was the recipient of prestigious Young Scientist award by DST-SERC under Fast Track Scheme. In the year 2010, he received CNRS scientist fellowship from France government. At present, he is Assistant Professor, Department of Chemistry, Bharathiar University and is a popular researcher in the fields of Coordination and Bio-Inorganic Chemistry.

Techniques on Textile Waste Water Treatment

Sri. S. Muthukumar

Sharadha Terry Products Limited

Mettupalayam, Coimbatore

Email: tvsstex@gmail.com

Textile processing is water intensive. Textile process produces waste water containing dyestuffs, auxiliaries and chemicals. Good water quality, more demands and increasing water cost makes good water management a must. We are committed to keep the water, land and atmosphere environmentally cleaner, greener and better by adopting clean technologies to reduce consumption and conserve the water and energy.

Sri. S.Muthukumar, is an esteemed alumnus of the Department of Chemistry of SRMV CAS. Presently he is associated with Sharadha Terry products, Coimbatore and working as a General Manager in Research and Development division. Having more than 30 years of rich experience in textile industry, he has developed several textile products, installed and commissioned many processing plants, and successfully improved sustainable and cost-effective manufacturing process. He was instrumental in the development of light weight micro cotton towels which are being used in White House and Pentagon of USA.

IT-03

Synthesis and characterization of new nanostructured electroactive polymers

Dr. P. S. Vijayanand
Department of Chemistry, Bannari Amman Institute of Technology
Sathyamangalam, Erode
Email: vijayps6@yahoo.co.in, vijayanandps@bitsathy.ac.in

A new type of soft templated in-situ polymerization method has been utilized to prepare conducting polymer nanostructures through a self-assembly process. Surfactants are the special class of molecules that are thermodynamically much stable aggregates of controlled nanoscale dimensions formed both in solution and also at the interfaces. The morphology of the synthesized polymer depends on the parameters such as effective area occupied by each surfactant head group, the volume and length of the surfactant tail within the hydrophobic core of the aggregate. Different morphological nanostructures like nanorods, nanospheres, nanoneedle, nanosheets of polyaniline copolymers were synthesized by utilizing soft-templates. The morphology of the nanoscaled structure also depends on the monomer concentration, surfactant concentration and the surfactant chain length. Reverse micro-emulsion is also a possible mechanism to prepare micro and nanostructures of conducting polymers through surfactants acting as soft templates.

Dodecylbenzene sulfonic acid (DBSA), a long chain molecule plays a major role as a structure directing agents for preparation of nanostructured polymer composites in the field of conducting polymers. Besides, it acts as a good surfactant and a very good dopant molecule.. The successful result of the polymer composites depends on the effective interaction of the nanomaterials with the polymer matrix. These interactions will be helpful to increase the charge transfer properties of the polymer composites when compared with the pristine conjugated polymers. The change of phase from microlevel to nanolevel provides enormous changes in their properties due to large surface area.

Dr. P. S. Vijayanand is a distinguished alumnus of the Department of Chemistry, SRMV CAS. He was one among the 40 UG students who passed out in 1995. He holds PhD from Anna University , Chennai in the field of Polymer Science. He was a post-doctoral fellow in Korea Advanced Institute of Science and Technology, South Korea and SEIKI University, Japan. At present, he is the Head (Assistant Professor, Level-III) of the Chemistry department of Bannari Amman Institute of Technology, Sathyamangalam, Erode.

IT-04

Quenching of ferromagnetism of ZnO upon Mn doping

Dr. S. Senthilkumaar
PSG College of Technology
Coimbatore – 641004
E-mail: sskumaarpsg@gmail.com

In this presentation, we report the changes in the room temperature magnetic property of ZnO on Mn doping prepared using Sol-Gel process. The zero field cooled (ZFC) and field cooled (FC) magnetization of undoped ZnO showed bifurcation and magnetic hysteresis at room temperature.

Upon Mn doping the magnetic hysteresis at room temperature and the bifurcation in ZFC-FCM magnetization disappear. The results seem to suggest that undoped ZnO is ferromagnetic while on the other hand the Mn doped ZnO is not a ferromagnetic system. We observe that on addition of Mn atoms the system shows anti ferromagnetism with very giant magnetic moments.

Dr. S. Senthil kumaar, is an illuminant alumnus of Department of Chemistry, SRMV CAS. He completed his post-graduation degree in the year 1991. He has 23 years of total teaching, research and industrial experience. He was the recipient of "Young Scientist Award" by the Tamil Nadu State Council for Science and Technology in the year 2003. His areas of research interest are Nano Catalysts for Organic reactions, Non-Toxic agricultural biomass for Environmental Remediation, Ceramics, and Nano Carriers for drug delivery for malignant cells. To his credit, he has published more than 50 research articles in international peer-reviewed journals. At present he is the Associate professor of Chemistry in PSG College of Technology, Coimbatore.

IT-05

SPECIFIC SOLVENT EFFECT AND HALOGEN BONDING: SOLVATOCHROMISM AND ULTRAFAST FLUORESCENCE SPECTROSCOPY OF HEMICYNANINE DYE IN CHLORINATED SOLVENTS

Dr. C. Selvaraju
National Centre for Ultrafast Processes
University of Madras
Chennai-600 113

The halogen bond is a net attractive interaction between an electrophilic region associated with a halogen atom in a molecular entity and a nucleophilic region in the same, or the another molecular entity. The halogen bond has been exploited in many fields of chemistry and materials science such as crystal engineering, soft matter, protein-ligand interaction, anion recognition and transport and catalysis. Halogen bonding exists as a type of specific solvent effect in chlorinated solvents and its influence on the ground and excited state dynamics was presented using the steady state and time-resolved spectral data obtained with cationic donor-π-acceptor pyridinium dye 1-ethyl-2-(4-(p-dimethylaminophenyl)-1,3butadienyl)pyridinium perchlorate [LDS-698] in chlorinated solvents. The ICT absorption maximum of LDS-698 cation shows negative solvatochromism with an anomalous bathochromic shift in chlorinated solvents. The specific halogen bonding interaction between the perchlorate anion and chlorinated solvents was confirmed by computational studies, which affect the ion-pair interaction and results in the anomalous red shift in the ICT absorption maximum of the LDS-698 cation. In chlorinated solvents, counter anion interaction with the LDS-698 cation is suppressed by the halogen bonding which decreases the dipolarity of the pyridinium cation and pushes ground structure close to the ideal polymethine state (IPS) with minimal bond length alteration. The ultrafast time-resolved fluorescence studies confirm the radiative relaxation from LE, ICT and TICT state. The higher fluorescence quantum yield and lifetime of LDS-698 cation in chlorinated solvents is due to the direct population of ICT state promoted by the halogen bonding interaction of the counter anion. In cationic polymethine dyes, the symmetry breaking induced by the ion-pair effect is reversed by the halogen bonding interaction of the anion with chlorinated solvents.

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Dr.C.Selvaraju, is a prominent alumnus of the Department of Chemistry of SRMV CAS. He was an under graduate student during the year 1991-1994. He holds PhD. in Chemistry from University of Madras in the field of Photochemistry. Presently, he is working as Assistant professor in National Centre for Ultrafast Processes, University of Madras. He has 15 years of research experience. His research areas of interest are Photochromism, thermochromism, Dynamics of solvent molecules in homogeneous and micro heterogeneous system and Ultrafast Spectroscopy

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IT-06

Renewable Energy Technologies for Sustainable Development

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The use of hydrocarbon fossil fuel for energy generation has contributes for global greenhouse gas (GHG) emissions into atmosphere. A special report in 2018 from Intergovernmental Panel on Climate Change clearly accounts on the impact of global warming by 1.5°C above pre-industrial level [1]. It is well known fact that nearly 65% of GHG emissions comes from burning fossil fuels; -coal, petroleum products, and natural gases and nearly 3% of total global GHG emissions accounts from municipal wastes to contributes for global warming [1]. The increase in GHG emission has led to serious environmental issues such as air-water-land pollution, global warming, climate change and grave health issues. In addition, the excessive utilization of fossil fuel has leads to geo-political tense coupled with resource depletion. IPCC clearly urge to mitigate GHG emission through the application of clean and renewable energy technologies for energy generation and green technologies for waste management, which includes waste to energy conversion technologies. Thus, there is an exponential development of renewable energy technologies such as solar, wind, hydro, ocean, geothermal, waste-to-energy, bio-energy and hybrid energy technologies for sustainable development. The first part of my presentation will focus on the fundamentals of various renewable energy technologies including waste to energy and India's potential and challenges for the progress of renewable energy technologies. The second part of my presentation will focus on our initiative to promote green campus in Pondicherry University [2]. The final part of my lecture will focus on research group, particularly on the application of plasmonic nanomaterials to tune and improve harvesting ability of solar energy [3], and graphene-based catalytic materials for ORR in fuel cell [4].

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Dr.R.Arun Prasath, is a prominent alumnus of the Department of Chemistry of SRMV CAS. He was an under graduate student during the year 1990 - 1993. He was also post graduate student of our Department from 1993 to 1995. He acquired his PhD from Anna University in the field of Polymer Science in the year 2002. He served as a post doctoral researcher in University of Strathclyde, United Kingdom and University of New South Wales, Australia. Also, he was conferred with several awards like DAAD fellowship (Germany), Dr.K.K.Majumdar Memorial Award (IISc, Bengaluru), DST-Fast track Young Scientist Award, BOF fellowship (Ghent University, Belgium). Presently, he is an Assistant Professor, Centre for Green Energy Technology, Pondicherry University, and his research areas include Energy materials and sustainability, Solar and catalytic hybrid materials. He enjoys the prestige of holding five international patents and several publications.

ORAL PRESENTATION

ORAL PRESENTATION

Synthesis, spectral, electrical, electrochemical, ESIPT behaviour and diode applications of oligobenzimidazoles

OP 01

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A ESIPT behaviour oligobenzimidazoles were synthesized by oxidative polycondensation of benzimidazole monomers. The structure of benzimidazoles monomers and oligobenzimidazoles (OBI) were confirmed by various spectroscopic techniques. The monomers BIP2, BIMP and BIBP are showing a dual emission, whereas BIP3 and BIP4 are showing only single emission. Due to the excited state intramolecular proton transfer (ESIPT) from the phenolic –OH to imine =N– in the intra molecularly hydrogen bonded monomer. The electrical conductivity of OBIs was showed good electrical response on iodine doping and conductivity increases with increase iodine doping time. The high carbines residue (~40%) at 500ºC in thermo gravimetric analysis shows that the OBIs are having reasonably good thermal stability. Oligomers have recorded high dielectric constant at low applied frequency of 50 Hz at 393 K. The I-V characteristics of oligobenzimidazoles p-n diodes showed rectifying nature with a typical forward to reverse current in the range 4 to 4 V. The high n values are caused by non-homogeneities and effect of series resistance.

Reference

[1] Siddeswaran Anand, Athianna Muthusamy, *J. Mol. Struct.* **2017**, 148, 254-265.

Preparation and characterization of a novel metal adsorbent from butcher litter material

OP 02

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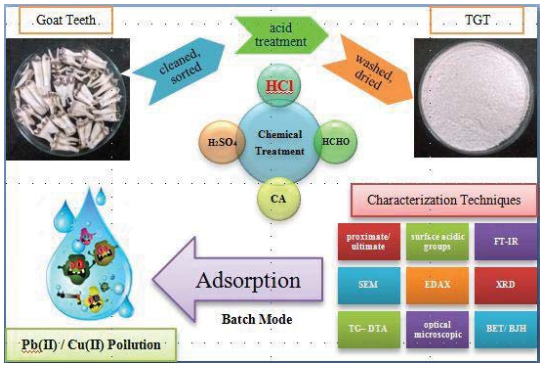
The elevated heavy metal concentrations in the environment pose a serious threat to all living beings. A new biomaterial was identified by impregnation of Goat Teeth in different acids and evaluation under pilot batch experiments in the removal of divalent ions. The best resulted adsorbent (TGT) was characterized using proximate /ultimate /surface acidic group studies, FT-IR, SEM/ EDAX, XRD,TG– DTA, optical microscopic and BET/ BJH techniques respectively. The metal ion loaded sorbents were also characterized by FTIR, SEM / EDAX analyses. The maximum adsorption capacities of 66.50 mg g^{1} and 60.32 mg g^{1} for Pb^{2+} and Cu^{2+} in single-ion system were determined under optimized batch parameters viz., particle sizes, dosages, initial metal ion concentrations, agitation time frames, pH of the media. Thence, the abundant, locally available, cheap waste material showed a greater efficiency after a simple acidic treatmentinmetal ion trapping, also can be utilized for other toxic water pollutants.

Keywords: acid treatment, adsorbent, characterization, metal removal, batch study



Pharmacological evaluation of bis(pyrazolium picrate) monohydrate - a combined experimental, quantum chemical, hirshfeld and molecular docking analyses

OP 03

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[b]*Department of Chemical Engineering, Sethu Institute of Technology, Virudhunagar, Tamil Nadu, India.*
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Biologically active Bis(Pyrazolium Picrate) Monohydrate (BPPMH) has been synthesized and crystallized by slow evaporation -slow growth technique at 27°C. Various functional groups in BPPMH were confirmed by spectral and structural analyses. The stability of BPPMH was authenticated by UV-vis spectrophotometric method at different time intervals. Optimisedgeometry was used to correlate the structural confirmation of BPPMH using B3LYP/6-311++G(d,p) level of basis set. Antimicrobial screening and its minimum inhibitory concentration analyses have been carried out using*Staphylococcus aureus* and *Aspergillusfumigatus*, and BPPMH shows excellent scavenging activity against $DPPH^{\bullet}$ and FRAP radicals. The experimental antioxidant activity of BPPMH was validated through Fukui function calculations. DNA binding analysis confirms the hypochromism through partial intercalation *via* minor groove binding and it was confirmed through UV absorbance/emission spectral analyses. Molecular electrostatic potential analysis and Fukui function calculationsof BPPMH indicate that there are plenty of nucleophilic, electrophilic and radical centres available for hydrogen bonding interactions with microbes and DNA.

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Synthesis, crystal structure, thermal, mechanical and laser damage threshold studies of an NLO active organic molecular adduct: 4-acetylpyridine: 4-aminobenzoicacid

OP 04

T. Daisy Rani and A. Chandramohan*

Post-Graduate and Research Department of Chemistry, Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore, Tamil Nadu, India.

A SHG active Organic molecular adduct, 4-acetylpyridine: 4-aminobenzoicacid (APAB)(1:1) was synthesized and single crystals grown by slow solvent evaporation solution growth technique at ambient temperature. The molecular structure was confirmed by NMR spectral studies and single crystal x-ray diffraction analysis. The title adduct crystallizes in orthorhombic system with non-centrosymmetric space group, *P*212121. FT-IR spectroscopic study was carried out to confirm the presence of various functional groups in the crystal. Optical transmittance window and lower cut off wavelength were identified by UV-Vis- NIR spectral study. The thermal stability was established by TG/ DTA analysis. The mechanical property was studied by Vickers Microhardness test. The relative SHG efficiency was investigated by modified Kurtz Perry powder technique and the value was found to be 1.39 times that of KDP. The laser damage threshold value was found to be 1.95 GW/cm2.

Keywords: Crystal structure, Crystal growth, optical materials and properties, Thermal analysis

Reference:

[1] T. Daisy Rani, M. Rajkumar, A. Chandramohan, Synthesis, crystal structure, thermal, mechanical and laser damage threshold studies of an NLO active organic molecular adduct: 4-acetylpyridine: 4-aminobenzoicacid, *Mater. Lett.,* **2018,** 222, 118-121.

Density functional theory (DFT) Studies of 1-methyl-1h-imidazol-3ium-2,4,6-trinitrobenzene-1,3-bis(olate)

OP 05

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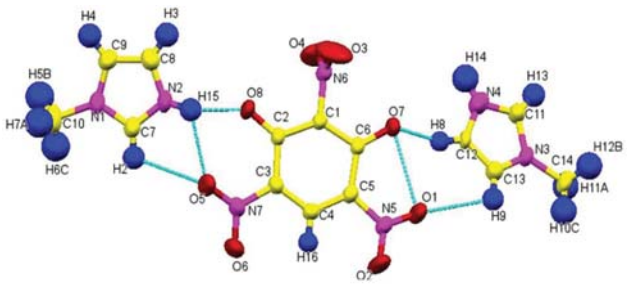
A new proton transfer organic crystal, namely, 1-methyl-1H-imidazol-3ium-2,4,6-trinitrobenzene-1,3-bis(olate)which belongs to the group of polarizable organic molecules, was prepared. Its realistic potential for optical applications is based on its simplicity of synthesis, good ability to crystallize, transparency, thermal stability and efficiency of the non-linear properties comparable to other compounds. The single crystal data was used to generate quantum mechanical computations, Density functional theory (DFT). Gaussian'09, a computer aided software with B3LYP/6-311 ++G (d,p) basis set has been used for quantum mechanical computations. Natural bond orbital (NBO), frontier molecular orbitals (FMOs) and molecular electrostatic potential (MEP) analyses show that the abstraction of an imido proton brings about a change in push-pull configurations resulting in a red shift for both absorption and emission spectra which subsequently leads to a high performance NLO optical material.



Tetranuclear palladacycles of 3-acetyl-7-methoxy-2*h*-chromen-2-one derived schiff bases: efficient catalysts for suzuki-miyaura coupling in aqueous medium

OP 06

S. Dharani[a], G. Kalaiarasi[a], D. Sindhujab, R. Karvembu[b], V. M. Lynch[c] and R. Prabhakaran[a*]

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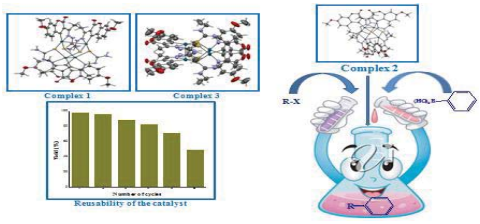
Tetranuclearorganopalladium(II) complexes **1-3** and mononuclear complex **4** have been synthesized by the complexation of 3-acetyl-7-methoxy-2*H*-chromen-2-one derived Schiff bases with potassium tetrachloropalladate $K_2[PdCl_4]$. Structural confirmation for the complexes (**1**-**3**) has been achieved by single crystal X-ray diffraction analysis. The ligands are found to bind with palladium ion through theirazomethine nitrogen, thiolatesulphur and C4 carbon of the coumarin moiety after C-H activation. Mononuclear nature of complex **4**was confirmed from its mass spectroscopic data. In complex **4**, coordination occurred *via* the lactone oxygen, azomethine nitrogen and thiolatesulphur atoms. A systematic study on the application of these complexes as catalysts in Suzuki-Miyauracoupling (SMC) has been done with different aryl halides and phenyl boronic acid in aqueous medium. Optimization of the reaction indicated that complex **2**is more efficient than the other complexes. An appreciable yield of the coupled products was observed with the minimum utility of catalyst (μmol). The C–C coupling has been confirmed by GC/GC-MS.



Preparation and characterization of a novel metal adsorbent from butcher litter material

OP 02

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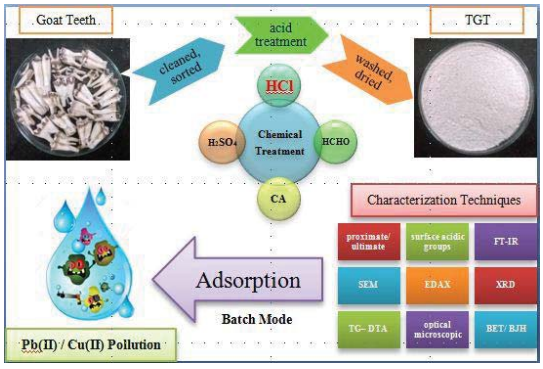
The elevated heavy metal concentrations in the environment pose a serious threat to all living beings. A new biomaterial was identified by impregnation of Goat Teeth in different acids and evaluation under pilot batch experiments in the removal of divalent ions. The best resulted adsorbent (TGT) was characterized using proximate /ultimate /surface acidic group studies, FT-IR, SEM/ EDAX, XRD,TG– DTA, optical microscopic and BET/ BJH techniques respectively. The metal ion loaded sorbents were also characterized by FTIR, SEM / EDAX analyses. The maximum adsorption capacities of 66.50 mg g^{1} and 60.32 mg g^{1} for Pb^{2+} and Cu^{2+} in single-ion system were determined under optimized batch parameters viz., particle sizes, dosages, initial metal ion concentrations, agitation time frames, pH of the media. Thence, the abundant, locally available, cheap waste material showed a greater efficiency after a simple acidic treatmentinmetal ion trapping, also can be utilized for other toxic water pollutants.

Keywords: acid treatment, adsorbent, characterization, metal removal, batch study



Synthesis and studies of bay substituted perylenediimide based d-a-d type small molecule acceptors for organic solar cell and antimicrobial applications

OP 08

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We report, the synthesis of a series of donor-acceptor-donor (D-A-D) type bay substituted perylene diimide (PDIs) derivatives (3a-3d) by the Suzuki coupling method and used as an acceptor for the small molecule-based organic solar cells (SM-OSCs). It has been evaluated for the anti-microbial activity against some of the bacteria and fungi. The synthesized small molecules were confirmed by FT-IR, NMR, and HRMS. The small molecules showed absorption up to 750 nm, which eventually reduced the optical band gap (E_g^{opt}) to < 2 eV. Small molecules showed thermal stability up to 400 °C. In the SM-OSC, the small molecules showed a power conversion efficiency (PCE) of <1% with the P3HT donor in bulk hetero-junction (BHJ) device structure. Additionally, the new small molecules showed antimicrobial activity against Gram-negativebacteria *such as Escherichia coli* (*E. coli*) Gram-positive bacteria such as *Bacillus subtilis* (*B. subtilis*) and anti-fungal activity against the C*andida albicans* (*C. albicans*), and *Aspergillus niger* (*A. niger*). Cytotoxicity studies were carried out against the breast cancer cell lines MCF-7 using MTT assay method. The results revealed that the small molecules was able to inhibit the cancer cells. LD_{50} calculated for the small molecules 3a-3d were between 200-400 µg/mL.

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Docking studies of cobalt (III)-terpyridyl complexes with DNA

OP 09

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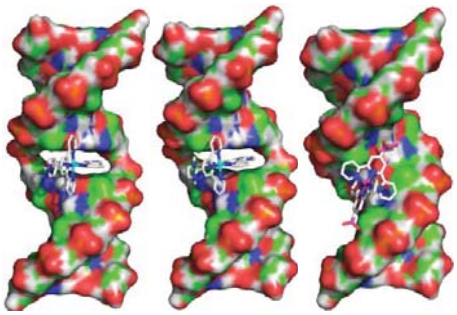
Computational studies play an important role in drug design and provide us with helpful information regarding molecular toxicity and thus reduce significantly the resource requirements in routine biological testing. Molecular modelling studies have been employed for the prediction of ligand selectivity, coordination number, lipophilicity, thermodynamic parameters, spectroscopic properties and helps in the prediction of site specific recognition by metal complexes in DNA. In the present investigation, molecular modelling studies were carried out for three different cobalt(III)-terpyridyl complexes, $[Co(ptpy)_2]^{3+}$(**1**), $[Co(itpy)_2]^{3+}$ (**2**)and $[Co(etpy)_2]^{3+}$ (**3**) where pyridylterpyridine (ptpy), imidazolyl terpyridine (itpy) and esterterpyridine (etpy) which throw more light on metal complex-DNA interaction in addition to experimental evidences.



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An efficient synthesis of 1, 4-thiazepinone fused pyrazolopyridines and their *in-silico* cytotoxicity studies

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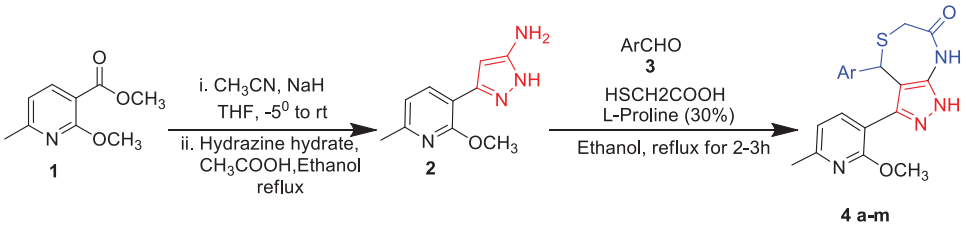
OP 10

A new series of 1, 4-thiazepinone incorporated pyrazolopyridines has been synthesized using L-proline as a catalyst through multi-component reaction which in turn subjected to the *in-silico* cytotoxicity studies against various cancer cell lines and almost all the compounds found to show good to moderate activity. Among the tested compounds, compound **4f** and **4k** are found to have least binding energy value and Z-score value. These compounds found to form more stable ligand-receptor complex amongst other compounds.



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[3] S. L. Schreiber, *Science* **2000**, 287, 1964-1969.

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Effect of silver dispersion on nanostructured poly (aniline-co-3-nitroaniline) copolymers

OP 11

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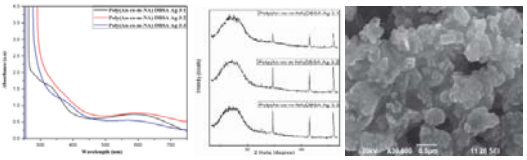
Conducting polymers have attained great interest of researchers due its potential applications in various fields such as electrochromic devices, rechargeable batteries, sensors, polymeric light emitting diodes and transistors. Among the conducting polymers polyaniline has been studied well due to its environmental stability, ease of synthesis and electrical conducting nature. A series of poly (aniline-co-3-nitroaniline) copolymer nanocomposites are synthesized by in-situ chemical oxidative polymerization method. The synthesized copolymers were characterized by UV-Visible, FT-IR, scanning electron microscopy (SEM), X-ray diffraction methods (XRD) and conductivity study. The copolymer was found to be soluble in common organic solvents like DMSO, NMP, THF and DMF. The UV-Visible spectra shows the two major peaks around 350 nm attributing the $\pi - \pi^*$ transition and around 590 nm indicating the n-π^* transition. SEM analysis shows highly agglomerated spherical morphology and the particle size ranges from 100-200 nm. XRD pattern shows that the nanocomposite is of crystalline nature. In FT-IR spectroscopy the appearance of a broad band at 2350 cm^{-1} corresponds to the C-H vibration of DBSA and confirms the formation of benzenoid and quinoid ring in the copolymer. The electrical conductivity is found to be higher than the homopolymer. The synthesized copolymer shows good solubility in various organic solvents than the polyaniline.

Keywords: aniline, 3-nitroaniline, copolymerization, silver nanoparticles.

UV Visible spectra XRD spectra SEM image



Eco-friendly biosynthesis of mixed metal metal oxides using cyathea nilgirensis holttum plant extract

OP 12

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Department of Chemistry, *Sri Ramakrishna Engineering College, Coimbatore, Tamil Nadu, India.*
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In this work we synthesize eco-friendly biosynthesis of mixed metal (Fe, Ni, Cr) oxide (MMO) particles via green process using *Cyathea nilgirensis holttum* plant extract via greener route. The synthesized particles were characterized using UV-Visible, FT-IR, XRD, SEM-EDX, elemental mapping and TEM analysis.UV-visible studies confirm the absorption of mixed oxide particles. The presence of biomolecules and metal oxides were confirmed by FTIR. Structural analysis using X-ray diffraction (XRD) revealed that mixture of oxides was formed. Morphology of mixed oxide particles observed by scanning electron microscope (SEM) suggests that most oxides particles were granules shaped. EDX analysis confirmed the presence of Fe, Ni, Cr & O were present. Elemental mapping analysis is also a valuable tool for confirmation of mixed particles.TEM images confirmed the biosynthesized mixed oxide were in nanoparticles in size. The successful synthesis of mixed iron, nickel and chromium oxides proved the biosynthesis of the mixed oxide particles by a plant extract is an effective processing method. The fraction of various oxides may be controlled by modifying the fraction of initial Fe nitrate, Ni nitrate and Crnitrate. This type synthesis method is cost effective, ecofriendly and used in electronic applications.

Key words: *Cyathea nilgirensis holttum.;* Mixed Oxides; biosynthesis; Characterization

Poly (*o*-phenylenediamine)/$MnCuFe_2O_4$ nanocomposites: synthesis, characterization, dielectric and magnetic properties

OP 13

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PG and Research Department of Chemistry, Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore, Tamil Nadu, India.
E-mail: muthusrkv@gmail.com

Poly *o*-phenylenediamine (PoPD)/$MnCuFe_2O_4$ nanocomposites with three different ratios of $MnCuFe_2O_4$ (10%, 20%, 30% w/w) were synthesized by *in-situ* oxidative chemical polymerization method ammonium persulphate used as oxidant. The structure, morphology and magnetic properties of synthesized PoPD/$MnCuFe_2O_4$ nanocomposites were characterized by FT-IR, UV-visible absorption spectra, X-ray diffraction, Scanning electron microscopy, Vibrating sample magnetometer. FTIR spectra and XRD were confirmed the formation of the PoPD/$MnCuFe_2O_4$ nanocomposites. The morphology of PoPD/$MnCuFe_2O_4$ nanocomposites is visualized through SEM and TEM. Dielectric properties of PoPD/$MnCuFe_2O_4$ nanocomposites at different temperature have been performed in the frequency range of 50Hz-5MHz.

Key words: PoPD, $MnCuFe_2O_4$, Dielectric constant, Magnetic material.

Synthesis and charecterization of $BiFeO_3$- entrappedalginate nanocomposites

OP 14

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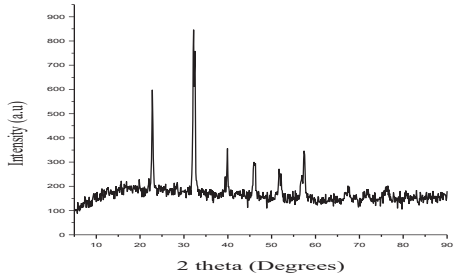
A novel type biopolymer composite composed of $BiFeO_3$ metal oxides and sodium alginate (SA) have been synthesized and characterized. The structural and grain size of BFO-SA particles was investigated by XRD. The surface morphology of synthesized material was confirmed by Scanning Electron Microscopy and the optical properties have been studied using UV–Vis spectrophotometer. The electrochemical nature of BFO – SA nanoparticles was investigated by Cyclic Voltammetric studies. The remarkable electrochemical characteristicsare attributed to the nanostructured electrode materials, generates a high electrode/electrolyte contact area and short path lengths for electronic transport and electrolyte ion. The approach is simple, innovative and can be easily extended to fabricate nano structural composites for super capacitor electrode materials.



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Studies on dual properties of photosensitive liquid crystalline polyethers

OP 15

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There is growing research and development interest in liquid crystalline polymers (LCPs) for optical and electro-optical uses. LCPs are organic materials that combine liquid crystal molecules with a polymer backbone. Main chain LCPs are more viscous than side chain LCPs and therefore are less functional for electro-optic applications. However, for photosensitive applications, the main chain polymers are of equal importance due to the presence of photoactive groups. The photoactivity can occur in the polymer backbone through polymerization processes or in the liquid crystal mesogen by isomerization processes, which can change the phase or alignment of the LC molecule. There are widespread potential uses of photosensitive LCPs, as demonstrated by the literature. Most uses are for optical applications: optical storage, holography, nonlinear optics, displays and imaging[1]. Two series of main chain thermotropic LC polyethers were synthesized by Claisen-Schmidt polycondensation of 4,4'-diformyl-α,ω-diphenoxyalkanes (series 1) and 4,4'-diformyl-2,2'-dimethoxy-α,ω-diphenoxyalkanes (series 2) with cyclopentanone, cyclohexanone and acetone. The study of thermal property by TGA revealed that cyclopentanone containing polymers are more stable than cyclohexanone and acetone containing polymers and also, showed that series 1 polyethers displayed better stability compared to series 2. The self-extinguishing property of synthesized polymers was studied by calculating limiting oxygen index values using Van Krevelen's equation. The influence of the length of methylene spacer on phase transition was investigated using DSC and it was noted that the isotropic temperature decreases with an increase in the spacer length. Further, a study of the odd-even effect revealed that the decoupling function of spacer plays a vital role on introducing substituent in the mesogen and varying the spacer length. Polarized optical microscopic study showed that cyclohexanone containing polymers exhibit schlieren nematic, oily streak and nematic droplet textures in both the series. The photolysis of LC polyethers revealed that EZ photoisomerization proceeds in the system. The liquid crystalline polymers containing photosensitive group in the main chain had not only the property of self-assembly as the liquid crystalline molecules, but also can generate anisotropy after being exposed at a certain wavelength of UV light so that which can induce the LC molecules rearrangement[2]. To support this photoisomerization phenomenon, polymer samples were subjected to irradiation under UV light for long time and then analyzed by solubility test, FTIR, NMR, TGA and DSC. The band gap energy was calculated from absorption spectra and proved that the presence of substituent and varying the length of spacers have a significant influence on their absorption and emission.

Fluoroquinolones as mediators to enhance inhibition property of aminothiazolyl coumarin for corrosion of mild steel in 0.5 m H_2So_4

OP 16

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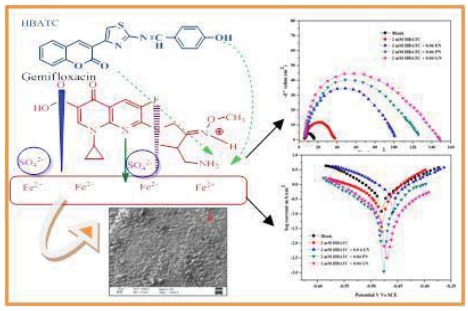
Ecofriendly fluoroquinolones (FQs) as mediators to promote inhibiting nature of the 3-(2-((4-hydroxybenzylidene)amino)thiazole-4-yl)-2H-chromen-2-one (HBATC) for the corrosion of mild steel in 0.5 M H_2SO_4 was inspected using weight loss and electrochemical studies. Synergistic effect was studied using 2 mM of HBATC and various concentrations of FQs. On comparison of % IE of individual HBATC and HBATC + FQs, the increase in % IE due to the effect of FQs confirms synergistic nature. Polarization study revealed the mixed mode of inhibition and the formation of protective layer was confirmed through surface morphological studies like FT-IR and SEM-EDAX. A suitable mechanism for corrosion inhibition was proposed based on the results obtained from weight loss and electrochemical studies.

Keywords: HBATC, FQs, synergism, mild steel, SEM-EDAX.



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Synthesis, growth structural and physicochemical characterization of organic single crystal: p-toluidinium- 5-sulphosalicylate

OP 17

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By utilizing the hydrogen bonding strategy, p-toluidinium- 5-sulphosalicylate an organic proton transfer molecular salt was synthesized and single crystals of it were successfully grown by slow solvent evaporation solution growth technique at ambient temperature. The ^{1}H and ^{13}C NMR spectra were recorded to establish the molecular structure of the title salt. The single crystal XRD analysis reveals that the title salt crystallizes in monoclinic crystal system with centrosymmetric space group, $P2_1/n$. Further, the title salt involves extensive intermolecular N-H...O, O-H...O and C-H...O as well as intramolecular O-H...O hydrogen bonding interactions to construct supramolecular architecture. The presence of the various vibrational modes and functional groups in the synthesized salt was confirmed by FT-IR studies. The thermal behaviour of title crystal was established employing TG/DTA analyses. The mechanical properties of the grown crystal were determined by Vicker's microhardness studies. Dielectric measurements were carried out on the grown crystal at a different temperature to evaluate electrical properties.

Keywords: Crystal structure, Hydrogen bonding, Fluorescence, Thermal analysis, DFT

Effective removal of congo red dye from an aqueous solution using magnetic activated carbon

OP 18

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Activated carbon/manganese ferrite (AC/$MnFe_2O_4$) magnetic nanocomposite has been prepared by using mixture of iron oxalate and manganese acetate as precursors via simple pyrolysis. The morphology and size of the iron oxide particles inserted into activated carbon matrix have been investigated by IR, PXRD, Scanning electron microscope and Transmission electron microscope. The magnetic nature of composites has been investigated by Vibrating Sample Magnetometer. The size of $MnFe_2O_4$ nanoparticles embedded in carbon shell in the range of 30-45 nm. The saturation magnetization (M_s), remanence (M_r) and coercivity (H_c) of the magnetic carbon nanocomposite were found to be 0.207 emu/g, 0.027 emu/g and 225 Oe, respectively. The nanocomposite AC/$MnFe_2O_4$ was applied to remove organic dye, congo red (CR), from an aqueous solution and the results show that the magnetic nanocomposite AC/ $MnFe_2O_4$ have the extraordinary adsorption capacity. Here, the tedious process of filtration is avoided by magnetic separation.

Keywords: Magnetic carbon; $MnFe_2O_4$; Magnetic nature; Congo red; Adsorption.

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Synthesis, characterization, stereochemistry and antimicrobial evaluation of *N*-acyltetrahydrobenzodiazepin-2-ones

OP 19

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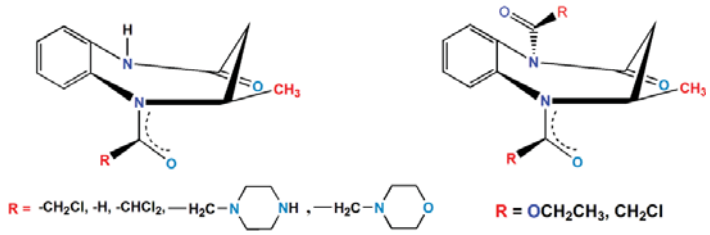
A few N_5-substituted and N_1,N_5-disubstituted tetrahydro-1,5-benzodiazepin-2-ones *viz*. N_5-chloroacetyl-, N_5-formyl-, N_5-dichloroacetyl-, N_1,N_5-diethoxycarbonyl- N_1,N_5-bischloroacetyl-, N_5-piperazinoacetyl- and N_5-morpholinoacetyltetrahydro-1,5-benzodiazepin-2-ones have been synthesized. The characterization and conformational analysis of these compounds have been carried out using IR and ^{1}H, ^{13}C, DEPT & 2D (COSY & HSQC) NMR spectral techniques. The coupling constants for the synthesized compounds are determined by irradiating the C4-methyl doublet. The appearance of *major&minor* conformers has been found in some of the benzodiazepin-2-ones and the spectral dataconfirm the equilibrium due to ring inversion over the N-C=O rotation. The spectral data and the extracted coupling constant values reveal that the substituted tetrahydro-1,5-benzodiazepin-2-onesprefer to adopt boat conformation. The antimicrobial activity of all the synthesized compounds has also been tested.



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Interactions of Voglibose and Pemetrexed with human serum albumin-multispectroscopic and docking studies

OP 20

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The binding interactions of drug molecules with the carrier protein is an important deterministic for their pharmacokinetic behavior. Voglibose, an antidiabetic drug and Pemetrexed, an anticancer drug were analyzed for their binding nature with Human Serum Albumin (HSA) using UV-Vis, fluorescence, circular dichroism and by molecular docking. The drugs quenched the HSA fluorescence through static and dynamic mode. The thermodynamic parameters obtained from the fluorescence data measured at three different temperatures showed that the interactions between both the drugs and HSA involved van der Waals forces and hydrogen bonds which are also substantiated by molecular docking results. The Gibbs free energy values calculated from the fluorescence experiment and by molecular docking are similar and proved the complex formation is spontaneous. The synchronous fluorescence and three dimensional fluorescence spectra further explored the variations in the micro environment of both tyrosine and tryptophan residues. The binding site of Voglibose was found to be site I and Pemetrexed in site III in HSA subdomains IIA and IB, respectively.

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Synthesis, characterization and solution state conformational preferences of *N*-formyl-2,7-diaryl-1,4-diazepan-5-ones

OP 21

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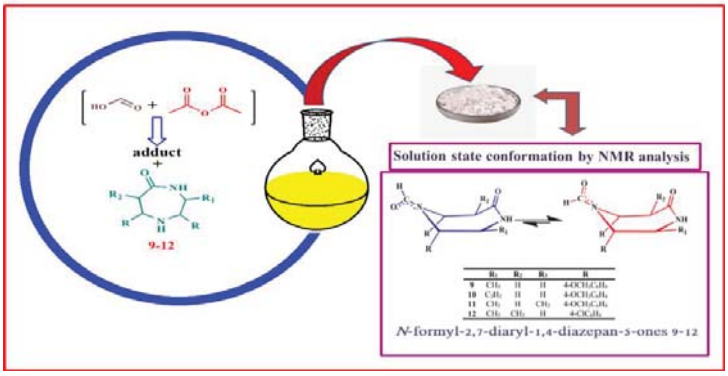
A series of *N*-formyl-2,7-diaryl-1,4-diazepan-5-ones **9-12** were synthesized from their corresponding diazepan-5-ones **5-8** by *N*-formylation. Initially, 2,7-diaryl-1,4-diazepan-5-ones **5-8** and 2,6-diarylpiperidin-4-ones **1-4** were prepared using Schmidt rearrangement and Mannich condensation reaction, respectively. Furthermore, all the synthesized compounds **9-12** were characterized unambiguously through IR, Mass, 1D and 2D NMR spectra. The compounds **9-12** showed doubling of NMR spectral signals due to the delocalization of nitrogen lone pair into the carbonyl Π cloud and thereby creating a partial double character at *N*-C(=O) bond which resulted in an equilibrium between *syn* and *anti* rotamers. Hence, the preferred conformations were arrived by considering the following: ^{1}H and ^{13}C NMR chemical shift values (δ, ppm), coupling constants (Hz), dihedral angles (°) and destabilizing strain factors. The NMR spectral data of *N*-formyl-1,4-diazepan-5-ones **9-12** suggested that the *syn* and *anti* rotamers of these compounds preferred to adopt an equilibrium between *flattened boat* conformations with the aryl groups at C-2 and C-7 occupying quasi-axial orientations.



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Synthesis and structural investigations of a novel organic crystal, N,N'-diphenylguanidinium 3,5-dichlorobenzoate

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OP 22

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N,N'-diphenylguanidinium 3,5-dichlorobenzoate (DPGCB), was synthesized and single crystals were grown from slow evaporation - solution growth method. The crystal structure is stabilized through N-H…O, C-H…O and C-H….Cl hydrogen bonding interactions. Hirshfeld surface analysis reveals that the van der Waals H…H (32.3 %) contacts plays the significant role in crystal packing. Optimized geometry demonstrates the formation of R_2^2 (8) graph set involving N-H…O hydrogen bond. Molecular electrostatic potential analysis proves the proton transfer mechanism in the formation of DPGCB. Z-scan study shows that the third order susceptibility of DPGCB is 1.80 x 10^{-6}esu which is due to strong electron cloud delocalization between two ionic moieties through hydrogen bonding association.

Keywords: Single crystal X-ray diffraction; Hydrogen Bonding interactions; Hirshfeld surface analysis; DFT; Z-scan study.

Green biosynthesis of silver nano particles using *Benkaramalabarica Lam*tirveng fruit extract

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OP 23

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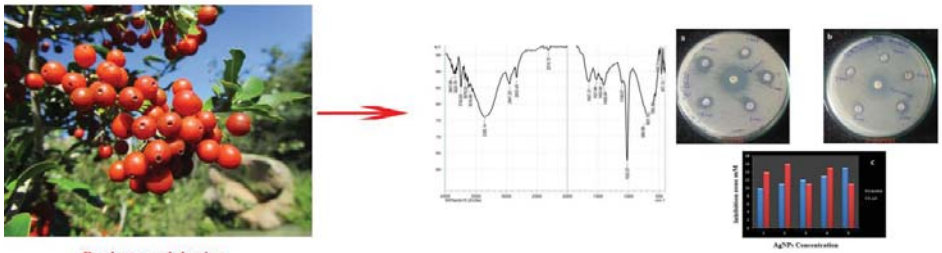
The hydro alcoholic extract of *B. malabarica Lam.* (Rubiaceae) contains high content of phenolic and flavonoid compounds with strong antibacterial activities, and it seems that this plant can be considered as a good candidate for metal nanoparticle synthesis. The AgNPs formation was observed as a color change of the mixture from green to dark-brownish. The X-ray diffraction pattern confirmed the presence of only Ag crystallites, and the dynamic light scattering estimates the average sizes of the AgNPs to be 30.25 ± 5.26 nm. Furthermore, Fourier Transform Infrared as well as UV-vis spectroscopy identifies ethylene groups as the reducing agent and capping agent for the formation of the AgNPs. Hydro alcoholic extract (96%) of *B malabarica* successfully produced quite small as 22.27 nm and the mean size of 200, spherical and poly dispersed NPs with medium aggregates. The conversion was fast and completed in 6 Hrs. The plant and the extraction method seem to be quiet attractive for industrial scale production of NPs. This green synthesis provides an economic, eco-friendly, and clean synthesis route to AgNPs. AgNPs in suspension showed activity against Gram-negative and Gram-positive bacteria with maximum bactericidal concentrations (MBCs) to be in the range from 50μl to 100μl.

Keywords: *B. malabarica Lam.,* Nano particles, Hydro alcoholic extract, amorphous materials, Nanosize



Benkara malabarica

Albizzia Lebbeck leaves extractas natural inhibitor against mild steel corrosion in acid medium

OP 24

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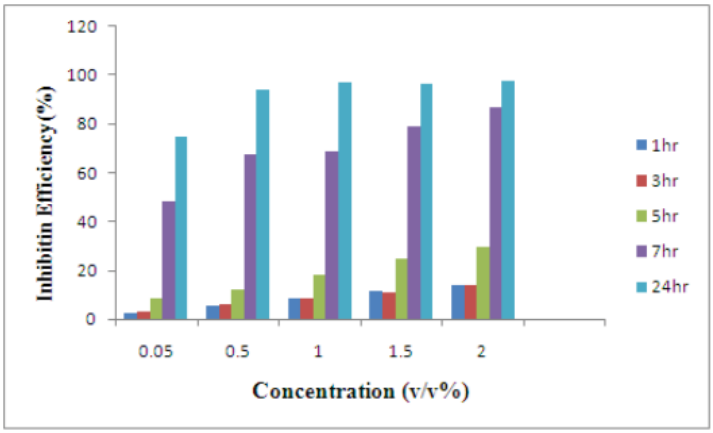
Corrosion inhibition of mild steel was monitored in the presence and absence of various concentrations of *Albizzia lebbeck* leaves extracts in 1N H_2SO_4. From the weight loss studies it was inferred that the corrosion rate decreases and the inhibition efficiency increases as the concentration of the inhibitor increases. The phytochemicals present in the leaves extracts prevents the corrosion rate of mild steel in acid medium. The results exhibited that leavesof *Albizzia lebbeck* was found to be good inhibitor having efficiency as high as 97.75% at 2% inhibitor concentration.

Key words: corrosion studies, mild steel, *Albizzia lebbeck*, sulphuric acid, inhibition efficiency



Plasticized guar gum and lithium nitrate as gel polymer electrolyte for lithium ion batteries

OP 25

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Advanced biodegradable plasticized gel polymer electrolyte has been prepared using guar gum as a host polymer (a biopolymer) and lithium nitrate as the doping salt. The plasticizer glycerol is added to the mixture. A series of thin films were prepared by solution casting technique. The interaction of the components in the solution was analyzed by FTIR technique. The amorphous nature of the electrolyte gave the best result for its nature by X-ray diffraction method. It has been found that the role of glycerol as a plasticizer had more effect. The morphology study of polymer electrolyte thin films were carried out by 3D Laser Profilometry assay and the results revealed that the polyelectrolyte thin films were considerably smoother. The thermal behavior of the films was done using TG/DTA analysis and the TG results demonstrated that increased stability of systems at higher temperature range than native Guar Gum. The DTA results predicted the decrease in decomposition temperature of Guar Gum-$LiNO_3$ gel polymer electrolyte system.

Porous organic frameworks for high-performance supercapcitors

OP 26

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Supercapacitors can be classified into two types based on the charge storage mechanism: electric double layer capacitor (EDLC) and pseudocapacitor. In EDLC, the energy is stored due to the adsorption of charges at the electrode/electrolyte interface, while for pseudocapacitor, theenergy is stored through faradic reactions [1]. To obtain excellent electrochemical performance, the exploration of advanced electrode materials is the key point [2].In this report, we prepared nitrogen-doped microporous carbon (N-MPC) via carbonization of a precursor triazine-based porous organic framework (POF). The N-MPCpresents many advantages for supercapacitor applications, including higher surface area (801 m^2 g^{-1}), porous structure, and uniform pore size. The supercapacitor performance of N-MPCwas evaluated in a 6 M KOH electrolyte and exhibited a high specific capacitance of 505 F g^{-1} at a current density of 0.5 A g^{-1}. The electrode showed excellent cycling stability with 89% capacitance retention after 10,000 cycles at a current density of 3.0 A g^{-1}.

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Experimental and DFT studies on induced focal-conic domains of smectic A* phase in hydrogen bonded ferroelectric liquid crystal

OP 27

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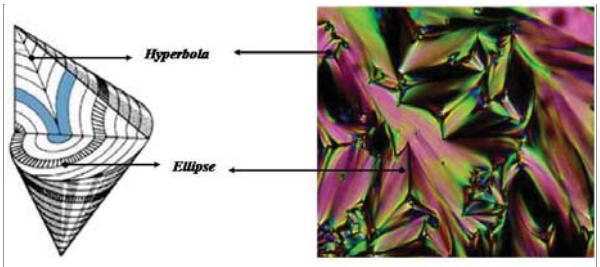
Hydrogen bonded ferroelectric liquid crystals (HBFLC) are designed and synthesized from non-mesogenic chiral proton donor compound of (R)-(+)-methylsuccinic acid (MSA) and mesogenic proton acceptor compound of 4-n-undecyloxybenzoic acid (11OBA).Textural changes and its thermal parameters are studied using polarizing optical microscope (POM) and differential scanning calorimetry (DSC). MSA+11OBA structure is optimized by B3LYP 63-11G(d,p) basis set.HBFLC complex had a strong dipole moment which is perpendicular to the long molecular axis leads to the formation of smectic phases. Smectic phase is stabilized by the dipole–dipole interaction in the HBFLC complex. Intermolecular interaction is analyzed by using natural bond orbital (NBO) studies. Stability of the Sm A* phase and its transition mechanism has been discussed with the help of HOMO-LUMO energies.



Schematic representation of focal-conic Sm A phase*

Conductive metallic nanowires based on polyol process

OP 28

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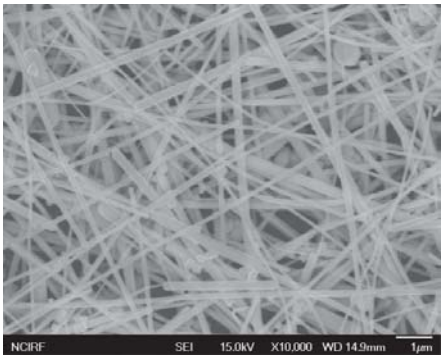
Facile method is introduced to prepare conductive nanomaterials for the development of next generation electronic and optoelectronic devices. A metallic silver nanowire is generated by effective polyol method. Latex blending is used to incorporate conductive metallic nanofillers into polymer matrix. Conductive metallic nanocomposites are characterized by FE-SEM, TGA, and XRD. Electrical conductive properties of metallic nanocomposites is also investigated. It is expected that this proposed methodology will open the door to generate proficient future conductive devices.



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Tunning bandgap energy of CdS nanoparticle by suitable non-metallic composite, its photocatalytic activity and adsorption process

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OP 29

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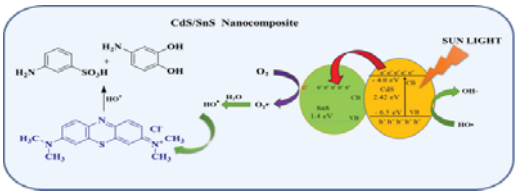
Cadmium Sulphide (CdS) is II-VI group semiconductor with a bandgap of about 2.42 eV. Tin (II) Sulphide (SnS) is composite with CdS nanoparticle to tune the band gap of CdS and increase the photocatalytic efficiency of CdS nanoparticles. In this study we prepared the pure Cadmium Sulphide (CdS) nanoparticles and SnS/CdS nanocomposite (with different ratio) by chemical precipitate method. Photocatalytic activity of pure and CdS and SnS/CdS nanocomposite by degradation of Methylene blue dye. The degradation efficiency of pure and nanocomposite are 97.33 and 97.78% at 3 hrs. Pure and nanocomposite has the same efficiency due to the hydroxyl radical generation. Removal of dye is studied by the adsorption process with an efficiency of about 50.05% for pure CdS nanoparticles at 1hr. For SnS and CdS nanocomposites the efficiency about 1.01, 1.01, 15.87, 2.65, 0.59, 4.95 %. Compared with the adsorption process photocatalytic degradation shows more efficiency to depollute the dye molecules.



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POSTER PRESENTATION

POSTER PRESENTATION

Unravelling siddha medicinal formulation- aya chendooram

PP 01

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Siddha system of medicine is one of the oldest traditional systems in the world. Though Siddha system has its own value, the concern on the availability of physiochemical and standardization data of most of the Siddha formulation is highly doubtful. Hence the standardization of Siddha drugs becomes highly essential in order to explore its potency and efficiency in the global market. The present study aimed at the characterization of the physic-chemical traits of the traditional Indian Siddha medicine, **Aya Chendhuram(AC),** using X-ray diffraction (XRD), Fourier Transform Infrared spectroscopy(FTIR), Differential thermal analysis(DTA), Thermogravimetry analysis (TGA), energy dispersive X-ray analysis (EDAX), Inductively coupling plasma-atomic emission spectroscopy(ICP-AES) and Scanning Electron Microscope (SEM). The present study revealed the major chemical entity in AC as α-Fe_2O_3 and the presence of heavy metals such as Lead and Mercury in minor quantity. The results of the present investigation provide evidence-based information on standardization part of this noble formulation.

Removal of heavy metals by graphene oxide/cellulose hydrogel

PP 02

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The present work aims at the synthesis of Graphene oxide by Modified Hummer's method, characterization of Graphene oxide and to prepare GO/Cellulose hydrogel as potential adsorbent for the removal of heavy metals. Graphene oxide was synthesized by modified Hummer's method and characterized using FT-IR Spectroscopy. GO/Cellulose Hydrogel was prepared using citric acid as cross linking agent and NaOH/Urea aqueous solution as binding agents. Due to the introduction of GO, the GO/Cellulose composite hydrogels exhibited good compressive strength. Adsorption studies for different heavy metals like Nickel and Copper were carried out using titrimetric method. The initial amount of Ni^{2+} was found to be 5.8g and the calculated adsorption capacity of GO/Cellulose was found to be 4.5g. The initial amount of Cu^{2+} was found to be 6.3g and the calculated adsorption capacity of GO/Cellulose was found to be 4.4g. Adsorption capacity of heavy metal ions increases with an increase in the GO/ Cellulose ratio and GO/ Cellulose hydrogel showed high adsorption rates.

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Synthesis of peptide nanomaterials with surface enhanced vibrational activity

PP 03

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This will describe the investigation on the synthesis and characterization of peptide nanomaterials through various synthetic methods. Various tools which are helpful to solve the structure and composition of the nanomaterials will be highlighted. In addition to the application of this nano particle in the field of sensing, catalysis, surface enhancement of vibrational activity is examined with different analyzes. The ability to chemically characterize microbial phenotypes in real time and nondestructively is a critical development for both industrial and clinical microbiology. Surface-enhanced Raman scattering (SERS) methods are of interest for this task because of their exceptional analytical sensitivity with nanometer scale localized selectivity With SERS, Raman scattering from a molecule is enhanced several orders of magnitude when it is in the proximity of a metal substrate.

Efficacy of nanoparticles from natural products in treating various diseases

PP 04

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Natural products have been used as medicine in treating various ailments traditionally. Most of the drugs used are of natural product origin. Development of nanotechnology and search for medicines with fewer side effects moved the interest toward the development of drugs from natural products. Certain polymeric nanoparticles along natural products, phospholipids, nanoparticles derived using natural products and metal nanoparticles synthesised using plant extracts were effective in treating various diseases.

Key words: polymeric nanoparticles, metal nanoparticles, phospholipids.

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Synthesis, molecular modeling and biological evaluations of novel pyrido-cyclopenta[*b*]indole as potential cytotoxic agents

PP 05

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Recently, developing multi bioactive indole derivatives have emerged as a more wise approach in drug discovery. In this regard, a series of new pyrido-cyclopenta[*b*]indole derivatives have been synthesized and the structures are investigated by spectral techniques and elemental analysis. Molecular docking studies have been carried out to understand the binding nature of the target molecule with the receptor p38 MAP kinase. The synthesized compounds were screened for cytotoxic activity against HeLa (cervical cancer) and MCF-7 (breast cancer) cell lines by MTT assay. The preliminary structure activity relationships were evaluated. Lipinski's rules were checked to discover the drug likeness nature of the target compounds.

Synthesis, characterization, thermal and electrochemical studies of oligo nitrobenzimidazoles

PP 06

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A series of oligobenzimidazoles were synthesized by oxidative polycondensation of benzimidazole monomers with NaOCl in aqueous alkaline medium. The structure of the synthesized monomers and oligomers were confirmed by various spectroscopic techniques. Cyclic voltametry measurements of monomers and oligomers were carried out at different scan rates to confirm the reversible and redox couple process. The monomer BINP2 and its oligomer are showing dual emission through excited state intramolecular proton transfer process. The band gap values of monomers and oligomers were calculated from both UV–Vis spectroscopic and cyclic voltammetric data. Theoretical band gap values of monomers obtained from DFT were compared with experimentally calculated band gap values. The electrical conductivity of I2 doped and undoped oligomers were measured using two point probe technique and are showing good correlation with the charge densities on imidazole nitrogen obtained from Huckel method. The conductivity of oligomers increases with increase in iodine vapour contact time up to 144 h. Among the oligomers, OBINP3 is having greater thermal stability as evidenced by its high carbine residue of around 65% at 600 °C in thermogravimetric analysis

Keywords: oxidative polycondensation, cyclic voltametry, Electrical conductivity, Dielectrics, band gap.

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Synthesis, Characterization and NLO Active of Hydrazone Polymers

PP 07

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A series of hydrazone polymers, Poly-2-{(2,4-dinitrophenyl) hydrazono)methyl}phenol (P-2DHP), Poly-3-{(2,4-dinitrophenyl) hydrazono)methyl}phenol (P-3DHP) and Poly-4-{(2,4-dinitrophenyl)hydrazono)methyl} phenol (P-4DHP) were synthesized by oxidative polycondensation of hydrazone monomers with NaOCl in aqueous alkaline medium. The structure of the monomers and polymers were confirmed by FT-IR, UV–Vis, ^{1}H and ^{13}C NMR spectroscopic techniques. The electrical conductivity of I_2 doped and undoped polymers were measured using two point probe technique and are showing good correlation with the charge densities on imidazole nitrogen obtained from Huckel method. The conductivity of polymers increases with increase in iodine vapour contact time up to 168 h. The TGA results showed that the polymer P-4DHP has highest thermal stability due to the greater the number of chain propagation sites than other polymers. The polymers are showing good SHG efficiency and thus it may be considered as a promising material for NLO application.

Keywords: Oxidative polycondensation, Hydrazone polymers, NLO, Electrical conductivity.

Structural activity of the kaempferol glycosides a DFT study

PP 08

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Numerous preclinical studies have shown kaempferol and its glycosides possessing a wide range of pharmacological activities including antioxidant, anti-inflammatory, antimicrobial, anticancer, cardioprotective properties etc., Detailed investigation of structural activity seems to be less explored for some of the active kaempferol derivatives. In the present work, afzelin(5,7-Dihydroxy-2-(4-Hydroxyphenyl)-4-Oxo-4h-Chromen-3-Yl6-Deoxy-Alpha-L-Mannopyranoside) and zuglanin(3-[(2S,3R,4R,5S)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy-5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one) two glycosyl derivatives of kaempferol are been theoretically investigated for their structural properties using density functional theory with the basis set 6-311G(d,p)++ under the level of theory B3LYP using Gaussian 09 package. Geometry optimization and thermochemical calculations are performed at room temperature 303K in vacuum. Computed global molecular descriptive parameter projects identical values between the two flavonoids. Frontier molecular orbital analysis displays energy gap about 4.14eV for afzelin and 4.03eV for juglanin. Accumulation of higher electron density is been witnessed around hydroxyl units present in B-ring of two flavones with the aid of electrostatic potential energy surface analysis and kinetic energy distribution analysis. On the basis of structural property observations made, afzelin and juglanin are theoretically validated as active antioxidants.

An electrochemical study to evaluate the inhibition activity of *Cyperusrotundus* to mitigate corrosion in stimulated concrete pore solution containing chloride

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PP 09

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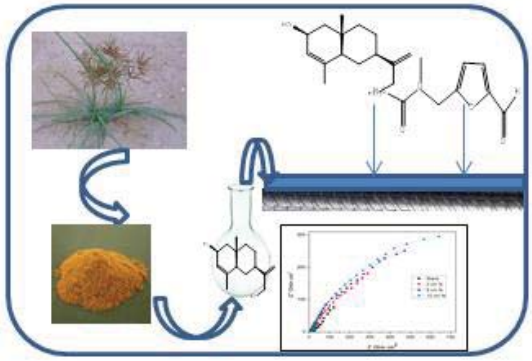
Concrete corrosion is one of the major factors limiting the life time of reinforced concrete buildings. In order to minimize the deterioration of steel embedded in concrete, ethanol extracts of *Cyperusrotundus* used for evaluating the rebar corrosion in stimulated concrete pore solution at selected concentrations of 2,6,12v/v% by electrochemical impedance and potentiodynamic polarization studies.Increase in R_{ct} evident for the formation of barrier. Polarisation studies representsanodic inhibition. The adsorption phenomena followed Langmuir adsorption isotherm indicating monolayer adsorption.

Keywords: Green inhibitor, pore solution, electrochemical techniques, adsorption.



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A review on green synthesis of silver nanoparticles

PP 10

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Nanotechnology is an emerging area that engages almost every technical discipline. It is a rapidly expanding area of research with huge potential to revolutionize our lives and to provide technological solutions to solve our problems in survival. Development of reliable and eco-accommodating methods for the synthesis of nanoparticles is a vital step in the field of nanotechnology. Silver nanoparticles are crucial because of their exceptional chemical, physical, biological properties and also their applications in varied fields. In the last decennium, numerous efforts were made to develop green methods for the synthesis of nanoparticles to avoid the hazardous byproducts. The bio-molecules from various plant components and microbial species have been used as potential agents for the synthesis of silver nanoparticles (AgNPs). This present review explains the methods of green synthesis for silver nanoparticles and their numerous applications. It also compares the efficient synthesis method of green synthesis via green routes over physical and chemical methods, which provides a strong evidence for the selection of suitable method for the synthesis of silver nanoparticles.

Moringa oleifera gum exudate as corrosion inhibitor on mild steel in sulphuric acid medium

PP 11

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The use of corrosion inhibitors has proven to be the easiest and cheapest method for corrosion protection and prevention in acidic media. These inhibitors slow down the corrosion rate and thus prevent monetary losses due to metallic corrosion on industrial vessels, equipment, or surfaces. Inorganic and organic inhibitors are toxic and costly and thus focus has been turned to develop eco-friendly methods for corrosion retardation. In the present study gum exudate obtained from the bark of *Moringa oleifera* tree has been used as an inhibitor on the corrosion of mild steel (MS) in 1M Sulphuric acid. The inhibitive effect of the natural product on the corrosion inhibition of MS in1 M sulphuric acid was studied using weight loss method. The experimental data showed good trend in inhibition efficiency which increased with increase in concentration of the gum but declined with rise in temperature. The adsorption follows Physisorption mechanism. From the trend in inhibition efficiency with the change in temperature and from thermodynamic parameters it has been found that the adsorption of MO on MS complies with Langmuir adsorption isotherm.

Electrochemical studies of layered double hydroxide for energy storage devices

PP 12

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Energy storage is as important as energy production and power generation. Storage of energy is portentous to be highly efficient and cost effective. Effectively energy can be stored by means of LDHs that can be synthesized using transition metals containing good electrical properties. Energy storage becomes more efficient when the particles form in nano-size. It can be attached to carbon nanotubes and can be incorporated as cathode in batteries. LDHs are a family of natural and synthetic compounds having general for $[M_{(1-x)}^{2+}M_x^{3+}(OH)_2]$ with divalent and trivalent metal cations occupying the octahedral interstices of the layers. Organic or inorganic anions are embedded in the interlayers of the lamellar edifices. Metals Mg, Zn, Ni, Al, Ga, Fe, Mn, Ca, In, V, Cr, Co and Cu are commonly used. The interlayer anion in LDHs is carbonate, as it has particularly high affinity for LDH formation. Other anions which have been reported to be used in LDHs include halides, oxoanions, oxometalates, polyoxometalates, and organic anions. The relatively mild reaction conditions for LDHs enables many organic and biological molecules to remain intact throughout the synthesis. As the properties of the LDH are altered based on the metal cations and interlayer anion, the applications of LDHs include catalysts, biomaterials, polymer additives, environmental materials, thin film applications, fire retardant additives, anti-corrosion coatings, and controlled drug release. The electrochemical properties of LDHs has created interest in its use as electrode modifiers/materials and sensors.

Keyword: Tranisition metal, Energy storage, Electrode modifiers

Metal corrosion inhibition by natural plant extract in aggressive medium

PP 13

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The serious consequences of corrosion have become a problem of worldwide significance. Corrosion prevention and control have become a perpetual struggle between man and nature.The use of inhibitors is one of the most practical methods for protection against corrosion, especially in acidic media. The present study focuses on acidic media due to the increasing demand for acids in process industries, such as mineral processing, fertilizer manufacture, oil refining, waste water processing and chemical synthesis, among others. Most of the corrosion inhibitors are synthetic chemicals, which are expensive and highly hazardous to the environment, hence the need for research into non-toxic organic corrosion inhibitors. The present work focuses the inhibition performance of leaves of *Alstoniascholaris* extract on mild steel in HCl solution by weight loss method, FTIR and SEM analysis. Weight loss method showed that the leaves extract acted as an effective corrosion inhibitor and its corrosion inhibition efficiency increased with the inhibitor concentration. FTIR study revealed the presence of possible functional groups in the plant extract.SEM investigation showed that the tested extract significantly protects mild steel samples in a hydrochloric acid environment.

Keywords: FTIR analysis, Inhibition efficiency, corrosion inhibitors, SEM, Mild steel

Palladium(II) hydrazone complexes: synthesis, characterization and DNA/BSA binding properties

PP 14

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Two new palladium (II) complexes of 3-hydroxy-naphthalene-2-carboxylic acid (2-oxo-1,2-dihydro-quinolin-3-ylmethylene)-hydrazide with triphenylphosphine and triphenylarsine as co-ligand have been synthesized and characterized by the aid of various spectral techniques. The DNA binding of these complexes and ligand calf thymus DNA (CT-DNA) was investigated by using various methods, which revealed that the compounds interacted with CT-DNA through intercalation. Binding properties of the free ligand and its complexes with bovine serum albumin (BSA) protein have been investigated using UV-visible and fluorescence spectroscopic methods which indicated the stronger binding nature of the palladium complexes to BSA than the free hydrazine ligand.

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Morphological and optical evolution of different organic acids used MoO_3 thin films by spin coating method

PP 15

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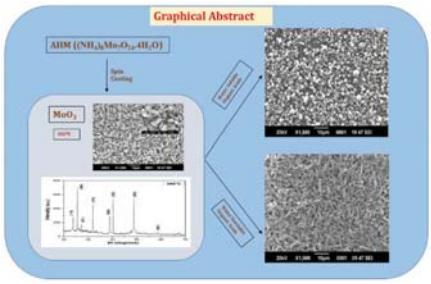
Molybdenum trioxide (MoO_3) thin films were prepared at room temperature (RT) and at different annealing temperatures of 250, 350, 450 and 550°C. We also prepared MoO_3 films using additives of water-soluble and water-insoluble organic acids. The thin films were coated using the spin coating technique and annealed at 350°C temperature. The effects of different annealing temperatures and different organic acid additives on MoO_3 films were characterized by structural and optical studies. From the XRD pattern, the structure of the MoO_3 films is found to vary with respect to increase in the annealing temperature. For RT and 250°C, the hexagonal structure was observed and for 350, 450 and 550°C, the orthorhombic structure was observed. The XRD pattern for all the organic acid additive used MoO_3 films exposed the orthorhombic structure. SEM images show hasty variations in the surface morphology for different annealed MoO_3 films and different additive used MoO_3 films. The EDX analysis confirmed the presence of Mo and O elements for all the films. The UV-Vis results show the absorbance and transmittance values. The band gap energy was found to be around 3.8 eV for all the MoO_3 films.



Synthesis, Growth, Spectral, Thermal and Optical Studies of a new organic crystal: 2-aminopyridiniumtrichloroacetate

PP 16

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A new organic salt 2-aminopyridiniumtrichloroacetate (APTC) has been successfully synthesized. The single crystals of APTC were grown by the slow solvent evaporation solution growth technique at room temperature using methanol as the solvent. The functional groups of the title salt was confirmed from the FT-IR spectral studies. The thermal stability of the complex salt was studied by TG/DTA thermal analyses. The lower cutoff wavelength and optical transparency window of the title salt was identified from the UV-Vis-NIR. Spectroscopic studies. The molecular structure of the title salt was confirmed from the ^{1}H and ^{13}C NMR spectroscopic studies.

Newer graphene oxide-PPD nanocomposite for silver ions

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PP 17

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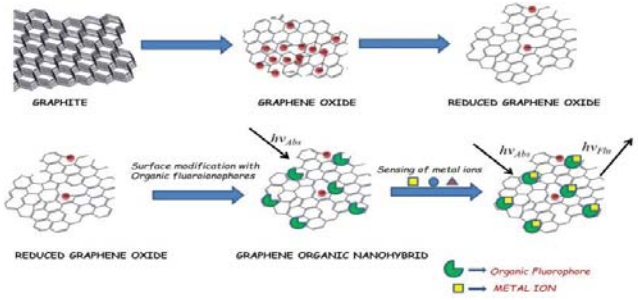
Graphene oxide (GO), a two-dimensional nano sheet produced by the oxidation of graphene, has notable characteristics such as good dispersibility and facile surface functionality. Metal ions are one of main source of pollutants of drinking water because a small amount of these species would cause detrimental effects on both environmental and biological systems. There are only a few reports on organic nanocomposites for the detection of metal ions by utilizing fluorescence spectroscopy. Therefore, based on the above, we have designed and synthesized novel GO-PPD nanocomposites by the hydrothermal method. These materials are characterized by XRD, SEM, UV-vis and Fluorescence spectroscopy. They are utilized as chemosensors for the detection of metal ions. All these details will be presented.



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Adsorption of heavy metals by graphene oxide/starch hydrogel

PP 18

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The present study aims at the Synthesis of Graphene oxide by modified Hummer's method. From the synthesized Graphene oxide, GO/Starch Hydrogel was prepared using citric acid as cross linking agent and NaOH/Urea aqueous solution as binding agents. Due to the introduction of GO, the GO/Starch hydrogels exhibited good compressive strength. Adsorption studies for different heavy metals like Nickel and Copper were carried out using titrimetric method. Adsorption capacity of heavy metal ions increases with an increase in the GO/ Cellulose ratio and GO/ Starch hydrogel showed high adsorption rates.

References

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An aerobic oxidation system for oxidation of primary and secondary alcohols using bipyridyl-cinchona based palladium catalyst

PP 19

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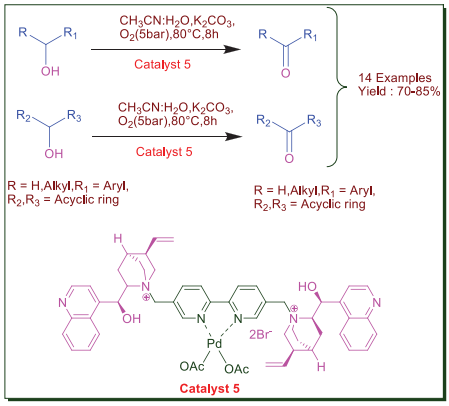
We have proposed an aerobic oxidation of primary and secondary alcohols to respective aldehydes and ketones using cinchona alkaloid based palladium catalytic system using molecular oxygen at moderate pressure. The above catalytic system is experimented for different oxidation systems, which includes different solvents, additives, bases, which are cheap, robust, non-toxic and commercially available in the industrial bench. The obtained products are quite appreciable in both yield and selectivity (70-85%).



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Structural and magnetic properties of PANI/ $MnCoFe_2O_4$

PP 20

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Ferromagnetic PANI/ $MnCoFe_2O_4$ nanocomposites have been synthesized by in-situ chemical polymerization of aniline in the presence of $MnCoFe_2O_4$ nanoparticles. The structure and morphology of PANI nanocomposites are characterized by Fourier transform infrared (FTIR), X-ray diffraction (XRD) and Scanning electron microscopy (SEM). Magnetic properties of PANI/ $MnCoFe_2O_4$ nanocomposites are also investigated. The PANI/$MnCoFe_2O_4$ nanocomposites under applied magnetic field exhibited the hysteresis loops of ferromagnetic nature at room temperature.

Keywords: Polyaniline, Nanocomposites, Ferromagnetic and SEM.

Investigation on the structural and optical properties of sonochemically synthesised $BiVO_4$for photocatalytic application

PP 21

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Bismuth vanadate ($BiVO_4$) is a well-known photocatalyst which has been extensively studied due to its visible light response ability and band gap of 2.4 eV. In this work, $BiVO_4$ has been successfully synthesised using facile sonication method, the precursor materials used are bismuth nitrate pentahydrate and ammonium metavanadate. The effect of ultrasonic frequency on the morphology and crystal structure of the synthesised samples has been studied by varying the frequency of ultrasonic vibration. An ideal frequency which yields better catalytic efficiency is figured out. The cyrstal structure and phases of the samples were analysed using X-ray Diffraction (XRD). The morphology has been investigated using scanning electron microscopy (SEM). The band gap has been determined using DRS. The crystal structure, morphology and catalytic efficiency of the samples prepared using sonication technique U-$BiVO_4$ has been compared with the sample prepared by normal magnetic stirring M-$BiVO_4$. The photocatalytic activities of the samples were evaluated by decolourization of Methyl Blue (MB) under visible light.

Keywords: $BiVO_4$, Ultrasonication, Photocatalyst, Methylene Blue

Structural and optical properties modification of nebulizer spray coated cd: zno nanocrystalline thin films

PP 22

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The Microstructure, electrical and optical properties of Pure ZnO and cadmium-doped ZnO thin films deposited by spray pyrolysis method have been studied. The ZnO thin films have hexagonal and polycrystalline structure. Scanning electron microscopy images revealed that the films have uniform size distributions with wrinkle network. The elemental analyses of the films were carried out by energy dispersive X-ray analysis. Photoluminescence measurements showed that the band gap decreases from 3.28 to 3.11 eV with increasing in Cadmium content. The increase in cadmium content leads to the broadening of the emission peak. The optical properties are experimentally analyzed. By varying Cd concentration, the band gap of pure and Cd doped ZnO films can be adjusted in a wide range from 3.26 eV for ZnO to 2.10 eV for 5% Cd doped ZnO.

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Synthesis, characterization and photophysical properties of AIE active conjugated polymer: facile encapsulation of AIE polymer into meso porous silica hallow nanospheres for bioimaging application

PP 23

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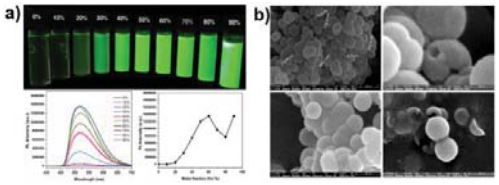
Polymeric luminogens are promising materials for applications in various areas, such as PLED, plastic lasers, fluorescent chemosensors and bio-probes.[1-2] In this journey a large number of conventional luminescent polymers usually undergo aggregation caused quenching, which limits the bright emission imaging application. In contrast, conjugated polymers with aggregation induced emission (AIE) characteristics are strong emission in their aggregate states and have been an ultimate field for developing highly emissive mesoporous silica nanoparticles for cell imaging application. In this work, tetraphenylethene (TPE) units, one of the typical aggregation induced emission (AIE) moieties, are utilized to construct a new functional AIE conjugated polymer, which exhibits the exciting property of AIE with hole transporting triphenylamine. An AIE active conjugated polymer was synthesized with good yield using conventional Wittig polymerization. Synthesized AIE polymer is weakly emissive in solutions. They however, in aggregate states emit intensively with absolute quantum yield up to 37%. For efficient cancer cell targeting, synthesized Green emissive AIE conjugated polymer was encapsulated into mesoporous silica nanoparticles (P-AIE-MSNPs) via simple non covalent approach, which afforded better emission. In addition, anti-EpCAM aptamer specific to cancer cell was functionalized on the surface of P-AIE-MSNPs for targeted cancer cell imaging.



a) Photographs of polymer in THF/water mixture under UV illumination. b) FE-SEM images of polymer encapsulated mesoporous silica hallow nanospheres

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Synthesis, spectroscopic studies and biological evaluations of nitrogen heterocyclic copper (I)/(II) metallacylces

PP 24

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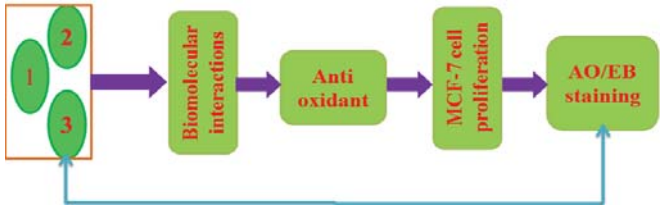
Nitrogen heterocyclic copper (I)/(II) complexes were synthesized and characterized by various physicochemical methods. X-ray diffraction analysis exposed the actual coordination nature of ligands to metal center. Compounds bind to nucleic acids *via* intercalative mode, which was further confirmed by viscosity measurements. The interaction of the complexes with albumin was studied by absorption and emission titration methods. The scavenging ability of the compounds against hydroxyl and DPPH radicals showed complexes have better ability than their parent ligands. *In vitro* anti cell-proliferation of the compounds revealed significant activity against human breast cancer cells (MCF-7) and found non-toxic against human normal keratinocyte cells (HaCaT). AO/EB dual staining assay of the cancer cells were pictured as apoptotic/necrotic pathway of cell death which is induced by the complexes. From the obtained biological results, it has been found that complex **3** exhibited better activity than ligands and complexes **1** and **2**.



Synthesis, characterization and biological activity of a charge transfer complex: 2-aminopyridinium-p-toluenesulfonate

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PP 25

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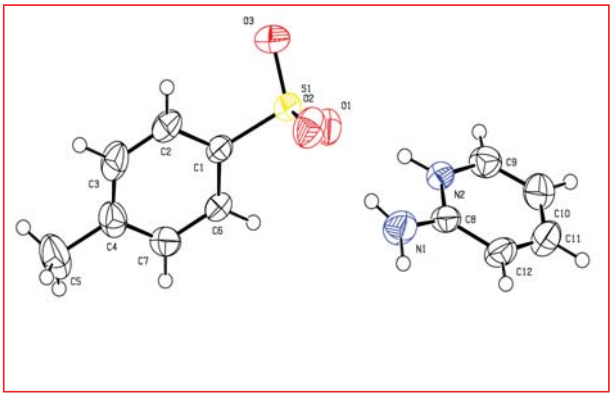
A single crystal charge transfer (CT) complex, 2-aminopyridinium-4-methylbenzenesulfonate (APTS) was synthesized and recrystallized by slow solvent evaporation solution growth method at room temperature. The complex has been characterized with the elemental analysis, UV-visible, infrared (IR), ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra. Thermogravimetric (TG) and differential thermal analysis (DTA) were reported the thermal behavior of the complex. Single crystal XRD studies showed that the orthorhombic nature of the crystal with space group Pbca. The biological activities of CT complex, such as DNA binding and antioxidant activity has been carried out. The results indicated that the compound could interact with DNA through intercalation and show significant capacity of scavenging with 2,2-diphenyl-2-picryl-hydrazyl (DPPH).



Menace to minimize the temple waste flowers by adsorption process

PP 26

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Temples generates more wastes particularly flowers every day. These temple waste flowers menace to the environment and livings. Every year approximately 80,00,000 tons of waste flowers are dumped in the rivers in India choking them to fatality. Dumping of large quantities of waste flowers produces foul smell, breeds insects and mosquitoes moreover it pollutes the soil fertility thus deteriorates the aesthetic value of land. Incomplete combustion of waste flowers releases toxic gases into the atmosphere which causes air pollution, acid rain etc. Recently the waste flowers are being used by many researches for many purposes such as composting, vermicompositing, extraction of essential oil, dyeing of cotton, wool, silk and production of biogas, etc. Also waste flowers used as cow feed, natural food colorounts, making holi colours, handmade papers, various ornamental purposes, incense sticks, rosewater, the flowers can also be incorporated into herbal products such as herbal colours, natural dyes as a result the waste flowers can be controlled to a greater extent. In order to utilize waste flowers effectively, it is necessary to involve both private and public sectors so that the importance of waste flowers management is sustained. In the present work, the temple waste flowers utilized as activated carbon by various physical and chemical processes such as biosorbent, direct pyrolysis, H_2SO_4, H_3PO_4, Na_2SO_4 and KOH and applied for the adsorption process, as a result this waste can be minimized at a greater extent.

Antimicrobial activities of CdO nanoparticles synthesized by hydrothermal method

PP 27

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CdO is an II-IV group n-type semiconductor coming under the nonstochiometric condition such as interstitial cadmium or oxygen vacancies. CdO nanoparticles having the direct band gap of 2.5 eV with an indirect band gap of 1.96 eV. CdO nanoparticles were synthesized by using hydrothermal method.The main raw materials used for CdO nanoparticles are cadmium nitrate and ammonium hydroxide as starting materials. This sample was characterized by XRD, FE-SEM with EDS and FTIR. It exhibits simple cubic structure with an average crystallite size of 27 nm. The surface morphological image displays spherical like structure with agglomeration. The vibrational stretching mode of Cd-O is 455 cm^{-1}. The optical energy bandgap is estimated as 2.56 eV. The significant antimicrobial activities were studied against gram negative (*Escherichia coli*) and gram positive (*Staphylococcus aureus*) bacteria. The zone of inhibition is found to be more for gram negative than gram positive bacteria.

Keywords: Crystalline size, Agglomeration, Band gap, Inhibition.

Influence of substrate temperature on MoO_3 thin films by the JNS pyrolysis technique for supercapacitor application

PP 28

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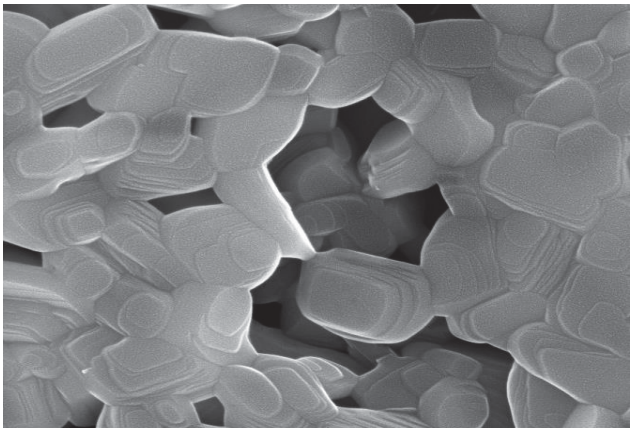
We have synthesized plate like one - dimensional (1D) MoO_3 thin films by using jet nebulizer spray (JNS) pyrolysis technique at different substrate temperatures from 300 °C to 500 °C. The XRD pattern exposed that the crystallite size of the films increases from 22nm to 52nm with respect to increase in the substrate temperature. The FESEM images showed the conversion of nanorods to micro sized plate-like structures by increasing the substrate temperature. The elemental presentation confirmed by EDS. Supercapacitive tests of electrode are performed with Cyclic Voltammetry. The better electrochemical performance of MoO_3 showed at 400 °C with the highest specific capacitance of 130 F/g.



Entropy generation in hydrodynamic nanofluid slip flow over a stretching sheet with non-uniform heat source/sink effect

PP 29

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Second law of thermodynamics to an electrically conducting incompressible nanofluid flow over a stretching sheet was investigated in the presence of non-uniform heat source/sink. The dimensionless governing equations for this investigation are solved analytically by hyper geometric function. Effect of such physical parameters are discussed for velocity, temperature and entropy generation profiles.

Keywords: Nanofluid, Partial slip, Stretching sheet, Magnetic field,Entropy generation, Non-uniform heat source/sink.

Influence of acetic acid on the structural, functional, optical, morphological, dielectric and electrical properties of polypyrrole by cop synthesis

PP 30

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Polypyrrole (PPy) was synthesized through chemical oxidative polymerization (COP) by varying weight percentages (10 wt.%, 30 wt.%, and 50 wt.%) of acetic acid. The structural functional, optical, morphological, dielectric and electrical properties of PPy were investigated by XRD,FT-IR, UV-Visible, SEM, electrical conductivity and impedance analysis. XRD analysis shows the formation of PPy and confirms the amorphous nature of the material. The average crystallite size of the PPy is about 113.2 nm. The presence of C=O and O-H stretching due to CH_3COOH carbonyl groups in the PPy samples is confirmed from the FT-IR peaks appearing at 2855 cm^{-1} and 2923 cm^{-1}. The absorption peak at 280 nm indicates π-π* transition in the heteroatom aromatic pyr role ring through the recorded UV-Visible spectrum. The calculated band gap value of the PPy samples is found to be 2.00, 1.75, and 1.50 eV. The SEM images reveal the globular structure of PPy. The room temperature impedance spectroscopy performs to find the dielectric and electrical properties of PPy, in the frequency from 50 Hz to 5 MHz. The AC conductivity remains constant up to 1MHz and its value increases slowly and attains a maximum at higher frequency which confirms the semiconducting nature of samples.

Synthesis of g-C_3N_4 loaded binary transition metal sulphide nanocomposites for photocatalytic applications

PP 31

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In this work, we synthesized a series of g-C_3N_4 loaded binary transition metal sulphide ($CuCo_2S_4$) nanocomposites by a facile solvothermal approach using biomolecule D-penicillamine as sulphur source. The phase structure, morphology, chemical composition, and optical properties were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), high resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), UV-vis diffuse reflectance spectroscopy (UV-vis DRS). The photocatalytic activities of the synthesized nanocomposites were evaluated using degradation of methylene blue (MB) dye under visible-light irradiation. The light absorption capacity and photocatalytic activity of $CuCo_2S_4$ were enhanced by the successful incorporation with g-C_3N_4. Experiments were carried out to find the optimum level loading of g-C_3N_4 in $CuCo_2S_4$ that enhanced the degradation efficiency of the nanocomposite compared to the pure $CuCo_2S_4$ towards the degradation of MB dye under the light irradiation. A possible mechanism for enhanced photocatalytic activity towards the pollutant degradation by the nanocomposites was proposed.

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Removal of toxic cation employing activated carbon/ carbon doped calcium alginate beads derived from *aallus aallusdomesticus* beaks

PP 32

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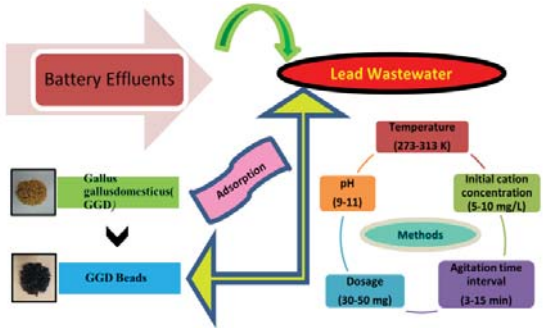
Wastewaters discharged from battery service centres contain lead as primary pollutant. In the view of this, the present study is focused on the collection and treatment of wastewaters from battery service centres in and aroundNamakkal. A novel biomaterial, *Gallus gallusdomesticus*(GGD) beaks were gathered from poultry units in Namakkal and utilized for the lead removal. GGD beaks were activated in Muffle furnace using HNO_3 (GGDBAC) and doped with calcium alginate beads precursor. (GGDCAB). Lead removal capabilities of GGDBAC and GGDCAB were optimized under variable sorption parameters and analysed using Atomic Absorption Spectrophotometer. The experimental results indicate, both the derived materials possess excellent lead removal, where GGDCAB registered a maximum (98%) against GGDBAC (92%) as evident from the recorded EDAX spectra. It is concluded that *Gallus gallusdomesticus* breeded at Namakkal, dump their beaks as litter pollutants which in turn are found to be efficient in trapping lead metal present in the battery discharges collected from Namakkal.

Keywords: battery service centres, lead, adsorption, biomaterial



Evaluation of corrosion rate of mild steel in sulphuric acid solution by ecofriendly plant material

PP 33

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Plant extracts are viewed as environmentally friendly and ecologically acceptable inhibitors. They are low cost, readily available, and renewable sources of materials. The extracts from their leaves, barks, seeds, fruits, and roots comprise of mixtures of organic compounds containing nitrogen, sulphur, and oxygen atoms and some have been reported to function as effective inhibitors of metal corrosion in different aggressive environments. Generally, the inhibitive effect of plant extract is attributed to the adsorption of organic substances on the metal surface, blocking active sites or even forming a protective barrier. The objective of this study is to evaluate the inhibitive effect of tuber extract of ***Dioscoriaalata*** *as* a green corrosion inhibitor on the mild steel in 1N H_2SO_4solution.The corrosion performance was studied using weight loss method, qualitative phytochemical screening and FTIR analysis. The preliminary screening showed the presence of chemical constituents in the plant extract. Weight loss method showed that decrease in corrosion rate of the metal with increasing inhibitor concentration at different immersion periods. FTIR study revealed the presence of various functional groups in the extract. The presence of phytochemicals in the tuber extract considerably prevents metal dissolution in acidic environment.

Keywords: Mild steel, Phytochemicals, Adsorption, Corrosion rate.

Naphthalene based fluorescent chemosensor for selective sensing of Ce^{3+}, HSO_3^- and colorimetric detection of Fe^{3+}

PP 34

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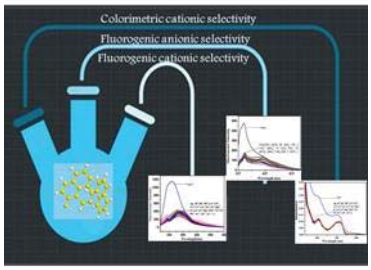
For past 100 years cerium element is extensively used in research and industrial fields.Cerium metal is used in the industrial areas such as for polishing glass, one of the most active components of catalytic converters in vehicles,fuel addictive,in the area of metallurgy also it exhibits a wide range of applications.HSO_3^- is an oxanion which are potentially used as antioxidants and shows biological activities like antimicrobial,antiviral etc. and to preserve beverages.It has been discovered bisulfite levels affects the leads to many diseases like asthma,gastrointestinal,allergic reactions etc.Fe^{3+}, plays a vital role in many biological processes,as it provides the oxygen-carrying capacity of heme and acts as a cofactor in many enzymatic reactions involved in the mitochondrial respiratory chain.Therefore, detection of Ce^{3+},$HSO_3^-$and Fe^{3+} by simple and cost-effective methods is important in biological and environmental concerns.Sensor 1 exhibits highly selective and sensitive recognition of Ce^{3+},$HSO_3^-$and Fe^{3+} by fluorescent and colorimetric detection modes, respectively.



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Preparation and characterization of nanoporous activated carbon from agro industrial by-products

PP 35

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In order to improve the efficiency of adsorbents which is prepared from oilcakes and also controlling the nutrient leaching level into aqueous system, activated carbons were prepared from oilcakes. Therefore activated carbons were prepared from coconut and neem oilcakes by pyrolysis of crude oilcakes over the temperature range 500-700°C followed by microwave activation in the absence of air at 1000°C. Pulverize the resulted activated carbons, passed through 120-200 ASTM mesh and determine the characteristics of the prepared activated carbon as per the procedure. The results shows that the prepared adsorbents have meso and micro porous morphological structure are evidence for good sorption capacity for heavy metal removal form plating industrial effluents, within 10 minutes of time intervals for the minimum sorbent dosage of 100mg/1000ml of effluent. Both kinetics and isotherms studies found that the sorption capacity of prepared nanoporous activated carbon is to be 8.91 and 5.15 mg/g respectively for the sorption of Nickel (II). The prepared nanoporous activated carbon withstand five cycles of retrieve without any lose.

Key word: Nano porous activated carbon, removal of Nickel (II).

Synthesis, characterization and magnetic studies of transition metal substituted cobaltite

PP 36

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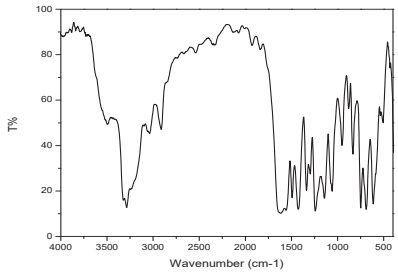
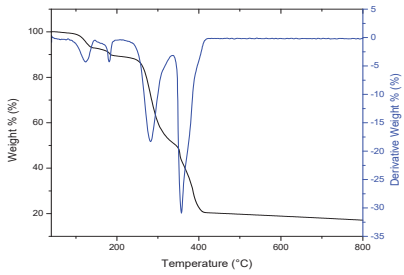
In the transition metal oxide string, spinel Co_3O_4 is well known for their gas-sensing, catalytic and electrochemical properties [1, 2]. In the present effort the ferromagnetic $Mn_xCo_{3-x}O_4$is synthesized from the precursor $Mn_xCo_{3-x}(PhOAc)_2(N_2H_4)_2$[3,4]. The physicochemical properties of the precursor is characterised by EDS, infrared spectroscopy (IR), thermal mass loss studies (TG-DTA) analysis. The as-prepared nanosample is characterized by XRD analysis. The average crystalline size is calculated using Debye-Scherrer formula, $D = K\lambda/ \beta \cos\theta$, is found to be around 14 nm. The elemental composition and morphology of the nanoparticle is studied by SEM-EDS analysis.It shows irregular foliated rock-like structure with agglomeration. The TEM micrograph shows spherical shaped nanoparticles with average particle size of 9-40 nm which is consistent with XRD details. The magnetization hysteresis (M-H) curve of synthesized $Mn_xCo_{3-x}O_4$ nanoparticle is obtained at room temperature. The M-H curve indicates the room temperature ferromagnetic behavior of the nanoparticle.





IR spectrum of the precursor TG/DTA spectrum of the precursor

Ruthenium (II) schiff base complexes: synthesis and characterization

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PP 37

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New ruthenium(II) complexes of 1-((6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methylene)-4-phenylthiosemicarbazidewith triphenylphosphine and triphenylarsine as coligand have been synthesized and characterized by the elemental analysis, IR, UV visible and NMR spectral techniques.The structure of the ligand and complexes were confirmed by using analytical and spectral techniques. The ligands act as tridentate, monobasic chelating ligand with O, S and N as the donor sites in all the complexes studied. An octahedral geometry has been tentatively proposedfor all the complexes.

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Naphthalene based "turn-on" fluorogenic and colorimetric sensor for detection of Al^{3+}& Fe^{2+} ions

PP 38

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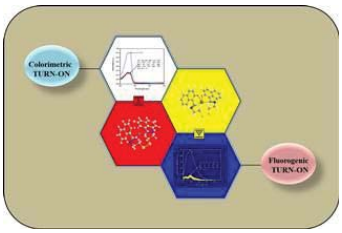
Aluminium is the third most plenteous (8.3% by weight) metallic element in the earth's crust after oxygen and silicon. Al^{3+} -ion extensively utilized in different fields, including pharmaceuticals, food packaging etc. The extreme introduction of human body to Al^{3+} -ion prompts numerous risky diseases such as the progression of bone disease in children, encephalopathy, Alzheimer's disease etc. Similarly, iron is the most imperative bioactive transition metal involved in living systems and also most essential trace element for human sustenance. Fe^{2+}-ion plays a crucial function in biochemical processes like oxygen transportation, cellular metabolism, DNA synthesis and also involved in electron transfer. The deficiency or overconsumption of Fe^{2+} -ion causes various diseases such as low blood pressure, heart diseases, kidney damages etc. Thus, in view of the reasons, development of reliable recognition methods for concentration level of Al^{3+}& Fe^{2+} -ion have consistently attracted in a lot of consideration in environmental and scientific fields. The sensor development and its ion detection will be presented.



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Treatment of textile dye coralene navy rdrlsr using TiO2/Zn electrode from TiCl3 in electrocoagulation processprocess

PP 39

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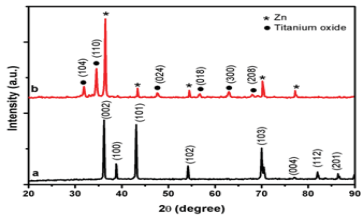
Treatment of textile dyeing wastewater and reuse of treated water is the need of the hour using electrochemical treatments which play a significant role in solving water crisis. This work primarily deals with the treatment of textile dyeing waste water followed by the utilization of waste material by electrocoagulation. The aim of the proposed study is to evaluate the performance of electrocoagulatiuon process using TiO_2/Zn electrodes by thermal decomposition of $TiCl_3$. The surface morphology of the electrode was studied by SEM, XRD analysis. The coralene navy RDRLSR was obtained from Devi Industries in Coimbatore. The operating parameters were compared for both zinc and TiO_2/Zn, where the decolourisation of dyeing waste water utilizing electrocoagulation technique with newly developed TiO_2/Zn electrode achieves high dye removal efficiency with less reaction time and energy in the coagulation process.

Key words: Electrocoagulation, dye, newly developed TiO_2/Zn electrode, reaction time



XRD of Zn, TiO_2/Zn

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Utilisation of chemical components of biological substances in alternative and complementry medicine- an awareness assessment

PP 40

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Health care systems have initiated strategies for intervention of complementary therapies to effectively improve the quality of life of patients. This is recognised as quality measure for optimal care by Joint Commission on Accreditation of Healthcare Organisations. The complementary medicine is used as complementary to allopathy and alternative medicines as an alternative to Allopathy. Though many systems are being in existence which has different origin, few systems like Ayurveda, Siddha, Unani, Homeopathy etc use the biological extracts containing the chemical constituents for effective curing of cause or symptoms of the patients. The study focuses on elucidating the extent of awareness to different complementary therapies in society as well as about the presence of underlying chemical constituents in the medicines that is being administered. The study design used is a self administered and structured questionnaire circulated through social media. The representative sample used for the study focus on student community who are the future of a nation. This would also be an eye opener in deciding the requirement of awareness creation to sustain the traditional systems of medicines among future generations.

Keywords: Complementary medicine, Alternative medicine, Biological extracts, Chemical constituents, Traditional medicine.

Decolourization of coralene red 3G by electrocoagulation using TiO_2/Zn electrode by the thermal decomposition of tip process

PP 41

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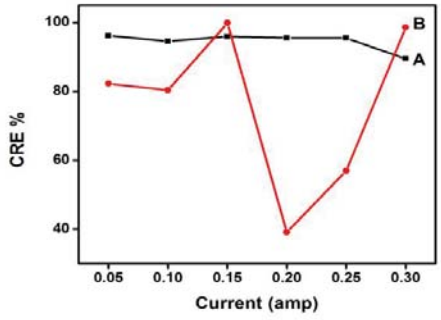
TiO_2/Zn electrodes were prepared by thermal decomposition of titanium tetra isopropoxide (TTIP) and characterized by SEM, XRD analysis. These newly developed electrodes were used in Electrocoagulation process for the decolourization of coralene red 3G and the operating parameters such as pH, electrolyte concentration, electrolysis time and applied current were investigated and the color removal efficiencies were compared for both thezinc and TiO_2/Zn in electrocoagulation. The Colour Removal Efficiency (CRE) was found to be high in coated electrode.This can be related to the increase in the generation of Ti^{4+} ions during electrocoagulation.

Key words: TiO_2/Zn electrode, dye, CRE, reaction time



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Highly sensitive coumarin-pyrazolone probe for the detection of Cr^{3+} and the application in living cells

PP 42

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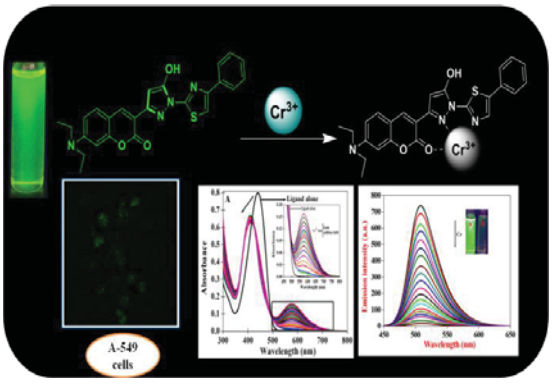
3-(7-(diethylamino)-2-oxo-2*H*-chromen-3-yl)-1-(4-phenylthiazol-2-yl)-1*H*-pyrazol-5(4*H*)-one**(COPYR)** was competently synthesized from methyl 3-(7-(diethylamino)-2-oxo-2*H*-chromen-3-yl)-3-oxopropanoate and 2-hydrazino-4-phenylthiazole. The interactions of receptor **COPYR** with various ions were investigated through absorption and steady state fluorescence spectral studies, respectively. The results reveals that the complexation of Cr^{3+} ions with **COPYR** results in 1:1 stoichiometry resulted in a quick color response from fluorescent green to colorless with significant quenching of fluorescence at 506 nm in DMSO medium. Theoretical calculations (DFT) confirm the photophysical changes such as absorbance and emission spectral changes. Furthermore, the confocal imaging of A-549 cells clearly points out that the synthesized probe **COPYR** could be applied for the examining Cr^{3+} in living cells.



Inclined magnetic field effects on viscous dissipative walter's liquid-b fluid flow over a stretching sheet with non-uniform heat source/sink

PP 43

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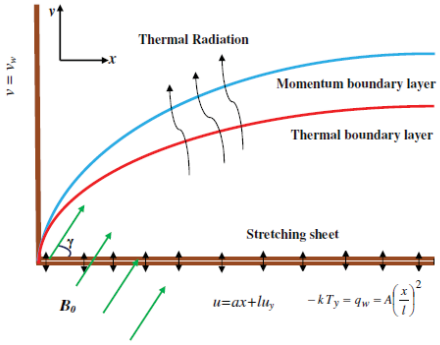
In this article, we have investigated the viscous dissipation effects on Walter's liquid B fluid over a stretching surface with non-uniform heat source/sink and inclined magnetic field. The basic governing equations are transformed into ODEs using similarity transformation and then solved analytically by using the confluent hypergeometric function. Results delineating the flow characteristics are presented through graphs and tables for the effect of various parameters. It is observed that the presence of the aligned magnetic field in both heat source and heat sink cases reduces the temperature profile.



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Synthesis and characterization of Co (II) hydrazine 5-sulpho salicylate

PP 44

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Single crystals of Cobalt (II) complex of the ligand hydrazine 5-sulpho salicylate have been prepared from the stoichiometric proportions of cobalt nitrate, hydrazine hydrate and 5-sulpho salicylic acid. Clear intense white platy like crystals of the synthesized compound have been characterized by elemental analysis, IR spectroscopy and Single crystal XRD. The compound crystallizes in the triclinic space group P1 with the following unit cell dimensions a = 7.0619 (6) Å, b = 7.2081 (7) Å, c = 11.5882 (10) Å, β = 550.91(9) Å, Z = 2. The crystal structure has been solved by direct methods and refined by full matrix least squares procedures to a final R value of 0.0425 for 8910 observed reflections.

Key words: Hydrazine, 5-sulpho salicylic acid, IR spectroscopy, Single crystal XRD

Studies on metal complexes of aromatic acid with aminoguanidine and its applications

PP 45

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A new series of transition metal complexes of aminoguanidine and 3 - hydroxy - 2-naphthoic acid of formula $(N_4H_7C)_2$ $[M\{(C_{10}H_6(O)(COO)\}_2].2H_2O$ where M(II) = Ni, Co, Cd and Zn have been synthesized and characterized by analytical and physicochemical techniques like elemental analysis, IR spectra, UV-Visible, TG-DTA and XRD analysis. The elemental analysis confirms the formulation of complexes. The IR spectra of these complexes show the formation of the complexes. Simultaneous TG-DTA studies show that the complexes decompose at 700ºC. All the complexes follow uniform degradation pattern with the formation of metal hydroxy naphthoate as intermediates and metal oxide as end product. The XRD studies show that all the complexes are isostructural in nature. A square pyramidal geometry has been proposed for the complexes. The complexes were screened for the antimicrobial activities and the results show that the zinc complex shows higher inhibition against gram positive and gram negative bacteria. Nano metal oxides were synthesized by using aminoguanidine complexes as precursors. The prepared nano metal oxides were characterized using IR, UV-DRS, XRD, SEM with EDAX, AFM studies. The synthesized nanoparticles shows a good photocatalytic activity against dyestuffs which was measured from UV-Vis spectra.

Magnetic and electrical properties of manganese cobalt ferrite doped poly(*o*-phenylenediamine)nanocomposites

PP 46

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Poly(*o*-phenylenediamine) (PoPD)/$MnCoFe_2O_4$ nanocomposites were synthesized by in-situ oxidative polymerization method. The different concentrations of $MnCoFe_2O_4$ nanoparticles were dispersed in PoPD.The synthesized PoPD/$MnCoFe_2O_4$ nanocomposites were characterized by XRD, FTIR, SEM, TEM and TGA. The dielectric properties of PoPD/$MnCoFe_2O_4$ nanocomposites were analyzed at different temperature and frequency. The hysteresis loops of $MnCoFe_2O_4$ and PoPD/$MnCoFe_2O_4$ nanocomposites were indicated ferromagnetic behaviour.SEM and TEM analysis illustrates that inclusion of $MnCoFe_2O_4$ nanoparticles in PoPD matrix. The $MnCoFe_2O_4$ nanoparticles were enhanced thermal stability of PoPD and thermal stability of PoPD/$MnCoFe_2O_4$ nanocomposites increases with increase in $MnCoFe_2O_4$ nanoparticles concentration.

Keywords: PoPD, $MnCoFe_2O_4$, Dielectric constant, SEM.

Supramolecular architectures in (2-amino-4,6-dimethoxypyrimidine-N)aquachlorido-(thiophene-2-carboxylato-O)cobalt(II)

PP 47

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Studies of cobalt complexes are of interest due to their potential applications in biological activity, NLO and magnetic materials. Recently, Thiophenecarboxylic acid, its derivatives and their complexes exhibit pharmacological properties. Cobalt (II) and copper(II) complexes of thiophenecarboxylate have many biological applications, for example, as antifungal and antitumor agents. The crystal structure of a complex namely (2-amino-4,6-dimethoxypyrimidine-N)aquachlorido-(thiophene-2-carboxylato-O)cobalt(II) monohydrate, $[Co(C_5H_3O_2S)Cl(C_6H_9N_3O_2)(H_2O)]H_2O$ were prepared and characterized by single crystal x-ray studies. The Co(II) ion has a distorted tetrahedral coordination involving one monodentate O atom from a thiophenecarboxylate anion, one N atom from amino pyrimidine (OMP) ligand, one chloride anion, and one water molecule. Furthermore, one water molecule is present in the crystal lattice. The amino group of the coordinated aminopyrimidine molecule and the coordinated carboxylate oxygen form an N-H...O interligand hydrogen bond generating a S(6) ring motif. The pyrimidine molecules also form base pair [$R_2^2(8)$ motif] via a pair of N-H...N hydrogen bonds. These interactions as well as O-H...O and O-H...Cl hydrogen bonds and π-π stacking interactions are generating a three supramolecular architecture. In addition to investigation of DFT studies using compared with the experimental results.

Inhibitive action of aqueous extract from *Ruellia Tuberosa* L on the corrosion of mild steel in HCL medium

PP 48

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The inhibitive effect of the aqueous extract of ***Ruellia Tuberosa*** **L**(RT) leaves on the corrosion of mild steel (MS) in hydrochloric acid medium was studied using weight loss and electrochemical methods. The inhibition efficiency increased with increase in concentration of the extract but decreased with rise in temperature. Furthermore, the inhibition efficiency synergistically increased on the addition of halide ions. Polarization measurement studies revealed that RT extract behave as a mixed inhibitor. Physical adsorption mechanism is proposed from the trend in inhibition efficiency with the change in temperature and from thermodynamic parameters. It has been found that the adsorption of RT on MS complies with Langmuir adsorption isotherm. The adsorption mechanism and surface morphology of the mild steel, both with and without the inhibitor, were studied using Fourier transform infrared (FT-IR) spectroscopy and field emission scanning electron microscopy (FESEM).

Keywords: *RuelliaTuberosa*, Mild steel, Corrosion, Potentiodynamic polarization,Electrochemical impedance spectroscopy.

Anticorrosion properties of methanol extract of plant leaves for the corrosion of mild steel in HCL medium

PP 49

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Anticorrosion properties of methanol extract of plant leaves on the corrosion of mild steel (MS) was studied using weight loss measurement, Potentiodynamic polarization spectroscopy, GC-MS analysis, Field Emission Scanning Electron Microscope and Energy - Dispersive X-ray Spectrometry. The results obtained indicated that the methanolic plant leaves extract is a good adsorption inhibitor for the corrosion of mild steel in HCl medium. The inhibition efficiency of methanolic extract of plant leaves were found to increase with increasing immersion of time and decreases with the increasing temperature. The polarization studies reveal that the extract acts as a mixed type inhibitor. The adsorption of methanolic plant leaves extract on mild steel surface is a spontaneous and exothermic reaction and is best described by Langmuir adsorption model. The values of activation and free energies obtained were within the range limits expected for the mechanism of physical adsorption. Field Emission Scanning Electron Microscopy confirms the adsorption of plant leaves extract on the MS surface. The GC-MS analysis was used for the identification of active phytochemical compounds in methanolic plant leaves extract.

Synthesis of gold@metal-organic framework composite for voltammetric determination of caffic acid

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PP 50

Caffic acid (CA, 3, 4-dihydroxycinnamic acid) is one of the phenolic compounds widely found in wines, cloves, coffee, star anise, olive oil, some vegetables and fruits. It has several pharmacological functions such as antioxidant, antibacterial, and immune-modulatory [1]. It is associated to the quality of this beverage and also various beneficial effects on health. The two hydroxyl group of CA significantly contribute to the unique antioxidant properties, thus the quantitative detection of the CA attain great significant to comprehend our daily diet [1]. Gold decorated Nickel-based metal-organic framework (Ni-MOF) was developed for highly selective determination of CA [2]. The Ni-MOF/gold composite was prepared by a simple hydrothermal method. The electrocatalytic activity of Ni-MOF/gold composite modified electrode was evaluated by the determination of CA using cyclic voltammetry and amperometry. The amperometric response of the composite electrode was linear in the 1 - 500 μM CA concentration range, with a 20 nM detection limit. The sensor electrode exhibited high sensitivity (0.15 $\mu A \cdot \mu M \cdot cm^{-2}$), reliable reproducibility, and good selectivity. The sensor, when used for the direct determination of CA in wine sample gave good recovery (98.5-101.0%).

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Flame retardant studies on phosphorous containing aromatic cardo polyesters

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PP 51

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Phosphorous containing cardo polyesters were prepared by interfacial polycondensation of phenylphosphonic dichloride with different bisphenols using a phase transfer catalyst at ambient temperature. The structures of the synthesized polymers were confirmed using FTIR, ^{1}H, ^{13}C and ^{31}P NMR spectroscopic techniques. The thermal properties of the polymers were studied by TGA and DSC under a nitrogen atmosphere. They showed high thermal stability, the maximum decomposition temperature being in the range of 475-523°C. The TGA data showed that all the synthesized polyesters showed high char yield at 700°C due to the presence of phosphorous atom in the polymer chain and hence they have good flame retardant properties. The flame retardancy of all synthesized polymers was investigated by limiting oxygen index (LOI) and vertical burning test (UL-94). The results show that the polymers had excellent flame retardancy;

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Structural characterization, experimental and theoretical calculations of a proton transfer crystal, 2-aminothiazolium 2, 4-dihydroxybenzoate

PP 52

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Single crystals of 2-aminothiazolium -2,4-dihydroxybenozate (2-AT24DHB) were grown by the slow evaporation solution growth technique. The structure was elucidated by single crystal X-ray diffraction analysis and the crystal belongs to the monoclinic system with space group P_c. The carbon skeleton and proto environment of (2-AT24DHB) was confirmed by NMR spectroscopy. Theoretical calculations were performed using density functional theory (DFT), to derive the optimized geometry, dipole moment, HOMO-LUMO energies and first–order molecular hyperpolarizabity, (β) (~ 84 times of urea). The atomic charge distributions of the various atoms were obtained by Mulliken charge population analysis. The molecular stability and bond strength of the molecule were investigated by applying the natural bond orbital analysis. Investigation of the intermolecular interactions and crystal packing via Hirshfeld surface analysis reveals that the close atom-atom contacts are associated with molecular interactions. Fingerprint plots of Hirshfeld surfaces were used to locate and analyze the percentage of contribution of various bonds. The grown crystals were further characterized by FT-IR, FT-Raman and TG/DTA.

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Influence of solvent in solvothermal synthesis of cu_3sns_4: morphology and band gap dependant photocatalytic dye degradation

PP 53

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Cu_3SnS_4 (CTS) with various morphologies have been synthesized via solvothethermal method. The influence of different solvents such as deionized water (CTS-DI), N,N-dimethylformamide (CTS-DMF) and poly ethylene glycol (CTS-PEG) has been investigated. XRD patterns of all the prepared samples exhibit tetragonal structure with preferential orientation along (1 1 2) direction. It is found that the solvents play a key role to tune the morphology and band gap. The morphology varied as irregular sheet like structure, mesoporous structure and feather like structure for CTS-DI, CTS-DMF and CTS-PEG, respectively. The band gap was found to be 1.33, 1.65 and 1.19 eV for CTS-DI, CTS-DMF and CTS-PEG, respectively. Photocatalytic dye degradation ofMethylene blue(MB) were tested using the prepared CTS samples. It is found that CTS-DMF with mesopours structure showsan enhanced photocatalytic activity. A more realistic mechanism for the photocatalytic activity of CTS-DMF is proposed.

Keywords: Cu_3SnS_4, Solvothermal, Methylene blue, Photocatalyst.

Synthesis and characterization of nanostructured poly(m-toluidine -co-3-aminobenzoic acid) copolymer in presence of dodecylbenzene suflonic acid

PP 54

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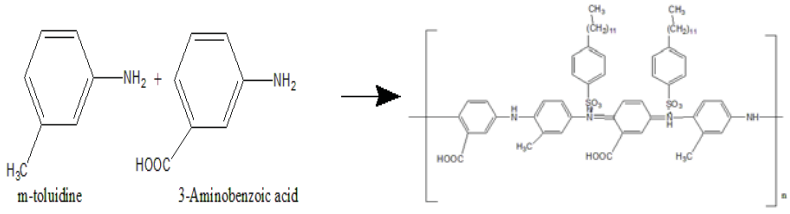
Novel series of poly(m-toluidine-co-3-aminobenzoic acid) copolymer has been synthesized with different monomer ratio between m-toluidine and 3-aminobenzoic acid in presence of dodecylbenzene sulfonic acid and ammonium persulfate as oxidant. The synthesized copolymer was readily soluble in common organic solvents like dimethyl formamide, dimethylsulfoxide and N-methyl pyrrolidone etc. The synthesized copolymers were analyzed with Uv-visible spectroscopy, FTIR spectroscopy, X-ray diffraction studies and electrical conductivity studies. The absorption spectra reveal π to π* transition at 316 nm, polaronic band at 400 nm and n-π* transition at 573 nm. These polaroinc bands are associated with the new localized electronic states which are close to the lower energy state that contains unpaired single electron. The FTIR spectra confirm the characteristic peaks of the copolymer. X-ray diffraction pattern reveal that the synthesized copolymer possesses amorphous nature. The surface morphology of the copolymer consists of large number of polymer chains that leading to form spherical shape. The electrical conductivity value of the copolymer was around 2.5 x 10^{-9} to 3.9 x 10^{-10} S/cm. The lower conductivity is due to the presence of the bulky methyl group in the copolymer.



Synthesis, characterization and pH sensing studies of 3-(6-methyl-1*H*-benzo[*d*]imidazol-2-*yl*)quinoline-2(1*H*)-one

PP 55

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In the present work qunoline derivative having methylated benzimidazole BIQM was designed and synthesized on the basis of flurophore-innophore principle. The synthesized compound was well characterized by IR, ^{1}H and ^{13}C NMR spectral studies. The fluorescence emission pH titration for BIQM were presented in Figure. BIQM showed an intense luminescent at 447 nm in the acidic solution revealed that the protonation of nitrogen atoms in BIQM compound leads a radiative relaxation process of excited molecules. Hence, the compound BIQM shows fluorescence in acidic pH range. Under high pH conditions, fluorescence quenching was observed with red shift from 447 to 460 nm. It illustrated that the base induced deprotonation of nitrogen atoms in BIQM provides availability of lone pair of electrons and leads to nonradiative molecular relaxation which was responsible for the fluorescence quenching of BIQM.

Keywords: Quinolines, benzimidazoles, fluorescence sensor, pH sensor

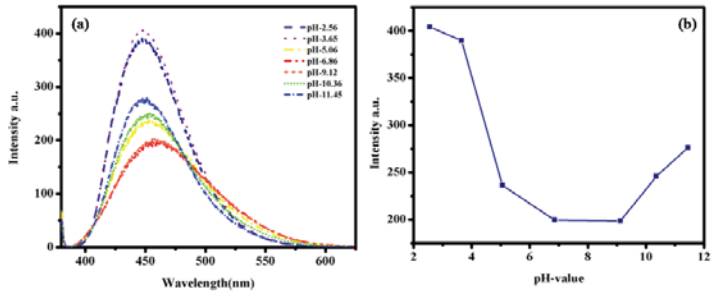

Fig. Fluorescence spectra of Compound BIQM (20 µM) at different pH values in aqueous ethanol medium (b) pH dependence of BIQM at 303 K at different pH values

Imperatorin-Functionalize Triangular Gold Nanoplates: Synthesis and Enrichment of Photothermal therapy

PP 56

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Aegle marmelos commonly known as **Bael** belongs to the *Rutaceae* family. .Extensive research had shown that Bael extracts are effective in inhibiting the growth of leukemic K562, B-lymphoid erythroleukemic HEL, melanoma Colo38, breast cancer cell lines MCF-7 and lung cancer A-549 cell lines.Au NPs are attracting enormous attention in applications for immunoassay drug delivery. Contrast enhancement, and thermal therapy for tumor treatment, due to their nanoscale size, oxide free components, bioconjugation property, biocompatibility, and unique optical properties. Triangle shaped gold nanoparticles absorb NIR radiation, which is a Prerequisite for photothermal activity and thus can serve as a suitable drug carrier. Imperatorin shows potent pharmacological activity and has been studied for its anti-inflammatory and antitumor properties. It also has shown an antiproliferative effect on several cancer cell lines.This study aims to isolate imperatorin from bael gum. These particles in turn shall be used to investigate biological activity on various cancerous cell lines, *invitro*. More specifically, photothermal and anticancer activity in A549 lung cancer cell lines shall be examined under optimized conditions

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Bronsted acid catalysed multicomponent reaction towards dihydropyridine derivatives via hantzsch reaction

PP 57

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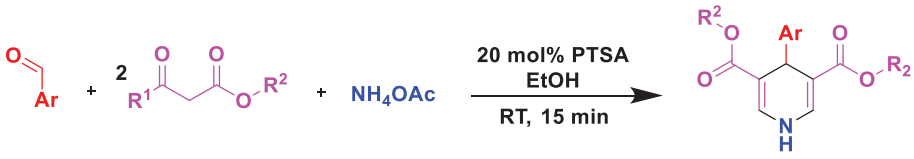
Pyridine derivatives are an important class of azaheterocycle found in many natural products, active pharmaceuticals, and functional materials. Among the rich versatile methodologies available in the literature forHantzsch reaction, still, it remains a valuable approach due to its simplicity. Here, we are intended to develop a simple and improved reaction methodology for Hantzsch reaction via Bronsted acid catalysis. The multicomponent reaction between ketone flanked ester, aromatic aldehydes and ammonium acetate under p-tolunesulphonicacid catalysis have successfully developed to synthesize a variety of dihydropyridine derivatives.



>80% yield
Wide substrate scope
Short reaction time

Keywords: Dihydropyridine (DHP), Hantzsch reaction, Bronsted acid catalysis,

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Synthesis, growth, spectral, thermal and optical studies of a new organic crystal: 2-aminopyridinium-3, 5-dihydroxybenzoate

PP 58

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A new organic salt 2-aminopyridinium-3, 5-dihydroxybenzoate (APHB) has been successfully synthesized. The single crystals of APTC were grown by the slow solvent evaporation solution growth technique at room temperature using methanol as the solvent. The functional groups of the title salt was confirmed from the FT-IR spectral studies. The thermal stability of the complex salt was studied by TG/DTA thermal analyses. The lower cutoff wavelength and optical transparency window of the title salt was identified from the UV-Vis-NIR spectroscopic studies. The molecular structure of the title salt was confirmed from the ^{1}H &^{13}C NMR spectroscopic studies.

Defluoridation of water by plate dip model using Zr^{4+} loaded polymer on Al plate

PP 59

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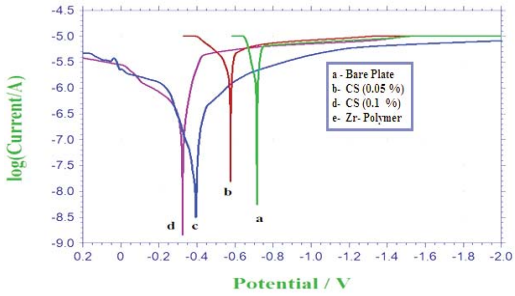
Aluminium and its alloys are widely used in almost all fields because of low cost. However, their surfaces are easily corroded by chemical reaction. We report here a simple method to fabricate zirconium loaded polymer coating on Al by electropolymerisation and electrodeposition techniques. This zirconium loaded copolymer coated Al plate was used as a novel adsorbent for fluoride removal without any filtration. The defluoridation experiments were carried out for various influencing parameters like contact time, pH and competitor anions for optimization. The adsorption capacity was found to be 3750 mg F^-/kg at pH 7. The adsorption isotherm data were well described by Freundlich isotherm model. The values of thermodynamic parameters indicate that the nature of fluoride removal is spontaneous and endothermic. The corrosion behavior of the coating in the 3.5% NaCl solution was investigated by EIS and potentiodynamic polarization. Based on corrosion parameters data, it was found that the zirconium loaded copolymer coating provided excellent corrosion resistance to aluminium and also this plate used as adsorbent, which has been successfully applied to remove fluoride from groundwater.



Growth, thermal and optical properties of *r*-2, *c*-6-bis (4-methylphenyl)- *c*-3, *t*-3-dimethylpiperidin-4-one – a new class of organic nlo material

PP 60

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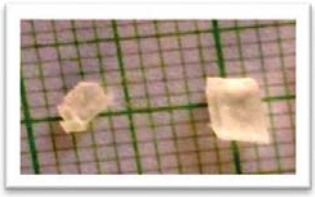
A new organic nonlinear optical crystalline material, *r*-2, *c*-6-bis(4-methylphenyl)- *c*-3,*t*-3-dimethylpiperidin-4-one(PT3DMPO) has been prepared. The single crystals of the title material with good optical quality have been grown from its benzene solution by slow evaporation solution growth technique at ambient temperature. The non-centro symmetric crystal belongs to orthorhombic system with space group Pna21. The grown crystals are characterized using the spectroscopic techniques such as UV-Visible, FT-IR and NMR spectra. The UV-Visible spectrum is recorded to find out the suitability of the title crystal for optical applications. The FT-IR, ^{1}H &^{13}C NMR spectra are recorded to confirm the presence of various functional groups and the molecular structure. The thermal stability of the crystal is established by TG/DTA analysis. The second harmonic generation (SHG) in the crystal is confirmed using the modified Kurtz-Perry powder test employing Nd: YAG laser as the source of IR radiation and the SHG efficiency is found to be closer to that of standard KDP**.**



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Synthesis, spectral and optical investigation of 2, 3-dimethyl quinoxilinium-4-chlorobenzenesulfonate

PP 61

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Novel optical active compound has been synthesized by slow solvent evaporation method at room temperature. The UV-Vis-NIR transmittance spectrum was recorded for find the suitability of the compound for various optical applications. The ^{1}H NMR and ^{13}C NMR spectra were recorded to confirm the different types of proton and carbon environments. The crystal structure has been confirmed by single crystal X-ray diffraction analysis. The presence of various functional groups in the compound has been ascertained by FT-IR spectral study. The thermal stability of the crystal was investigated using Thermogravimetry and differential thermal analyses.

Keywords*:* Optical activity, FT-IR, NMR, X-ray diffraction analysis

Synthesis, characterisation of thiourea compound: crystal structure, DFT and molecular docking studies

PP 62

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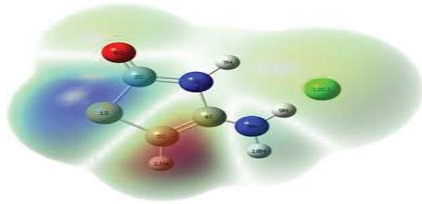
Over the past few years, thazolidine compounds have been many reports on their applications in biology including antibacterial, antifungal, anticancer, antioxidant, anti-inflammatory, antimalarial, antiviral activity and also used as catalyst.[1] Thiazolidin-4-one ring systems are known to act as analgesic, antibacterial, anticonvulsant, antiparasitic, herbicidal agents, and potent anti-HIV agents[2]. Thiourea reacts with monochloroacetic acid to form a cyclic product of 2-Imino-4-oxo-1, 3-thiazolidine hydrochloride. The 2-Imino-4-oxo-1, 3-thiazolidine hydrochloride compound was prepared and characterized by Single crystal X-ray diffraction studies, Hirshfeld surface analysis, DFT, antimicrobial and molecular docking studies. The compound has more stabilized within the active sites of O, N and S groups. The active sites of O, N, S groups involves in the many biological applications are presented.



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Physicochemical characterizationand quantum chemical calculations for the molecular adduct, 2-amino-4, 6-dimethylpyrimidine: itaconic acid

PP 63

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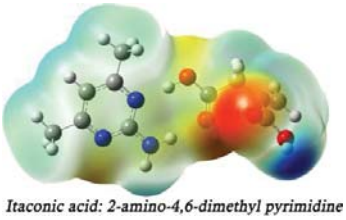
The molecular structure of a molecular adduct, itaconic acid:2-amino-4,6-dimethylpyrimidine (IADAP) was optimised and the microscopic optical properties were analysed. Quantum chemical calculations of the organic molecular adduct, were carried out using B3LYP/6-311G(d,p) level of theory. The calculated geometric parameters were in good agreement with experimental values. TD-DFT method was used to analyse the electronic transitions in the molecule. An electrostatic potential study revealed the nature of reactive sites based on the electron density of different sites. To correlate the molecular structure with optical properties, static and frequency-dependent hyperpolarizabilities, calculations were done using three different methods. The results reveal that the charge-transfer and hydrogen-bonding interactions are responsible for optical properties. The intermolecular interaction between the heterocyclic pyrimidine moiety and carboxylic acid of IADAP induces photoluminescence at 450 nm.



Itaconic acid: 2-amino-4,6-dimethyl pyrimidine

Keywords: Organic crystals; Hydrogen bonding; DFT; Emission; Hyperpolarizability.

Supramolecular assemblies in 2-amino guanidinium 4-methyl benzene sulphonate -hirshfeld surface analysis and computational calculations

PP 64

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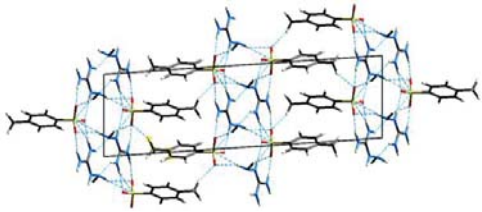
An organic compound, 2-aminoguanidinium 4-methyl benzene sulphonate (AGMS) with assemblies of hydrogen bonding interaction was crystallized at room temperature. Fingerprint plots of Hirshfeld surface analysis spells out the interactions in various directions. The molecular structure of AGMS was optimised by CAM-B3LYP method at 6-311G (d,p) basis set and the geometrical parameters were compared. Electrostatic potential calculations of the reactants and product illustrate the reason behind the transfer of proton. Hyperconjugative interactions which are responsible for the second hyperpolarizabilities were accounted by NBO analysis. Static and frequency dependent optical properties were calculated. The hyperpolarizabilities of AGMS increase rapidly at frequencies 0.0428 and 0.08 a.u. compared to static one.



Keywords: Single crystal XRD, Hirshfeld Surfaces, Hyperpolarizability, NBO analysis

Adsorption characteristics for the removal of methylene blue dye from an aqueous solution using activated carbon developed from *tecoma stans* leaves

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PP 65

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The present paper used to describe the efficiency of low-cost and eco-friendly activated carbon prepared from the leaves of *Tecoma stans* for the removal of Methylene blue dye from an aqueous solution. Batch mode experiments were conducted and the parameter which influences the extent of adsorption such as initial concentration of Methylene blue dye solution was studied. The adsorption kinetics of Methylene Blue dye onto activated carbon followed the first order Lagergren rate equation. Characterization of the adsorbent were studied using FTIR, SEM and EDAX. The percentage removal of Methylene blue dye was increased from 28.86 to 43.36 using 300 mg of the adsorbent when the initial concentration of the dye solution used was varied from 100 to 350 mg/L in 60 minutes of contact time at room temperature.

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Impact of nicotine on human sperm motility parameters in vitro

PP 66

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Human seminal plasma contains varieties of trace and macro elements including zinc(Zn),copper(Cu),magnesium(Mg), and iron(Fe) that have important roles in normal functioning of semen and it's quantity, quality. The imbalance of these chemical elements has been reported in several pathologic and male infertility disorders. The aim of this experimental study is to evaluate the effects on nicotine on sperm motility and unconventional sperm parameters.

Keywords: Human sperm, Effect of nicotine, Sperm parameter

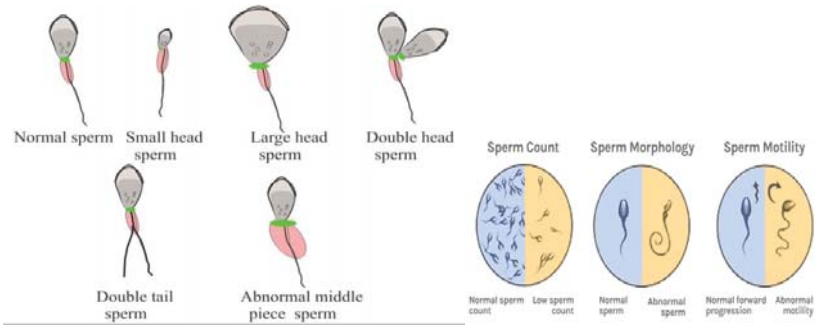

Fig: Sperm Morphology,Sperm Count

Dual functional fluorescent chemosensor for discriminative detection of Ni^{2+} and Al^{3+} -ions and its imaging in living cells

PP 67

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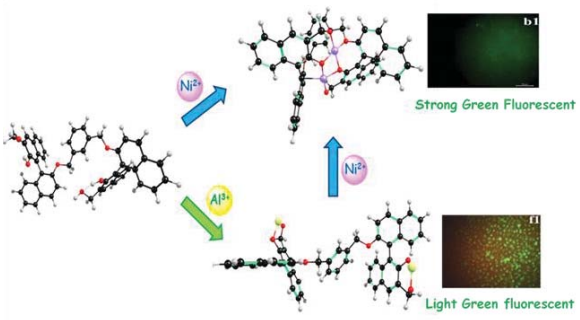
Nickel and Aluminium have been of great importance in the field of medicine, environment and industrial applications. Development of Sensors for detecting these metal ions is of current need. Therefore, on the continuation of our research based on the 1,1'-binaphthyl based fluorophores, we developed a twin-functional fluorescent chemosensor for the recognition of Ni^{2+} and Al^{3+}-ions. All those findings were supported by NMR, Mass spectrometric and theoretical studies. In addition, sensing of Al^{3+} ions is sucessfully applied into the live cells for bioimaging studies and logic gate applications. All the above details will be presented.



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Synthesis, growth, spectral, thermal and optical studies of a new organic crystal: 4-dimethylaminopyridinium-2-chlorobenzoate.

PP 68

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A new organic salt 4-dimethylaminopyridinium-2-chlorobenzoate (APCB) has been successfully synthesized. The single crystals of APCB were grown by the slow solvent evaporation solution growth technique at room temperature using methanol as the solvent. The lower cutoff wavelength and optical transparency window of the title salt was identified from the UV-Vis-NIR spectral studies. The molecular structure of the title salt was confirmed from the ^{1}H and ^{13}C NMR spectroscopic studies. The functional groups of the title salt was confirmed from the FT-IR spectral studies. The thermal stability of the title salt was established by TG/DTA thermal analyses.

Growth of non-linear glycine oxalate crystal and its characterizations

PP 69

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Semi-organic nonlinear optical (NLO) single-crystals of Glycine Oxalate (GO) with sizes up to 22 × 30 × 10 mm3 have been grown by the slow-evaporation technique method. It crystallizes in the monoclinic system, with a = 11.225 Å; b = 6.582 Å and c = 10.658 Å. Transmittance spectra of the grown crystal shows that the optical transmission in the entire visible region with the cut off wavelength of 275 nm. The powder second harmonic generation (SHG) measured by using the Kurtz and Perry technique indicates that GO is a phase-matchable NLO material with a SHG efficiency of 0.26 times that of KH_2PO_4 (KDP). TGA and DSC studies reveals the relationship between the structure and the thermal properties. Furthermore, laser-induced damage threshold measurements show a threshold up to 5.224 GW cm−2. The dielectric and AC Conductivity studies were carried out to study the variation of dielectric constant with frequency and temperature. All the results demonstrate that the semi-organic crystals GO is promising in NLO applications.

Keywords: Semi organic non-linear single crystals, second harmonic generation.

Synthesis, spectral characterization, electrochemistry and binding studies of new copper (ii) 3-acetyl-2[h]-chromen-2-one substutited thiosemicarbazone complexes

PP 70

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A series of four new thiosemicarbazone copper (II) complexes have been synthesized and characterized by spectroscopic techniques such as IR, UV- Vis, ^{1}H-NMR, ESR, Mass and cyclic voltammetric methods. Based on the spectral studies it is concluded that complexes (**1-4**) containing tridentate monobasic, ONS chelated thiosemicarbazone ligand coordinated through thiolate sulphur, hydrazinic nitrogen and oxo oxygen atom of coumarin moiety resulted in an octahedral geometry by forming a six member and a five member chelate rings. The binding ability of the complexes (**1-4**) to CT-DNA has been studied by absorption, emission titration, EB- displacement and cyclic voltammetric methods. Protein binding studies of compounds are monitored by absorption and fluorescence studies. Three dimensional studies show the microenviromental changes in binding BSA with compounds. Further the complexes (**1-4**) were tested for antibacterial activities against human pathogens such as *Staphylococcus aures, Escherichia Coli,* and *Pseudomonas Aeruginosa.* The results reveal that complexes (**1-3**) have better antibacterial activity than the conventional antibiotic *ampicillin* against both gram positive and gram negative organisms.

Synthesis and crystal structure of $[Co(Hqui)_2(H_2O)_2]$ - a convenient route to prepare nanocrystalline spinel cobaltite

PP 71

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The solid solution precursors of cobalt quinolinate hydrates complex $[Co(Hqui)_2(H_2O)_2]$ was successfully prepared and characterized by various physico-chemical techniques. Although there have been numerous characterized structures originating from quinolinic acid (H_2qui), however, predictable unusual structures still can be assembled when appropriate experimental conditions are modified. The prepared water assisted cobalt quinolinate complex is used as the solid solution precursors for the synthesis of the spinel cobaltite at low temperature by convenient method (i.e., thermal decomposition). The cobalt precursors were characterized by spectroscopic, thermal and powder X-ray diffraction studies. The crystal and molecular structure of cobalt quinolinate compound is crystallized in monoclinic crystal system with *P21/n* space group. Generally, the quinolinate anion (qui^{2-}) acts as a tridentate ligand to create polymeric structure, but in this complex, the anion attains bidentate (O, N) mode to generate monomeric structure and it is rare. The parent acid ($\lambda_{em.}$ = 383 nm) and its complex display a strong fluorescence emission at 405 nm upon excitation at 320 nm. The prepared cobalt compound exhibits endo-followed by exothermic decomposition to produce cobalt oxides around 450 ^oC by simultaneous TG-DTA method. The cobaltite (Co_3O_4) are derived from the cobalt quinolinate solid solution precursors by heating the complex at 450, 550 and 650 ^oC in a silica crucible for 3 hrs in muffle furnace. The high homogeneity of *spinel* cobaltites nanoparticles were characterized by infrared spectra, UV-visible, powder X-ray diffraction, scanning electron microscope coupled with EDX analysis and transmission electron microscope studies.

Rapid access to indeno[1,2-c]quinolines via Brønsted-acid catalyzed cascade reaction

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PP 72

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A Brønsted acid catalyzed annulation strategy has been developed to construct indeno[1,2-c]quinolines. This tandem synthetic method proceeds through a sequential electrophilic addition followed by a FriedelCrafts type reaction. A variety of tetracyclic compounds were obtained in moderate to high yields under mild reaction conditions in a short time.

Keywords: Indeno[1,2-c]quinolines, Brønsted acid catalysis, cascade reaction, Polycyclic heterocycles, Alkynes

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Template synthesis, structural variation, thermal behavior and antimicrobial screening of Mn(II), Co(II) and Ni(II) schiff base Complexes

PP 73

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Complexes of Mn(II), Co(II) and Ni(II) with ligands derived from the condensation of benzyl carbazate with 3-acetylpyridine have been synthesized using a template method. The complexes have the compositions $[M(NCS)_2(bc\text{-}3ap)_2(bc)].H_2O$; M = Co (**1**) or Ni (**2**), $[Mn(NCS)_2(bc\text{-}3ap)_4].2CH_3OH$ (**3**) and $[M(NCS)_2(bc\text{-}3ap)_4].2H_2O$; M = Co (**4**) or Ni (**5**) [where **bc** = benzyl carbazate, **3ap** = 3-acetylpyridine]. Characterization of the products involved elemental analysis, IR, UV-vis and ^{1}H NMR, and in the case of **1**, **3** and **4** single crystal X-ray structures have been determined. These are all six coordinate with octahedral coordination geometries. For **1** to **5** the charges of the M(II) cations are balanced in each case by two thiocyanato ligands, mutually *cis* for **1** and **2** but *trans* for **3-5**. In these six-coordinate complexes, **1-5**, the benzyl carbazate derived Schiff base ligands bind to the metal atoms in a *trans* monodentate fashion *via* the pyridine N atoms, two for **1** and **2**, and four such ligands for **3**, **4** and **5**. In addition to the thiocyanato anions, the remaining coordination positions are filled by bidentate chelate carbazate molecules for **1** and **2**. Thermal reactivity of the complexes was studied by TG-DTA. In addition, antimicrobial screening confirmed that all of the complexes have a moderate to good range of activity against both Gram-positive and Gram-negative bacterial strains and also against fungi.

Magnetite Fe_3O_4 nano-oxide from aqueous leaf extract of *Coccinia Grandis*: synthesis, characterisation and anti-cancer evaluation

PP 74

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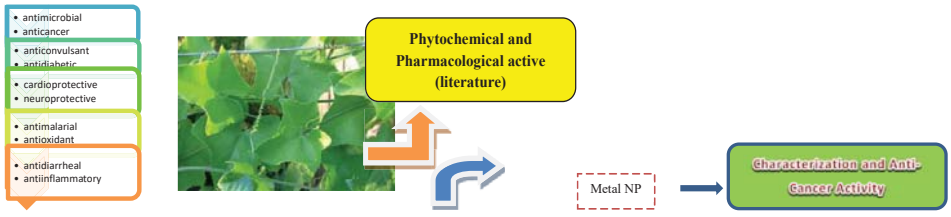
Coccinia plants (Ivy) belonging to Cucurbitaceae family have their own importance in traditional medicines, including Ayurveda, practiced in India. The present study was investigating the anticancer activities of the metal nanoparticles derived from the hydromethanolic extract of the leaves of Coccinia grandis L. Voigt. (Cucurbitaceae). The powder XRD pattern of the synthesized Fe_3O_4-NPs showed its be high purity crystalline nature and are approximately cubic in structure. The synthesized nanoparticles were affirmed to be Fe_3O_4 but not maghemite (γ-Fe_2O_3) by comparing the XRD patterns with the standardmaghemite JCPDS file no.: 01-089-3850.The anticancer activities of the magnetite nanoparticles have been evaluated by using in vitro assays and were compared to standard anticancer drugs such as cisplatin, Doxorubicin.



Performance of TI_2O_3/ZN electrodes verses Zn by electrocoagulation process for disperse dye removal

PP 75

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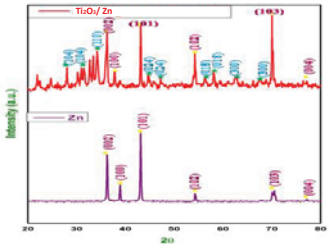
Electrocoagulation methods are being used for the alternative treatment process for the remediation of textile waste water. This work primarily deals with the treatment of textile dyeing waste water followed by the utilization of waste material. The purpose of the proposed study is to evaluate the potential of electrocoagulatison process using Ti_2O_3/Zn electrode prepared by spray pyrolysis using $TiCl_3$ and compared the performance with Zn electrodes. The surface morphology, structural analysis and percentage composition of the elements of the Ti_2O_3/Zn electrode was studied by SEM, XRD and EDS analysis. The efficiency of electrocoagulation treatment process to treat synthetic waste water containing Coralene Navy RDRLSR, Coralene Red 3G, Rubru RD GLFI dye was studied for the effect of operational parameters. The result indicates that this process was able to achieve color removal (97.2%) at pH 8.5, with 34.42% less energy consumption with Ti_2O_3/Zn compared with zinc electrodes.

Keywords: Electrocoagulation, Disperse dye, Ti_2O_3/Zn, Reaction time, energy



XRD Pattern for Zn and Ti_2O_3/Zn

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Coleus aromaticus leaves extract as corrosion inhibitor for mild steel in hydrochloric acid medium

PP 76

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The leaves extract of Coleus aromaticus (CA) as corrosion inhibitor for mild steel (MS) in 1 M HCl was studied using weight loss, potentiodynamic polarization measurements (PDP) and electrochemical impedance spectroscopy (EIS). The enhancement of inhibition efficiency was observed with increase in concentration of the extract. The effect of temperature on the corrosion of MS in hydrochloric acid with and without the addition of CA extract was studied in the temperature range of 303-333 K. It was found that the inhibition efficiency declined on increasing the temperature. Physical adsorption mechanism is proposed from the trend in inhibition efficiency with the change in temperature and from thermodynamic parameters. The adsorption of the molecules of the CA extract on the MS surface was in accordance with the Temkin adsorption isotherm. Polarization studies showed that the CA acts as mixed type inhibitor with predominant cathodic behaviour. FTIR and optical profiler images confirmed the adsorption of CA on MS surface.

A simple bis-salicylaldehyde based chemosensor for the detection of Ce^{3+} ions in aqueous media

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PP 77

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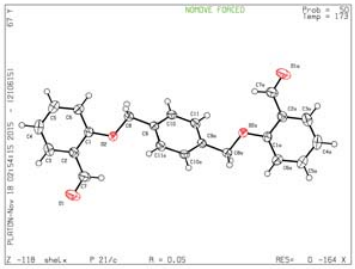
Heavy metal ions can have severe effects to human health and environment. Hence, methods for the rapid detection of metal ions with high selectivity and sensitivity receive much attention. In recent days, cerium metal is becoming the most precarious heavy metal ion and affects the environment such as the air, soil, and water. Many industries are started to use cerium metals due to its different oxidation states and adaptability nature. Moreover, cerium is widely used in agriculture, nuclear energy, metallurgy, microelectronics, therapeutic application, magnetism, glass and ceramics.Although many instrumental techniques are widely available, there is a necessity to develop new innovative techniques to detect cerium in the environment. Herein, we have designed salicylaldehyde basedreceptor, for the selective sensing of cerium-ions. The salicylaldehydebased sensor is very sensitive and selective towards the cerium metal ions. All the above details will be presented.



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Effect of dopant concentraion on optical, structural and electrical characterizations of silar deposited zinc doped cadmium sulphide thin

PP 78

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The Zn doped CdS thin films were prepared on cleaned glass substrates by SILAR deposition technique using cadmium acetate, zinc acetate and thiourea as precursor solution with deposition cycles of 75 dippings for various (3, 6 and 9) Zn mol%. The prepared samples were annealed in air. The prepared thin films were characterized for their structural, micro structural and optical properties by XRD, FESEM and UV-Visible spectroscopy. The XRD analysis shows that, the prepared samples are polycrystalline and it exhibits cubic structure. The morphology of the Zn doped CdS thin films characterized by FESEM revealed that the film consisted of mixture of nanoparticles and the EDAX results showed the presence of Zn and CdS in the prepared thin films. The optical properties of the deposited films were characterized by UV-VIS. Optical band gap was blue shifted with increase in Zn doping which is associated with Moss-Burstein (MB) effect. The electrical properties of the CdS thin films characterized by Hall measurements. It is observed that, for increase in Zn doping concentration, the resistivity decreases, conductivity and Hall mobility increases with Zn doping concentration. CdS film coated with 6 mol % Zn concentration had higher carrier concentration, mobility and lower resistivity than other two samples.

Spectral thermal and DFT analysis 4-dimethyl aminopyridinium 3,5 dichlorosalicylate

PP 79

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A new charge transfer complex (4DAPDCA) has been synthesized by the reaction between an electron donor, 4-dimethylaminopyridine with the electron acceptor, 3,5-dichloro salicylic acid. Single crystals of the compound, 4DAPDCA, were harvested and characterized experimentally using a variety of physico-chemical techniques. The experimental work included the use of UV–vis, FT-IR and ^{1}H NMR and ^{13}C NMR and TG-DTA studies. Both FT-IR and NMR studies asserted the occurrence of proton transfer during the reaction. For supporting the experimental results, DFT computations were carried out using B3LYP/6-31G(d,p) method to compute the optimized structures of the reactants and complex, their geometrical parameters, reactivity parameters, molecular electrostatic potential map and frontier molecular orbitals. The analysis of DFT results strongly confirmed the high stability of the formed complex based on hydrogen bonding interactions.

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Synthesis, growth, spectral, thermal and optical studies of a new organic crystal: 2-nitroanilinium-l-tartarate

PP 80

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A new organic salt 2-nitroanilinium-L-tartarate (NALT) has been successfully synthesized. The single crystals of NALT were grownby the slow solvent evaporation solution growth technique at room temperature using methanol as the solvent... The functional groups of the title salt was confirmed from the FT-IR spectral studies.The lower cutoff wavelength and optical transparency window of the title salt was identified from the UV-Vis-NIR spectral studies. The molecular structure of the title salt was confirmed from the ^{1}H and^{13} C NMR spectroscopic studies. The thermal stability of the title salt was established by TG/DTA thermal analyses.

Physico- chemical and biological parametric evaluation on ground water, surface water and bilge's from industries – an overview

PP 81

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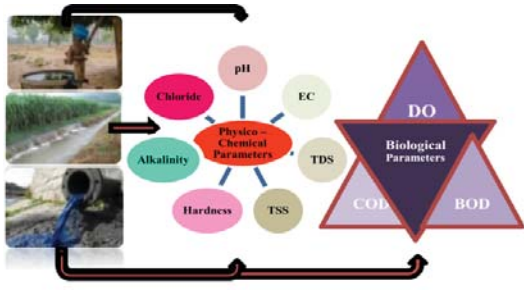
Water is an obligatory natural resource on earth and safe drinking water is the primary tool of every human being. Discharge of toxic chemicals, fungicides and organic manure promotes algal growth, increase in the concentration of heavy metals which finally leads to bad taste, corrosiveness, staining or frothing. Thus the analysis of the water quality is very important to preserve and protect the natural eco system. A comparative assessment of the quality of ground water, surface water including effluent from industries was carried out in and around Dindigul, Erode,Tirupur and Coimbatore districts. Around, fourteen samples (bore well, water tanks and effluents from industries) were taken for parametric evaluation under lab scale by optimizing few of the Physico- chemical parameters viz., p^H, EC, TDS, TSS, hardness, alkalinity, acidity, chlorides, and biological study such as DO, chemical oxygen demand (COD) and biochemical oxygen demand (BOD). The obtained results are compared with WHO standards for recommendations. The results revealed that, most of the analyzed parameters were in high concentration at the sampling stations. Thenceforth, water quality management practices should be carried out periodically to prevent/ protect the water resources.



Preparation, thermal and anti-bacterial studies of Zr(IV) sulphonate containing neutral hydrazine

PP 82

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Para toluene sulphonic acid is interesting molecule owing to the presence of three potential donor oxygen atoms. The above said acid and can be deprotonated easily in aqueous solution. Sulphonic acid are known to act as bridging as well as monodentate and as charge compensating anion. Bridging mode of the para toluene sulphonic acid is only known in the case of actinides. In transition metal complexes it is known to act as monodentate and in some cases as charge compensating anion. In this connection our aim is to prepare the zirconium sulphonate complex encompasses neutral hydrazine with appropriate experimental condition. The isolated complex is characterized by various physico-chemical techniques. Physico-chemical studies reveal the compositions of the complex has **$[Zr(PTS)_4(H_2O)_2].2N_2H_4$**. The IR spectrum of the complex shows O-H stretching frequency in the region 3450 cm^{-1} revealing the presence of water molecule. The asymmetric and symmetric stretching frequencies of the sulphonate groups appears around 1350 cm^{-1} and 1175 cm^{-1} which shows the presence of sulphonate moiety .The N-H and N-N stretching frequencies of hydrazine moiety has been observed around the region of 3240 and 945 cm^{-1} confirming the presence of neutral bidentate chelating hydrazine.

The simultaneous TG-DTA studies shows the complex decompose continuously to yield metal oxide as the final product. In all these observation the proposed structure of the complex shows six coordinated octahedral structure with two coordinated water molecule. The title complex shows higher anti-bacterial activity.

Corrosion inhibition of mild steel in HCl by the fresh juice of *Alternanthera Sessilis* leaves

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PP 83

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The corrosion inhibition of mild steel in 1 M hydrochloric acid by the fresh juice of *alternantherasessilis* leaves was studied using weight loss and electrochemical techniques. Results obtained indicate that the fresh juice is effective in hydrochloric acid medium and the efficiency decreases with increase in temperature. Thermodynamic parameters show that the physisorption of the inhibitor molecules on mildsteelsurface obeys Langmuir adsorption isotherm. The adsorbedfilm on the metal surface has been analyzed by FTIR and FE-SEM studies. Polarization measurements show that fresh juice is an inhibitor of mixed nature.

Keywords: Mild steel, Weight loss, EIS, PDP, FT-IR, FE-SEM.

MHD nano-second grade fluid flow over a stretching sheet with second order slip and thermal jump effects

PP 84

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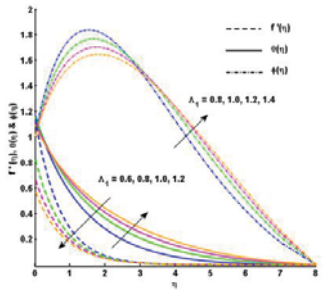
The present examination is for the most part centered on the flow of an incompressible magnetohydrodynamic nano-second grade fluid over a stretching sheet implementing the second-order slip and thermal jump model. To analyze the problem elaborately, numerical simulations are carried out. For that the partial differential equations that were employed to characterize the flow were transformed to ordinary differential equations with the aid of similarity transformations. Solving them with the much known Runge-Kutta strategy in association with shooting iteration technique, the outcomes for the nano-second grade fluid velocity, temperature, concentration, the local skin friction coefficient, the local Nusselt number and the local Sherwood number are discussed. Some of the notable results of second grade, thermophoresis and Brownian motion parameters along with Lewis number are brought out, which might be relevant for future research work.



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Dielectric relaxation and ac conductivity of chitosan-graft-polyaniline

PP 85

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The Chitosan-graft-Polyaniline (Chit-g-PANI) samples have been synthesized by chemical oxidation method with various grafting percentages, GPs (GP = 35%, 54%, 66% and 83%). Dielectric properties and AC conductivity of Chit-g-PANI have been investigated in the frequency range from 50 Hz to 5MHz between 303 and 393 K. The degree of grafting was confirmed through FTIR studies. The dielectric behavior was analyzed using real and imaginary parts of dielectric constant (ε′), dielectric loss (ε″), loss factor (tanδ), electric modulus (M′ and M″) and impedance (Z′ and Z″) measurement. The studies have been discussed and their results are reported along with suitable depictions.

Ovalbumin directed bright red fluorescent gold nanoclusters as selective colorimetric and fluorometric nanoprobe for cyanide detection

PP 86

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The iron oxide nanoparticles are prepared by hydrothermal process using the raw materials like iron chloride ($FeCl_3.0H_2O$) and ammonium hydroxide (NH_3OH). The concentration of 0.1 mole is chosen for synthesis of iron oxide nanoparticle and annealed at 400ºC. The pH is maintained at 8 during the sample preparation. The XRD analysis for iron oxide nanoparticles are confirmed the rhombohedral structure with good crystallinity. The average particle size is predicted as 24 nm. The morphology of iron oxide nanoparticles is visualized from Scanning Electron Microscopy (SEM). Energy Dispersive X-ray Spectrum (EDS) is identified the stoichiometry of prepared iron oxide sample. The photocatalytic behavior of iron oxide is tested under UV irradiation for the removal of methylene blue in the water. The removal efficiency of the iron oxide nanoparticle photocatalyst is also estimated from the degradation level dye pollutant of organic dye to show its robustness.

Keywords: Particle Size, Morphology, Stoichiometry, Irradiation, Efficiency

Tuning of optical band gap and enhancing the photocatalytic activity by ZNS/SNS nanocomposites

PP 87

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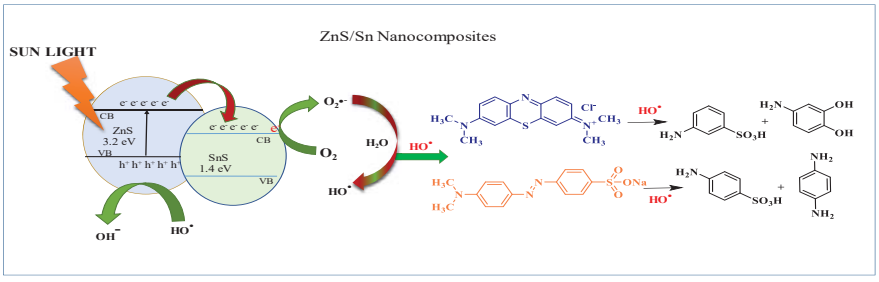
Semiconductor nanoparticles of pure ZnS and different percentage of ZnS/SnSnanocomposites are prepared by simple co-precipitation method utilizing low dopant concentrations (0–1%) and employing poly(vinylpyrrolidone) (PVP) as a capping agent, which adsorbs to the nanocrystal surface, is generally added to control the size of the nanocrystal and to prevent agglomeration of the synthesized crystals at room temperature. The obtained ZnS and ZnS/SnSnanocomposites had cubic and hexagonal structures respectively with average particle sizes of 2.5 nm. The tuning of band gap of the material can promotes the photocatalytic activity in visible light.The composites in ZnS nanoparticles directly affects the photocatalytic activity due to the change in position of CB and VB. As anticipated, the ZnS/SnSNanocomposites show good photocatalytic activity in decomposing MB compared to pure ZnS. Photocatalytic studies of pure ZnS and ZnS/SnSNPs showed better degradation of MB as compared to that of MO.



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Synthesis, characterisation and antimicrobial evaluation of pyrazolino cyclohept[*b*] indole derivative

PP 88

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Cyclohept[*b*]indoles [1] are crucial building blocks in organic synthesis and the core structures of numerous biologically active compounds. Cyclohept[*b*]indoles[1] containing molecules have also been widely used as organic materials[2].Due to these interesting properties, a number of synthetic approaches to the Cyclohept[*b*]indoles[1]framework have been described. This work describes a strategic approach for the synthesis of efficient precursor 2-(4-methoxy)benzylidine-1-oxo-1,2,3,8-tetrahydrocyclohept[*b*]indole which can obtained by aldol condensation[3] of the 7-methyl-1-oxo-2,3,4,5-tetrahydrocyclohept[*b*]indole with anisaldehyde under basic conditions. Pyrazolino carbazoles were derived by the treatment of 2-(4-methoxy)benzylidine-1-oxo-1,2,3,8-tetrahydrocyclohept[*b*]indole with hydrazinehydrate in sodium methoxide under proper condition .

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One pot direct synthesis of reduced graphene oxide and its characterization

PP 89

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The direct one-step synthesis of reduced graphene oxide (rGO) from graphite was prepared by modified Hummers method. As synthesized rGO were characterized using Fourier transform infrared (FT-IR) spectroscopy and Raman spectroscopy. Further, the rGO formation was confirmed by X-ray diffraction (XRD) studies. The morphology and elemental compositions were studied using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDS), respectively. Further, the anti-microbial activity of the synthesized rGO was tested against human pathogens.

Keywords: Reduced graphene oxide (rGO), XRD, Raman Spectroscopy, Hummers method.

Biological application of 2-aminopyrimidine and p- nitro aniline-formaldehyde terpolymer resin

PP 90

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The terpolymer resin-2APNAF was prepared by using 2-aminopyrimidine and *p*-nitro aniline with formaldehyde. The synthesis of 2-aminopyrimidine-*p*-nitroaniline-formaldehyde terpolymer by condensation polymerization techniques in 1:1:2 and 2:3:5 mole ratios in presence of dimethyl formamide as a reaction medium. The synthesized terpolymer are characterized by elemental analysis, FTIR, UV-Visible and NMR (^{1}H & ^{13}C) and the molecular weight of the terpolymer is determined by gel permeation chromatography. And further to be screened for antibacterial and antifungal activities by disc diffusion technique. The result it has been proved that 2APNAF-Cu had excellent antimicrobial activity compared to the ligand. Due to their excellent activity, they can be successfully used as antibacterial and antifungal agents. The solubility parameter shows that the terpolymers are insoluble in almost all the known solvents like benzene, ether, ethanol and $CHCl_3$, whereas the terpolymer is soluble in organic solvents like THF and DMSO

GPR120 homology modeling and docking studies with GPR120 homology model and GPR40 receptor

PP 91

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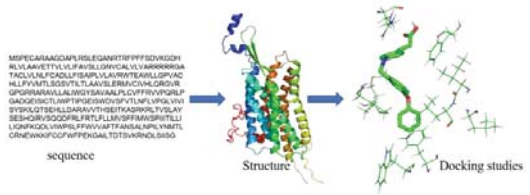
GPR120 is a validated therapeutic target for the treatment of obesity and type 2 diabetes mellitus, many of the pharmacological compounds have been reported however none of the molecules available in drug market due to its poor pharmacokinetic properties. Since the function of GPR120 is important in diabesity patients. GPR120 agonists are also selective towards GPR40 even it is having only 12% sequence identity. So discovery of novel GPR120 agonists with both high potency and selectivity is highly desirable. GPR120 homology modelling was performed to generate 3D model of GPR120 by using Orexin2 receptor (5WQC) as a template and model was validated. Compounds derived from hybrid design and scaffold hop methods from reported GPR120 agonists given a way to know the relation between GPR120 and GPR40. The common residues which are important in activation in the binding site like ARG183, ARG258 in GPR40 and ARG99 in GPR120 along with this influence of hydrophobic residues may lead to more selectivity towards GPR40. A docking simulation approach using GPR120 homology models and GPR40 receptor could be useful in predicting GPR120 receptor-selective agonists which may lead to discovery of novel GPR120 agonist with both potency and selectivity.



Sequence to structural studies of GPR120

Study of Photocatalytic Behaviour of Hydrothermally Prepared Iron Oxide Nanoparticles

PP 92

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The iron oxide nanoparticles are prepared by hydrothermal process using the raw materials like iron chloride ($FeCl_3.0H_2O$) and ammonium hydroxide (NH_3OH). The concentration of 0.1 mole is chosen for synthesis of iron oxide nanoparticle and annealed at 400 ^oC. The pH is maintained at 8 during the sample preparation. The XRD analysis for iron oxide nanoparticles are confirmed the rhombohedral structure with good crystallinity. The average particle size is predicted as 24 nm. The morphology of iron oxide nanoparticles is visualized from Scanning Electron Microscopy (SEM). Energy Dispersive X-ray Spectrum (EDS) is identified the stoichiometry of prepared iron oxide sample. The photocatalytic behavior of iron oxide is tested under UV irradiation for the removal of methylene blue in the water. The removal efficiency of the iron oxide nanoparticle photocatalyst is also estimated from the degradation level dye pollutant of organic dye to show its robustness.

Keywords: Particle Size, Morphology, stoichiometry, irradiation, efficiency

Characterization of smectic blue phase hydrogen bonded ferroelectric liquid crystals for optoelectronic applications

PP 93

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New type of blue phase hydrogen bonded ferroelectric liquid crystal (HBFLC) mixture has been designed and synthesized from cholesteryl stearate (CHS) and 4-n-decyloxybenzoic acid (10OBA). Optical, thermal and structural properties are studied using polarizing optical microscope (POM), differential scanning calorimetry (DSC) and X-ray diffraction technique (XRD). Formation of hydrogen bond between the donor and acceptor atom is confirmed using Fourier transfer infrared (FT-IR) spectroscopy. A noteworthy observation is that the induced smectic blue phase and its enhanced span width have been detailed in the present communication. Band gap energy (4.1eV) is experimentally determined using UV-Vis spectrometer for the present CHS+10OBA HBFLC complex clearly reveals the usage of smectic blue phase in diode fabrications. The other liquid crystal parameter such as, transition temperature, enthalpy value and thermal stability factor are calculated and discussed.

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Microwave assisted synthesis, biological evaluation and molecular docking studies of novel pyrido[2,3-a]carbazole derivatives

PP 94

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A new series of 2,3-thiophene-5,6-dihydro-11H-pyrido[2,3-a]carbazole-4-one derivatives, are synthesized from microwave irradiation reaction which has not been reported yet. The binding of this set of compounds with calf thymus DNA (CT-DNA) are investigated by electronic absorption spectroscopy, which indicates that pyrido [2,3-a]carbazoles can strongly bind to CT-DNA *via* intercalation mechanism. Gel electrophoresis assay demonstrates the ability of synthesized compounds to cleave the pBR32 *via* oxidative pathway. Further, investigation about the antioxidant properties showed that all synthesized compounds have a significant radical scavenging potency against DPPH and OH radicals. The cytotoxicity activities of all the synthesized carbazole derivatives are evaluated against three different cancer cell lines (HeLa, MCF-7 and HEp-2), which showed that the compounds exhibited substantial cytotoxic specificity on HeLa cell line over the other cancer cell lines. In order to understand the nature of the interaction of these molecules, we carried out molecular docking studies using the Check Point Kinase 1 protein inhibitors. The docking results provide some useful insights about the future design of more potent inhibitors.

Keywords: Microwave irradiation, DNA binding/cleavage, Radical scavenging activity, Cytotoxicity, Molecular docking.

Kinetic and equilibrium adsorption studies of methylene blue from aqueous solution using low-cost adsorbent

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PP 95

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This study investigates the potential use of activated carbon prepared from copper pod flowers for the removal of methylene blue dye from simulated wastewater. The parameter studied included contact time, initial dye concentration, carbon dosage, temperature, and pH. The characterization of the adsorbent was carried out using Fourier transform infrared spectroscopy, scanning electron microscope, and X-ray diffraction data.The kinetic data were modeled using pseudo-first-order model, pseudo-second-order kinetic model, and intraparticle diffusion. The adsorption followed second-order rate equation. The adsorption equilibriums were analyzed with Langmuir and Freundlich isotherms. The experimental data were better interpreted by Freundlich isotherm model Langmuir isotherm model. Adsorption capacity values obtained from the Activated carbon developed from the copper pod flowers can be used as an alternative to highly efficient and low-cost abundant materials for methylene blue dye removal from wastewater.

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A highly sensitive non-enzymatic glucose biosensor by electrochemical behaviors of silver doped on 1d hydroxyapatite with flower like 3D MOS_2

PP 96

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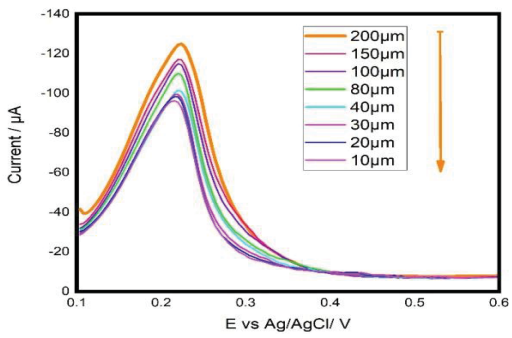
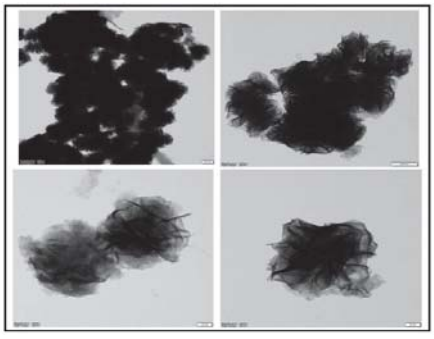
A novel and high sensitivity of non-enzymatic glucose biosensor was developed by silver nanoparticles on combined 1D HAP and flower like MoS_2. The facile fabrication and stability indicates promising capability for large scale manufacturing. The hydrothermal process improves the crystalinity of HAP and MoS_2. Nano composites and silver nano particles was doped by a simple sonication technique. The crystalinity and morphology of the prepared nano composites were characterized using varies analytical techniques such as SEM, TEM,UV and XRD. The electrocatalytic and eletcroanalytical studies of all these fabricated electrode were characterized by cyclicvoltametry(CV) and square wave voltammetry (SWV).



Square Wave Voltammetry(SWV)



HR-TEM Image of MoS_2

Preparation, characterization and anticancer activity of silver nanoparticles reduced by *Cymbopogon Citratus*

PP 97

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The present study investigated the anticancer properties of silver nanoparticles (AgNPs) synthesized using water extracts of the *Cymbopogon citratus*. AgNPs were characterized by ultraviolet-visible spectroscopy, transmission and scanning electron microscopy, and energy dispersive X-ray fluorescence spectrometry. The AgNPs were unwavering and small at 4.35 ± 2.79 nm in size. The *in vitro* anticancer effect of AgNPs was resolute on cervical (HeLa), liver (HepG2), and leukemia (CEM-ss) cell lines using fluorescence microscopy, flow cytometry, caspase activity determination, and MTT assays. After 72 h treatment, AgNPs was shown to be significant cytotoxic to the cancer cells in a dose- and time-dependent manner. The IC_{50} values of AgNPs on the HeLa, HepG2, CEM-ss, cell lines were 8.65, 12.14, 15.45, µg/mL, respectively. The anticancer effect of AgNPs is via the inherent apoptotic pathway. The study showed that AgNPs is a good aspirant to be developed into a chemotherapeutic compound for the treatment of cancers especially cervical cancer.

Spectral, optical, thermal, hirshfeld and computational calculations of a new organic crystal, 1H-benzo[d][1,2,3]triazol-3-ium-3,5-dinitrobenzoate

PP 98

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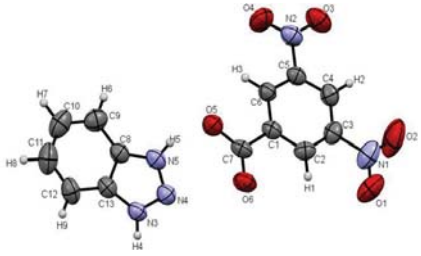
A molecular complex, 1H-benzo[d][1,2,3]triazol-3-ium-3,5-dinitrobenzoate, (BTDB), was synthesized, crystallized and characterized by CHN analysis and ^{1}H, ^{13}C NMR spectral studies. The crystal is transparent in entire visible region as evidenced by UV-Vis-NIR spectrum. TG/DTA analysis shows that BTDB is stable up to 150 ºC. Single crystal XRD analysis was carried out to ascertain the molecular structure and BTDB crystallizes in the monoclinic system with space group P21/n. Computational studies that include optimization of molecular geometry, natural bond analysis (NBO), Mulliken population analysis and HOMO-LUMO analysis were performed using Gaussian 09 software by B3LYP method at 6-311G(d,p) level. Hirshfeld surfaces and 2D fingerprint plots revealed that O···H, H···H and O···C interactions are the most prevalent. The first order hyperpolarizability (β) of BITB is 44 times greater than urea. The results show that the BTDB can be used for various opto-electronic applications.



Synthesis and characterization of Ruthenium(II) quinoline thiosemicarbazone complexes

PP 99

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Two new ruthenium(II) thiosemicarbazone complexes (**2** and **3**) have been synthesised from the reactions of $[RuHCl(CO)(PPh_3)_2]$, $[RuHCl(CO)(AsPh_3)_2]$ with, 4-methyl-1-((6-methyl-2-oxo-1,2-dihydroquinolin-3-yl)methylene)thiosemicarbazide HL(**1**), were prepared and characterized by various physico-chemical and spectroscopic methods. The thiosemicarbazone act as tridentate, monobasic chelating ligands with ONS as the donor sites and are preferably found in the thiol form in the complexes studied. An octahedral geometry has been tentatively proposed for all the complexes.

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Ultrasonic, DFT, FT-IR and MD simulation studies on hydrogen bonding interactions in aqueous solutions of ethylene glycol

PP 100

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The density, viscosity and ultrasonic velocity measurements were carried out in aqueous ethylene glycol (EG) solutions at different concentrations and temperatures to illustrate the hydrogen bonding interactions of EG with water. The main acoustic parameters such as isentropic compressibility (β_s), acoustic impedance (Z), hydration number (H_n), intermolecular free length (L_f), classical sound absorption $(\alpha/f^2)_{class}$ and shear relaxation time (τ) were calculated based on the experimentally measured values. These parameters have been utilized to study the solute-solvent interactions in aqueous EG solutions. These results suggest that the clusters of likely complex of an EG molecule form hydrogen bonding with two water molecules in aqueous phase. Meanwhile, the quantum chemical calculations were also performed to investigate the existence of intramolecular hydrogen bonding in EG molecule itself and intermolecular hydrogen bonding between EG and water molecules in an interacting complex. The equilibrium structure of most favoured conformations of EG monomer like tTt, $g^+G^+g^-$, tG^+g^- and an interacting complex $g^-G^+g^- 2H_2O$ in gas and solvation phases and vibrational frequencies have been computed by using theDensity Functional Theory (DFT) method at B3LYP/6-31+g(d) level of theory. The solution phase study was carried out using Onsager's reaction field model in water solvent. When two water molecules are considered explicitly with an EG ($g^-G^+g^-$) molecule the computed vibrational frequencies are in good agreement with the main features of the experimental spectrum. The total optimization energy (E_{total}), intramolecular and intermolecular hydrogen bond lengths and dipole moment (μ_m) of an interacting complex are also presented. The glass transition temperature (T_g) of roughly semi diluted EG-water ($g^-G^+g^- H_2O$) system was computed through Molecular Dynamics (MD) simulation method. MD simulation was performed with isothermal-isobaric (NPT) ensemble. The Radial Distribution Functions (RDFs, g(r)) of oxygen-oxygen atoms of solute-solvent molecules with respect to temperature were also computed for understanding the intermolecular hydrogen bonding interactions and discussed within the light of solute-solvent interactions.

Preparation and characterization of pure and Ce doped WO_3 thin films for PN junction diode application

PP 101

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The present research deals with synthesis of $Ce_2(WO_4)_3$ thin films for different doping concentrations of Ce (0, 5, 10 and 15wt.%). Further 15wt.% of n-$Ce_2(WO_4)_3$/p-Si junction diode were prepared at the substrate temperature of 500°C by JNSP technique. The prepared films were analyzed by the structural, optical and electrical properties. I-V characterization was performed for diode measurement in darkness and under the halogen lamp.

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Exploration on metal oxide nanoparticles for humidity sensor applications

PP 102

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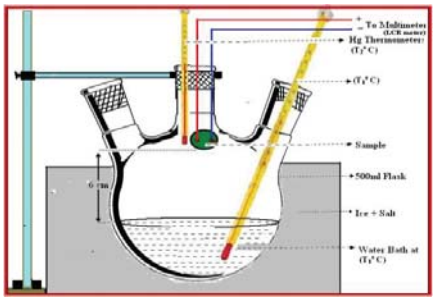
ZnO, SnO_2, NiO, Fe_2O_3 nanoparticles has been synthesized by chemical precipitation method. The samples are characterized by structural, optical, electrical properties. The prepared samples are dissolved in ethanol and N-Methyl-2-pyrrolidone (NMP) solvent. XRD pattern shows the crystalline nature of the oxide nanoparticles. UV-VIS spectra are recorded for the samples dissolved in ethanol and N-Methyl-2-pyrrolidone (NMP) solvent. The electrical conductivity and dielectric constant of the samples in pellet form are measured and the results are discussed. The applications of synthesized metal oxide nanoparticles as humidity sensors are analyzed based on the resistance variation due to the absorption/desorption of water vapor. The fabricated sensors showed better sensitivity, linearity, and quicker response time.



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Hierarchical flower like CZTS & CCTS semiconductors for photocatalytic dye degradation and electrocatalytic hydrogen evolution

PP 103

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Quaternary semiconductors based on CXTS (X= Zn, Co) attracts the attention of photocatalysis, photovoltaic and electrocatalysis applications for its cost effective and earth abundant nature. Owing to its morphology and optical properties, they gain an effective result in their applications. In this work, CZTS (Cu_2ZnSnS_4) &CCTS (Cu_2CoSnS_4) are prepared by hydrothermal method to explore its properties in photocatalysis for dye degradation and in electrocatalysis for hydrogen evolution reaction. XRD analysis confirmed the tetragonal structure. SEM results reveals flower like morphology and UV absorption is also analyzed for both CZTS and CCTS. The photocatalytic activity of CZTS and CCTS for the degradation of MB dye under visible region and electrocatalytic water splitting of hydrogen evolution has been evaluated. The impact of recombination of charge carriers on the photocatalytic degradation and the effect of surface activity in hydrogen evolution reaction has been discussed

Keywords: CZTS and CCTS, hydrothermal, flower like, photocatalyst, electrocatalyst, hydrogen evolution

Cardiospermum Halicacabum leaves extracts as an inhibitor for mild steel corrosion

PP 104

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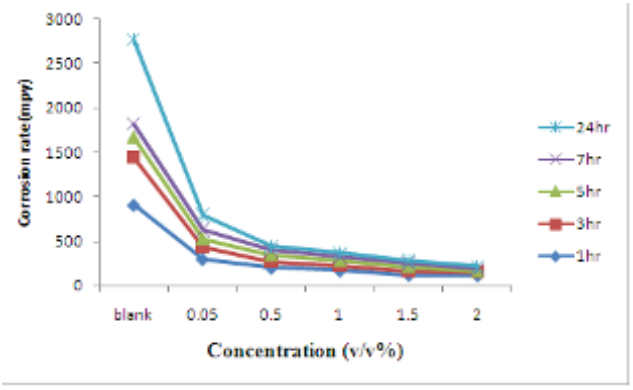
Cardiospermum halicacabum leaves extracts act as good inhibitor for mild steel in 1N sulphuric acid medium. The protection efficiency of the inhibitor depends on its concentration and immersion time. From the report we have found that leaves extracts of *Cardiospermum halicacabum* was found to be good inhibitor having efficiency as high as 97.79% at 2% inhibitor concentration. As the concentration increases corrosion rate decreases and inhibition efficiency increases. The study of effect of immersion time on inhibition efficiency shows that the inhibitor is effective even for longer immersion periods at low concentration.



Formation of hetero binuclear Ru(III)/Fe(II) cyclopentadienyl complexes of acetylferrocene-4(*N*)-substituted thiosemicarbazones: synthesis, spectral characterizations and nucleic acid/serum albumin binding interactions

PP 105

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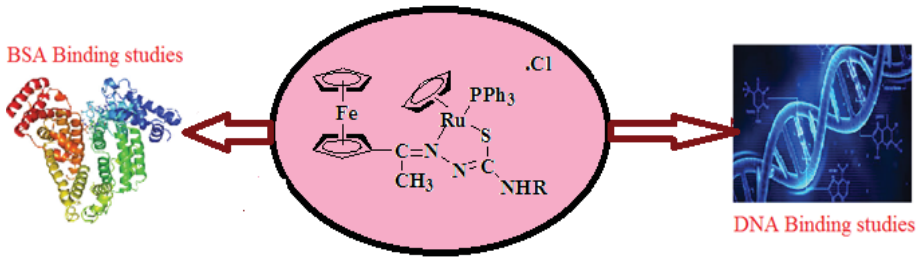
A series of four new hetero binuclear Ru(III)/Fe(II) complexes of acetylferrocene-4(*N*)-substituted thiosemicarbazones [AF-Rtsc] (where, R= H, CH_3, C_2H_5 and C_6H_5)have been synthesized and characterized by various spectral techniques like IR,UV-Vis, ^{1}H-NMR, EPR and HR-MS. The ligands coordinated to ruthenium metalby utilizing theirazomethine nitrogen and thiolate sulphur atoms. The binding interaction of the ligands and complexes were studied by taking calf-thymus DNA (CT-DNA) and bovine serum albumin (BSA)through absorption and emission titration methods. The complexes exhibited better binding affinity than their parent ligands. The interaction was found as intercalative binding with CT-DNA and static quenching mechanism was found when the complexes interacted with BSA.



Structural, spectral, physiochemical, computational studies and pharmacological screening of a new organic salt: 2, 6-Diaminopyridinium-2-nitrobenzoate

PP 106

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A new organic salt, 2,6-diaminopyridinium-2-nitrobenzoate (DAPNB) has been synthesized. The single crystals of DAPNB were harvested by the solution growth-slow evaporation method. ^{1}H and FT-IR spectral studies clearly show that the exact environment of protons and the functional groups present in the single crystal. The material was thermally stable up to 205°C. The suitability of this material for optical applications was assessed by optical absorption, transmittance and photoluminescence spectroscopic techniques. Natural bond orbital (NBO) analyses reveal the strength of intermolecular hydrogen bonding interactions in DAPNB. Molecular electrostatic potential analysis was performed to get additional information on the formation of hydrogen bonding interactions in DAPNB. Hirschfield analysis was performed to quantify the covalent and noncovalent interactions by using Gaussian 09 software by B3LYP method at 6-31G basis set level. Finally, DNA binding property of the title salt with calf thymus-DNA has been examined by electronic absorption and emission spectroscopic studies and the result shows that DAPNB could interact with calf thymus-DNA through electrostatic interaction and antioxidant study results reveal that DAPNB has good capacity for scavenging DPPH radical.

Ultrasound assisted synthesis and characterization of 3-methyl-2, 6-bis (p-methoxy phenyl) piperidin-4-one and its derivatives

PP 107

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Ultrasound irradiation differs from conventional energy sources (such as heat, light, or ionizing radiation) in time, pressure, and energy per molecule. The use of ultrasound waves in organic synthesis has attracted an increasing interest over the last years. Use of ultrasound waves as alternative source of energy is of great interest in the area of green and pharmaceutical chemistry. A series of two novel derivatives *N*-acetyl and *N*-chloroacetyl piperidin-4-one (**2**-**3**) are synthesized in good yield from the parent compound 3-methyl-2,6-bis(p-methoxy phenyl)piperidin-4-one(**1**). The derivatives are synthesis from acetyl chloride and chloroacetyl chloride in the presence of catalyst triethylamine and solvent benzene by using ultra-sonication as one of the green chemistry tools. Parent piperidin-4-one (**1**) and its *N*-acetyl and *N*-chloroacetyl derivatives(**2**-**3**) respectively have been characterized using IR, ^{1}H, ^{13}C,DEPT-135 & 2D NMR and mass spectral studies. The result of ultra-sonication methods gives minimum reaction time and maximum yield. All synthesized compounds are compared with ultra-sonication method and conventional method.

Reference:

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Biopolymer – SPIO tethered curcumin magnetic nano gel towards anticancer screening

PP 108

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According to WHO's recent report a whopping one Crore people have been diagnosed with cancer and around 70 % of them (Seven Million people / annum) have been reported to die annually due to this deadly disease. Though the conventional chemotherapy could combat this worst danger, it's been heavily suffered by several precincts such as severe toxicity, lack of targeted drug delivery, triggering multi-drug resistance, etc. In order to overcome these limitations and to achieve better results, there are several advancements in global medical research methodologies have been attempted over the several years. Choi et.al., reported Photodynamic therapy by conjugating photosensitizer with iron oxide as supramolecular assembly. Sulaimanet.al., reported on the synthesis and characterization of magnetic iron oxide through phytochemical means and explored the in-vitro free radical scavenging properties of the same against DPPH as model system for the evaluation of cytotoxicity and DNA cleavage of human breast cancer cell lines. Towards this, the presentation will cover the synthesis and characterization of SPIO embedded Curcumin as a novel systemin targeting carcinoma cell line.

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Synthesis of Ni(II) and Cu(II) 3-acetylcoumarin thiosemicarbazone complexes and CT-DNA binding studies

PP 109

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Reactions of $NiCl_2.6H_2O$ and $CuCl_2.6H_2O$ with 3-acetylcoumarin thiosemicarbazone and 3-acetylcoumarinphenylthiosemicarbazone resulted the new complexes(**1-4**).The new complexes were characterized by IR and UV spectroscopic techniques. From spectral studies it is concluded that the ligands coordinated as ONS tridentate monobasic, through thiolate sulphur, hydrazinic nitrogen and oxo oxygen atom of coumarin moiety. The electron transfer properties of the new complexes (1-4) were studied by cyclic voltammetry. Further, the complexes (1-4) were subjected to CT-DNA binding studies by using absorption, emission and electrochemical studies.

Synthesis, characterization and antiproliferative activity of dispiro pyrrolidines containing 2-thioxothiazolidin-4-one nucleus

PP 110

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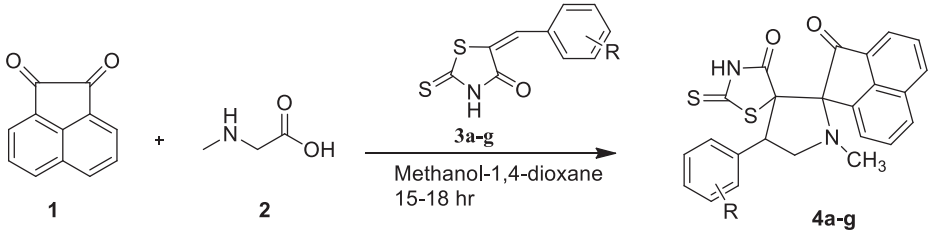
Seven dispiro pyrrolidines has been accomplished by [3+2] cycloaddition reaction from acenaphthenequinone and sarcosine with several dipolaro files, such as substituted 5-benzylidene-2-thioxothiazolidin-4-ones in methanol and 1,4-dioxane by conventional method. Further to characterized the synthesized compounds by IR, ^{1}H and ^{13}C NMR spectral data. The cytotoxic activity of the synthesized compounds was carried out by MTT assay. Among all the synthesized compounds, **4d** was found to be more potent with human cervical cancer line with an IC_{50} value of 5.5 µM.

Key words: Rhodanine, acenaphthenequinone, sarcosine, antiproliferative activity.



New pyridine based chemosensor for the detection of tryptophan

PP 111

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Amino acids are the basic building blocks of protein in our body, which play an essential role in adaptable body functions including protein synthesis. Among the natural alpha amino acids, tryptophan is majorly involved in multiple biotransformations in living organisms. Lack of tryptophan in human body causes metabolic disorder, Alzheimer disease, liver damage, nausea, blurred, edema, slow growth, dry month, hair depigmentation, lethargy, muscle and fat loss. Though there are several methods are available to detect tryptophan, they have several lacunas including high cost, stability of the sensor molecule etc. Herein, we have developed a new pyridine based fluorescent chemosensor which gives turn on signal after binding with tryptophan. This will be tested in different environment parameters in near future to create an impact in the biomedical field. All those results will be presented

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Synthesis, characterisation and biological study of pyrazolino and isoxazolo cycloocta[*B*]indole derivatives

PP 112

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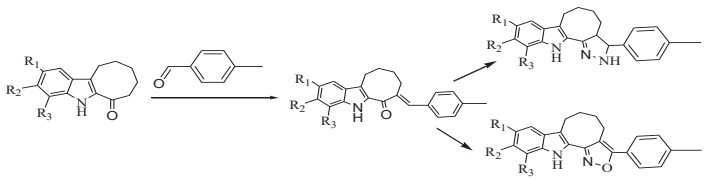
The cycloalkane[*b*]indole ring system is good; including the structurally complex mycotoxins[1] such as paxilline, paspaline, and yuehchukene[2]. An efficient route for the synthesis is attained by employing methyl-benzaldehyde to condense with a precursor cycloocta[*b*]indole derivative to give condensed product namely,2-(4'-methyl-benzylidene)-1-oxo-1,2,3,4,5,6-hexahydrocycloocta[*b*]indole **(3).** Using that further compounds were prepared namely, pyrazolinocycloocta[*b*]indole and isoxazolocycloocta[*b*]indole derivatives by allowing the condensed product to react with hydrazine hydrate and hydroxylamine hydrochloride, which results in 3-(4'-methyl-phenyl)-4,5,6,7-tetrahydro-2*H*-pyrazolino[4',5':7,8]cycloocta[*b*]indoles**(4)** and 3-(4'-methyl-phenyl)-4,5,6,7-tetrahydroisoxazolo[4',3':7,8]cycloocta[*b*]indoles **(5)** formation respectively. Physical properties and melting point are noted forthe resulting products and are characterised using FT-IR, NMR, and CHN analysis.Their biological activities[3] were studied against bacterial and fungal strainsusing disc diffusion method[4], which shows moderate activity.



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Photocatalytic degradation of methylene blue with pulse electrodeposited $CuInAlSe_2$ films

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PP 113

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$CuInAlSe_2$ films were deposited by the pulse electrodeposition technique at room temperature. The duty cycle was varied in the range of 6 – 50 %. Single phase chalcopyrite films were obtained. The grain size varied in the range of 10 nm – 18 nm with decrease of duty cycle. Band gap of the films increased from 2.27 eV to 2.40 eV with increase of duty cycle. Methylene blue dye degradation was studied with the films deposited at different duty cycle. Films deposited at 50 % duty cycle exhibited maximum photocatalytic degradation. The dye could be degraded upto 95 % in 60 min, The optimum conditions for maximum photocatalytic degradation was established, pH value of 11, dye loading of 20 mg/L and amount of photocatalyst of 50 mg/L was optimum. Reusability of the photocatalyst was tested by measuring the degradation of methylene for four consecutive cycles. A decrease if only 3 % was observed.

Hypothetical studies on hydrogen bonded liquid crystal mixture derived from mesogenic and non-mesogenic carboxylic acid

PP 114

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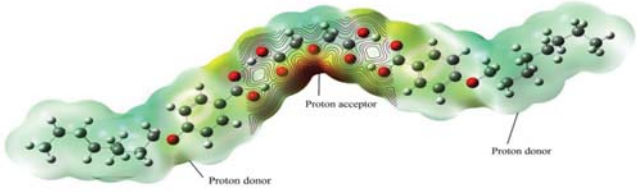
Hydrogen bonded liquid crystal (HBLC) mixture derived from diglycolic acid (DGA) and 4-n-octyloxybenzoic acid (8OBA) is optimized by B3LYP 6-311G basis set (d,p).Induced liquid crystal phases are confirmed by polarizing optical microscopy (POM).The formation of hydrogen bondingin LC is confirmed using the Fourier transform infrared (FT-IR) spectroscopy. The experimental FT- IR data is correlated with the theoretical data and validated. The O-H…O bond angle, bond length and electrostatic potential (ESP) has been investigated by DFT. Natural bond orbital (NBO) studies revealed the O-H…O stabilization energy in the present HBLC mixture. Also, lone pair (LP) to π* transition confirms the existence of intermolecular hydrogen bonding in the HBLC mixture. The band gap energy of DGA+8OBA HBLC mixture is calculated as 5.18eV which is more useful parameter to identify suitable HBLC materials for photonic application. Mulliken analysis shows the clear evidence of the charge distribution in different molecules.

Keywords: Hydrogen bond, FT-IR, POM, NBO and ESP.



Synthesis, spectral characterization and biological activities of some novel mannich bases of 1, 3, 5 – triazine substituted uracil derivatives with formaldehyde and piperazine

PP 115

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The compound 2,4-diamino-5-(2-carboxy phenyl)-6-(2-hydroxy phenyl)-1,3,5-triazine**1** is treated with uracil to yield 2-[4-Amino-2-(2-hydroxy-phenyl)-6-(2-oxo-2,3-dihydro-1H-pyrimidin-4-ylideneamino)-2H-[1,3,5]-triazin-1-yl]-benzoic acid **2**. The compound **2** is then subjected to reaction with formaldehyde and piperazine to furnish 2-[4-Amino-2-(2-hydroxy-phenyl)-6-(2-oxo-1-piperazin-1-ylmethyl-2,3-dihydro-1*H*-pyrimidin-4-ylideneamino)-2*H*-[1,3,5]triazin-1-yl]-benzoic acid**3**.The title compounds have been screened for their antimicrobial activity against different micro-organisms, which show better activity against gram positive and gram negative micro-organisms. The structure of the newly synthesized compounds has been established on the basis of physical properties, FT-IR, ^{1}H and ^{13}C NMR spectral data.

Synthesis, characterization and biological studies of new class of aminoacid based schiff base

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PP 116

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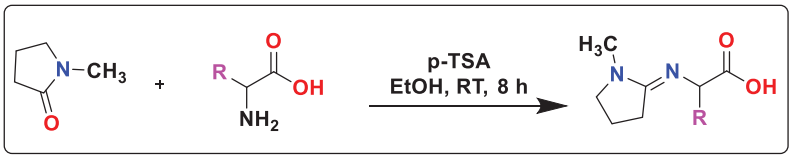
New class of Schiff base prepared from N-Methyl 2-pyrrolidone and various amino acids via transamination mechanism. We have employed *p*-toluene sulphonic acid as a suitable acid catalyst. The current work focused on the design, syntheses, and characterization of theSchiff base. The Schiff basecharacterized by IR Spectroscopy. In future work these compounds will be used as a ligand for complexation reaction. Further, the Schiff base will be captured by suitable metals for biological studies.

Key words: Schiff base, Transamination reaction, Biological studies, Metal complexe



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Modelling and fixed bed column adsorption of Ni(II) onto *citrus limetta*

PP 117

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The biochar (activated carbon) derived from *Citrus limetta* peel waste biomaterial, was tested for the removal of nickel (II) ions from aqueous solution. The fixed-bed column adsorption experiments were carried out to investigate the adsorption capacity of *Citrus limetta* peel biochar for the removal of Ni(II) from aqueous solution. The biochar (= CLPBC) characterization was accomplished using FTIR, SEM and EDAX techniques. The Effects of flow rate of aqueous solution (1-3 ml/min), bed height (10, 15, 20 cm), and initial Ni(II) concentration (50,75, 100 ppm) on the breakthrough characteristics were investigated. Three models used to analyze the column experimental data, and model parameters evaluated were used to fit the adsorption data: Modified response, Thomas, and Yoon-Nelson. The column data fitted well with the Thomas, Modified Dose and the Yoon-Nelson model. The results of the present study suggest that CLPBC can be used beneficially for nickel(II) removal from aqueous solution. All models were good and were found to yield a better fit and hence, these were used to predict the adsorption of Ni(II) ions in the fixed bed column. The CLPBC was shown to be a suitable adsorbent for adsorption, or removal, of Ni(II).

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Multicomponent one step synthesis of substituted benzo[*h*][1,6] naphthyridines

PP 118

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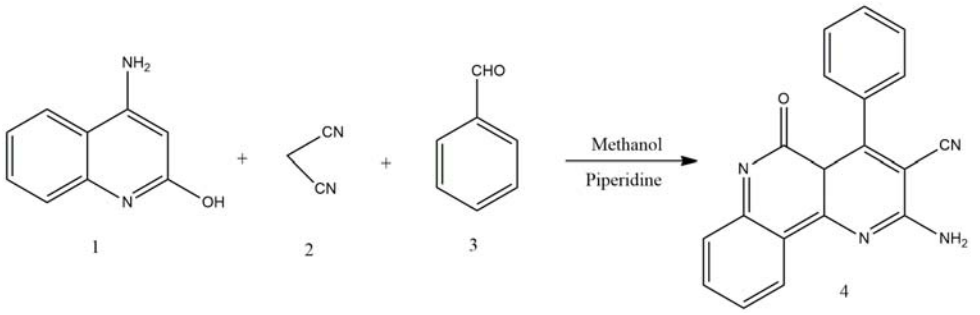
Heterocycles are the core unit for synthesizing pharma and agro products. They are mainly used as antitumor, antibiotic, anti-inflammatory, fungicidal and insecticidal agents. Pharmacological applications of these unit lead us to synthesise nitrogen contain hetero compounds. In our present work, we synthesized ring fused nitrogen compounds i.e, Naphthyridine derivatives, in multi component one pot method using versatile precursors 4-amino-2-hydoxy quinolone (1), malononitrile (2) and benzaldehyde(3) by conventional and non-conventional methods in the presence of base. The yield obtained are also compared.

Keywords: 2-amino-3-cyano benzo[h][1,6]naphthyridine, 1,6 Naphthyridine, Malononitrile, Microwave synthesis.



1 2 3 4

Synthesis, characterization and photoisomerization studies of azomethine based phosphorous containing flame retardant polyesters

PP 119

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In this study azomethine polyphosphonates were synthesized by solution polycondensation of phenyl phosphonic dichloride with various azomethine diols such as [4-(4-hydroxy phenyl)iminomethyl] phenol, [(4-(4-hydroxy-3-methoxy phenyl) iminomethyl)] phenol and [4-(4-hydroxy-3-ethoxy phenyl)iminomethyl] phenol using triethylamine catalyst at ambient temperature. The structure of the synthesized polymers was confirmed by using Fourier transform infrared and ^{1}H, ^{13}C, and ^{31}P nuclear magnetic resonance spectroscopic techniques. The thermal properties of the polymers were studied by thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC) under nitrogen atmosphere. The TGA data showed that the synthesized polyphosphonates produce high char yield at $600^{0}C$ due to the presence of phosphorous atom in the polymer chain and hence have good flame-retardant properties. One of the synthesized polyphosphonate was blended with commercial DGEBA resin in various weight percentage and cured with TETA. The polyphosphonates blended epoxy thermosets have tensile strength in the range of 5.286 – 40.53MPa, and the percentage of elongation at breaks of 4.36 – 18.55. It was found that incorporation of polyphosphonates into epoxy thermoset decreased the tensile strength from 40.53 MPa to 5.286MPa. Whereas the elongation at break value increased with increase in the weight of polyphosphonate. The influence of polyphosphonates on the flame retardancy of blended thermosets was examined by limiting oxygen index (LOI) and vertical burning (UL-94) tests and found that the polymer samples achieved an increased UL-94 rating and the LOI values were in the range of 23.5 - 26. The photoisomerization property was examined with UV spectroscopy and the polymer showed a rate of trans to cis isomerization ranging 10–30 s, whereas reverse process took around 110 min in solution. UV studies suggested that this material may be used in the field of rewritable applications.

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Employment of modified *Camellia sinensis* stem in anion eviction from aqueous matrices

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PP 120

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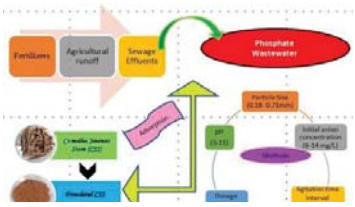
Phosphate ions from various sources viz., fertilizers, agricultural runoff and sewage wastewaters discharged into water bodies either directly or indirectly may cause eutrophication and death of aquatic plants. The present study investigates the utilization of tea plant stem C*amellia sinensis,* for the removal of phosphate anions. The chosen material, discarded as litter are collected from Balacola in Ooty and broken into small pieces, washed, dried and pulverized, sorted into different particle sizes(CSSD). Excess alkaline nature is neutralized with 0.1N H_2SO_4 (TCSSD). FTIR, SEM and EDAX characterization studies are carried out. Sorption efficiency is experimentally verified through Batch Equilibration method under varying operational adsorption parameters. Absorbance values are recorded using UV/VIS spectrophotometer. 98.7% phosphate removal is registered under fixed particle size 0.18mm, 200 mg dosage, 10 mg/L initial concentration, 9 mins contact time, pH 5 at room temperature. Validation using Langmuir and Freundlich isotherms, revealed Freundlich with a better linear fit. It is concluded that the selected material possesses excellent capability for the uptake of phosphate anions, extended to mitigation of domestic wastewaters in near future.

Key words: biomaterial, phosphate, batch process, adsorption, isotherms



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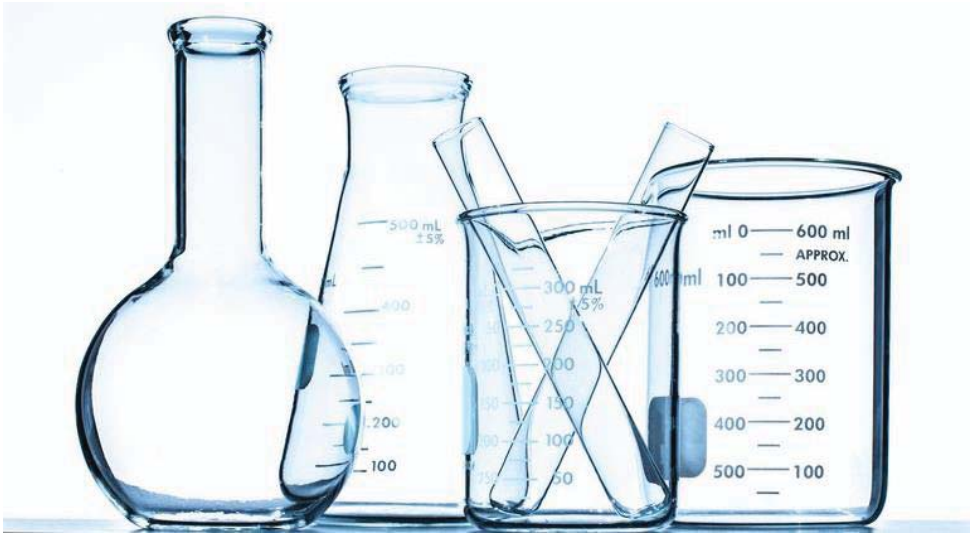

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