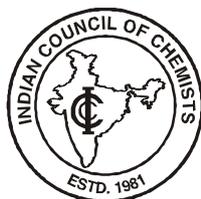


# INDIAN COUNCIL OF CHEMISTS



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**XXXVI  
ANNUAL CONFERENCE  
2017**

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**ABSTRACTS BOOK**

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School of Chemistry  
Andhra University  
Visakhapatnam-530003 (A.P.)

on  
**26<sup>th</sup> - 28<sup>th</sup> DECEMBER, 2017**

*Editor : Prof. R.K.S. Dhakarey*

## Welcome

Dear Fellow Researchers & Scientists

*On behalf of the Indian Council of Chemists, it is my pleasure and honour to welcome you all to the XXXVI Annual Conference of ICC from 26<sup>th</sup> - 28<sup>th</sup> December, 2017 at School of Chemistry, Andhra University, Visakhapatnam-530003 (A.P.).*

*The leading researchers and key opinion leaders in Chemistry have been invited to facilitate sessions and deliver lectures at XXXVI National Conference of ICC.*

*A series of scientific and educational activities have also been planned for delegates participating during the conference. There will be vast range of learning opportunities at invited talks, oral, poster presentations and symposium session. Participants can also look forward to expanding their network at various networking events such as conference lunch, dinner and cultural programme. Apart from the scientific programme, there are many tourist attractions in and around Visakhapatnam. You can enjoy there too.*

*Thank you for your participation.*

**Prof. R.K.S. Dhakarey**  
Secretary, ICC

## **PROVISIONAL PROGRAMME**

### **Tuesday, 26th December, 2017**

08:30 to 10:00 AM	Registration and Kit Distribution
10:00 to 01:00 PM	Inauguration, Award Ceremony and Keynote Address
01:00 to 02:00 PM	Lunch
02:00 to 02:30 PM	Sectional Presidents Address in respective sections
02:30 to 05:30 PM	Invited Lectures and Paper Presentations
05:30 to 07:00 PM	Poster Presentations
07:00 to 08:30 PM	Cultural Programmes
08:30 PM onwards	Dinner

### **Wednesday, 27th December, 2017**

09:00 to 01:00 PM	Symposium on Marine Chemistry (common to all delegates)
01:00 to 02:00 PM	Lunch
02:00 to 06:00 PM	Invited Lectures and Paper Presentations
06:00 to 07:00 PM	Poster Presentations
07:00 to 08:00 PM	ICC General Body Meeting (to be attended by fellows only)
08:00 PM onwards	Dinner

### **Thursday, 28th December, 2017**

09:00 to 01:00 PM	Invited Lectures and Paper Presentations
01:00 to 02:00 PM	Lunch
02:30 to 04:00 PM	Valedictory Function

**ADVISORY COMMITTEE**  
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**ANDHRA UNIVERSITY**  
**VISAKHAPATNAM-530003 (A.P.)**

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## **Instructions for the Preparation of Poster Presentation**

Your poster should be displayed as per the poster board number given in the abstract book. Posters will be displayed during the Poster Sessions and must be mounted from the start of sessions and removed upon conclusion of sessions on the scheduled day. Authors are requested to stand next to their poster boards during the Poster Sessions.

- 1 You should be printing and bringing your poster to the conference.
- 1 The dimensions of poster **should NOT exceed 90 cm wide × 120 cm high.**
- 1 Please prepare your poster to fit the dimensions specified. It is recommended that poster be prepared on one sheet. Alternatively presenters may display their material on several smaller sheets.
- 1 Allocate the top of the poster for the title and authors as stated on the submitted abstract.
- 1 The text, illustrations, etc. should be bold enough to be read from a distance of two meters.
- 1 Double sided tape and technical equipment will be available for the mounting of posters. Staff will also be available to assist you.
- 1 DO NOT write or paint on the poster boards. DO NOT use nails, push pins, screws, or any tools that will puncture the poster boards.
- 1 Please use the board that displays the same number assigned to you.

For any help kindly contact the concerned **Sectional President** or **Prof. Ajay Taneja**, Joint Secretary-ICC.

## **Acknowledgements**

*The Indian Council of Chemists is going to hold its XXXVI Annual Conference at A.P. on 26<sup>th</sup> - 28<sup>th</sup> December, 2017 and the abstract book containing the abstracts of papers selected for presentation in the Conference is in your hands. The Council justifiably feels proud of its achievements during the past 36 years of its existence.*

*The Council is grateful to Prof. R. Murali Krishna, Prof. P. Vani, Dr. P. Shyamala, Dr. K. Basavaiah, Dr. V. Siddaiah, Staff Members and Students of School of Chemistry, Andhra University, Visakhapatnam for their utmost cooperation in organizing the Conference.*

*The Council on its own behalf and on behalf of the Organizing Committee thanks all those who have helped in preparing and publishing this Abstract Book. The assistance given by Dr. C.P. Singh, Dr. Manoj Rawat, Dr. S.C. Goyal and Prof. Ajay Taneja is gratefully acknowledged.*

*Some of the abstracts have been edited by Sectional Presidents, due to paucity of funds and also on account of pressing limitations on the space available, a few others have also been condensed and as such some inadvertant omissions might have occurred for which ICC offers its apologies.*

**Prof. R.K.S. Dhakarey**

*Editor*

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## **ABBREVIATIONS**

AIL	- Analytical Invited Lecture
AO	- Analytical Oral
AP	- Analytical Poster
IIL	- Inorganic Invited Lecture
IO	- Inorganic Oral
IP	- Inorganic Poster
OIL	- Organic Invited Lecture
OO	- Organic Oral
OP	- Organic Poster
PCIL	- Pharmaceutical Invited Lecture
PCO	- Pharmaceutical Oral
PCP	- Pharmaceutical Poster
PIL	- Physical Invited Lecture
PO	- Physical Oral
PP	- Physical Poster
CYSA	- Contestent for Young Scientist Award
SMC	- Symposium

## **Life Time Achievement Awardee Lecture**

### **KAZA'S Carbons- Tools of Defluoridation of Drinking (Potable) Water**

**Kaza Somasekhara Rao**

*Acharya Nagarjuna University P.G. Campus, Nuzvid, A.P.*

*E-mail : sr\_kaza1947@yahoo.com*

Commercially available activated carbon is used in medicine, dyeing industry, pharmaceutical industry and as adsorbent in industrial sector. The cost depends upon purity, quality and physical form. Our group started intensive studies on Palmyra male Inflorescence (which is waste from Palmyra tree in fields) with a focus around GIGO (Garbage [or bio-waste] in gold out) philosophy and practices of biotechnologists. With the progressive extensive utility in diverse application areas, this group of materials have become popular as KAZA'S Carbons (KAZACs). This type of carbon first time I had prepared, i.e., I had invented and named in the name of myself, these carbons that are prepared hereafter were as KAZA'S carbons. Critical fluoride content and fluorosis effect on Human Health presented. Laboratory method and large scale (House hold) method for removal of fluoride in drinking water using KAZA's carbons will be discussed.

**To be presented in  
Environmental & Analytical  
Chemistry Section**

**Prof. W. U. Malik Memorial Awardee Lecture**

**Pharmacological Applications of Coumarins:  
an Approach to Natural Products**

**Kallappa. M. Hosamani**

*Professor of Organic Chemistry, Karnatak University, Dharwad,  
Karnataka - 580003*

Interest in the biological and industrial potentialities of heterocyclic moieties containing bioactive oxygen heterocycle has resulted in the development of various synthetic procedures for the introduction of potent functional groups in the novel coumarin nucleus. Because of significant potential therapeutic properties of such heterocycles in medicinal chemistry has resulted the prominent place and generated much interest in the synthesis of new classes of novel heterocyclic systems such as coumarin derivatives, thereby to explore their pharmacological properties. Thus, coumarins occupy an important place in the realm of natural products and synthetic organic chemistry. Hence, coumarins comprise a group of natural compounds found in a variety of plant sources (obtained from Tonka beans by Vogel in the year 1820) in the form of benzopyrene derivatives.

Coumarins are the elite class of oxygen heterocycles having wide applications in medicinal chemistry, being known as anti-cancer, anti-oxidants, anti-allergic, anti-thrombotic, anti-viral, anti-tuberculosis, anti-mutagenic, anti-HIV, analgesic, hepatoprotective, enzymatic inhibitors, vasorelaxants, mild adrenergic activities, CNS depressant, antimicrobial agents, fish toxin and bactericidal agents. In addition to biological activities they are used as additives to food and cosmetics<sup>5</sup> and optical brightening agents. Thus, a series of coumarin derivatives were selectively prepared under microwave irradiation as well as by conventional methods. These compounds have been characterized by spectroscopic studies and by the X-ray diffraction technique. Based on the computational study, some potent compounds have been screened for their anticancer activity, in-vitro antitubercular activity, cytotoxicity and DNA cleavage study.

**To be presented in  
Pharma & Bio-Chemistry Section**

**Prof. S.P. Hiremath Awardee Lecture**

**Diversity Oriented Synthetic Strategies  
for the Carbazole and Carboline  
Derivatives**

**Mandava V. Basaveswara Rao**

*Department of Chemistry, Krishna University, Machilipatnam, A.P.  
E-mail : vbrmandava@yahoo.com, professormandava@gmail.com*

Organic synthesis methods that allow rapid access to large number of structural arrays is growing rapidly, which served as a new driving force for advancement of synthetic organic chemistry. In order to synthesize large number of molecules with high level of diversity and complexity, organic chemists are looking for exploring new methods to design and evolve new molecules, strategies for new molecules leading to new source of diversity and improving the quality of compound libraries. Efforts have been directed to diverse new flexible modular methodologies that will allow many structurally diverse compounds to be prepared efficiently in high yields and in excellent purity and will work on wide variety of substrates and be compatible with wide range of functional groups. Schriber has called it as diversity oriented synthesis<sup>1</sup>.

One of the richest source of diversity in drug discovery are small molecule heterocycles, which in addition to exhibiting biological activity, also serve as rapid scaffolds for further display of broad range of functionalities. For several years Prof. M.V. Basaveswara Rao and his research group has been engaged in design and development of new efficient methodologies for a wide variety of heterocycles, displaying a range of skeletal and functional group diversity. The biological properties of heterocycles in general make them one of the prime interests of the pharmaceutical industry, biotechnology

industry and as well as for opto-electronic industry. we have initiated work on the synthesis of heterocycles with an aim to understand their properties towards bioactivity like, antibacterial, anti-malarial, antifungal, anti cancer, free radical scavenger, etc. and also towards Non Linear Optic materials. We have synthesized indole skeletons initially and utilized them for making other heterocycles, like carbazoles and carbolines and their fused derivatives.

**To be presented in  
Pharma & Bio-Chemistry Section**

**Prof. Kaza Somashekhar Rao Awardee Lecture  
Women Scientist Award**

**Antimicrobial, Spectral, Fluorescence and  
Thermal studies of Co(II) and Ni(II)  
Complexes of Schiff base derived from  
2-chloro-5-nitrobenzaldehyde with 4-amino-  
5-mercapto-3-propyl-1,2,4-triazole**

**Kiran Singh**

*Department of Chemistry, Kurukshetra University, Kurukshetra  
E-mail : kiransinghkuk@yahoo.co.in*

The cobalt(II) and nickel(II) metal complexes have been synthesized from the Schiff base derived from 4-amino-5-mercapto-3-propyl-1,2,4-triazole with 2-chloro-5-nitrobenzaldehyde. The Schiff base and its metal complexes were further characterized by various physicochemical techniques (IR, <sup>1</sup>H-NMR, Visible, Fluorescence, thermal analysis, elemental analysis and magnetic moment measurements. IR spectra and thermal studies supported the coordinated water molecules in metal complexes. On the basis of these studies octahedral geometry for Co(II) and Ni(II) complexes have been proposed. Further, synthesized complexes have been checked for their biological properties against the bacteria (*E. coli*, *P. aeruginosa*, *B. subtilis* and *S. aureus*) and two fungi (*S. cerevisiae* and *C. albicans*).

**To be presented in the  
Inorganic Chemistry Section**

**Dr. Arvind Kumar Memorial Awardee Lecture**

**Tunable Hierarchical Morphological Metal  
Oxide Nanostructures for Sunlight Driven  
Environmental Remediation**

**Parag V. Adhyapak\***

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Hierarchical nanostructured functional metal oxide semiconductors are of prime importance due to their diversified application areas such as photocatalysis, optoelectronics, microelectronics, sensors, renewable energy, LED's etc. Among these various applications, photocatalysis is the important application area from viewpoint of environmental remediation where hierarchical nano-sized metal oxides are effectively employed preferably due to their inherent photo-stability and non-toxicity. However, to realize their industrial-scale application, the key challenge is the tunable -morphology oriented large scale synthesis using facile yet scalable method. Our efforts in this direction are presented by citing the study of few semiconducting metal oxides viz. ZnO, CuO, Sn3O4 etc. We have explored various capping agents under different experimental conditions to generate distinctive nanostructures with hierarchical morphologies such as nano-rods, nanoflakes, nanoflowers, burger/donut-like, cabbage-like structures, sea urchins, microballs etc. Various methods such as chemical precipitation, hydrothermal, sonochemical etc. were employed to generate these nanostructures. It has been demonstrated that the structural, morphological and optical properties of the samples can be perfected by fine-tuning the synthesis protocol. For instance, spherical and vesicular nanomorphs of CuO were formed by chemical precipitation method whereas,

platelet type and sheet-like CuO nanomorphs were obtained by hydrothermal method etc. The solar energy driven photocatalytic performance of the resultant nanostructures has been evaluated for degradation of the representative heteropolyaromatic pollutant dyes viz. Methylene Blue (MB), Rhodamine B, Methyl orange etc. In nutshell, ecofriendly metal oxides nanostructures are the promising candidates for futuristic environmental remediation.

**To be presented in  
Physical Chemistry Section**

**Prof. S. T. Nandibewoor Awardee Lecture**

**Mixed Sulfur Donor Ligand Complexes of Antimony(III): Synthesis, Structural investigation, Characterization, Power XRD, FAB<sup>+</sup> Mass, Supramolecular association, Single Crystal X-ray, Thermal (TGA, DTA, DSC) and Antimicrobial Activities**

**H.P.S. Chauhan**

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The 1,1 dithiolato, 1,2 dithiolato and other sulfur donor ligands and their antimony(III) complexes have found their applications in a number of ways like in analytical methods, in production of petroleum derivatives, for regeneration of cracking catalysts, lubricants oil additives and as antiviral agents, antidotes, antimicrobial as well as antitumor drugs. These complexes have wide range of structural possibilities: Ligands can behave as monodentate, bidentate (bridging and chelating) and bimetallic- triconnective and small ligand bite, substituents organic groups as well as antimony(III) has a stereochemically active lone pair of electrons. Polymeric supramolecular assemblies also play important role in deciding the geometry of the molecules.

In view of the above antimony(III) compounds with sulfur donor ligands have been synthesized by the reactions of antimony(III) precursors with 1,1 dithiolato, 1,2 dithiolato and other sulfur donor ligands, in different suitable molar ratios in anhydrous organic solvents with different sets of yellow solids or semisolids are soluble common organic solvents. These compounds have been characterized by physicochemical, spectral [UV-Vis, FTIR, Far IR, NMR (<sup>1</sup>H and <sup>13</sup>C)], Power XRD, FAB<sup>+</sup> Mass and Thermal (TGA, DTA and DSC) studies. Thermal studies have been carried out in inert atmosphere and the last thermal decomposition product was formed to be pure Sb<sub>2</sub>S<sub>3</sub> which is used in a number of ways.

The single crystal studies of *tris*(*N,N'*-dimethyl-dithiocarbamato-*S,S'*) antimony(III) found to be a dimer with Sb...S and C-H...S interaction as well as chloro*bis*(*N,N'*-dimethyldithiocarbamato-*S,S'*) antimony(III) also found it to be a dimer with C-H...Cl interaction as in supramolecular structure.

Some of these compounds have been screened in vitro against four human pathogenic bacterial species, two Gram-positive [*Staphylococcus aureus* (ATCC 9144) (G+) and *Bacillus subtilis* (ATCC 6051) (G+)] and two Gram-negative [*Escherichia coli* (ATCC 9637) (G-) and *Pseudomonas aeruginosa* (ATCC 25619) (G-)] and two fungal species [*Aspergillus niger* (ATCC 9029) and *Penicillium chrysogenum* (ATCC 10106)].

**To be presented in  
Inorganic Chemistry Section**

**Symposium on  
"Recent Developments in Understanding  
Chemistry of Marine Environment"**

**Chairman Remarks**

**P. Shyamala**

*School of Chemistry, Andhra University, Visakhapatnam-530003 (A.P.)*

## **SMC-IL-01 : Chemical Exploits of the Oceanic Black-Box**

**Nittala S. Sarma**

*Department of Physical and Nuclear Chemistry & Chemical Oceanography,  
Andhra University, Visakhapatnam – 530 003  
E-mail : nssarma@rediffmail.com*

The fundamental contributions of Chemistry in understanding the fascinating problems in Ocean science will be presented.

The birth of the subject of Oceanography followed the voluminous data and samples collected during the HMS Challenger Expedition (1872 – 1876). The expedition team and the investigations were essentially biological and physical (including geological), and only one chemist James Buchanan was there on board. In the early days, chemical analyses required in different disciplines were performed by non-experts. Determination of sea salts through titration of chloride elevated Robert Boyle of the Boyle's law fame to the status of father of chemical oceanography. The quantification of macronutrients led the biologist Alfred Redfield to postulate his famous Redfield Ratio of nutrient elements. Developments in seawater chemical equilibria and elemental speciation gave fundamental insights into the oceanic processes e.g., authigenesis, sediment accumulation, red-ox excursions, carbon burial, hydrothermal inputs and gas exchange.

The residence time concept, chemical flux estimations and biogeochemical cycling of elements especially N, P, Si, C, Fe, Mn, S and gases paved the way for understanding and assessing the role of oceans in climate modulation due to anthropogenic inputs of CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O and other trace gases. Climate change is a hotly debated topic now.

The arrival of Harold Urey of deuterium fame and a Noble Laureate in chemistry marked a beginning of the measurement and over-arching application of isotopes in different phases of the ocean – water, precipitates, particles, organisms, sediments, fossils and rocks for understanding the biology, geology and physics of the ocean. A new discipline paleoceanography evolved that helped track the past events and quantify their impact. Isotope geochronology is fundamental to any sediment, rock or ice sheet study, nowadays.

Urey's students Cesare Emiliani and Harmon Craig took the ideas further. Emiliani is considered as the father of the marine isotope stratigraphy, an area that enanciated the concept of the marine isotope stages and showed that the cycling of global climate is in sync with the Milankovich cycles, attributed to the Earth's orbital changes.

Craig discovered hydrothermal vents and led the GEOSECS program which made fundamental contributions in the chemistry of the sea. The thermohaline oceanic circulation in the form of the global conveyor belt was postulated by Wallace Broecker based on the measurement of radiocarbon. The radiocarbon's measurement was also applied by Steeman-Nielsen to measure biological productivity precisely and this led John Ryther to synthesise data to derive global productivity pattern and relate it to fish production.

One of the most famous experiments of the 20<sup>th</sup> century was the Miller-Urey experiment which showed that complex organic compounds, including amino acids, could be generated and in large quantities by abiotic synthesis from H<sub>2</sub>O, CH<sub>4</sub>, NH<sub>3</sub> and H<sub>2</sub> under anoxic condition, an environment that mimicked that of the primitive Earth.

The sea is considered as the last frontier yet of proven promise for the development of drugs that can cure the dreaded diseases. Chemists teamed up with biologists and pharmacologists to introduce anticancer drugs yondelis and aplidin of ascidians and the pain killer prialt of snails. Andhra University made pioneering contributions in this area.

Biomarkers is a fascinating area that works on chemical clues to the past - sources and their timing as well as the environmental variables acting on the fossils. Petroporphyrins found in petroleum settled the dilemma regarding the mechanism of petroleum formation and favoured the organic over the inorganic hypothesis. Long chain alkenones of prymnesiophyte algae, found in marine sediments revealed the sea surface temperature, free from interferences unlike the oxygen isotope method. More recently, tetra ether index (TEX<sub>86</sub>) is used for the same purpose for better precision. Alkanes have source specificity, and recently, we showed that the coastal marine sediments preserve information of the changing terrestrial discharge through the last couple of centuries. We also showed for the first time that humic matter, soluble and insoluble, forms from lipid matter synthesized chemoautotrophically in hydrothermal regions with implications for ocean productivity and carbon burial respectively.

The few glimpses referred above explain why ocean chemistry currently plays a central role amongst ocean science disciplines. Chemistry in general connects with all scientific pursuits and the new discipline of biogeochemistry is born which has been attracting utmost attention of scientists, general public and administrators equally.

## **SMC-IL-02 : Are Indian Coastal Seas Really Polluted? – Myths and Effects from Western India**

**G. V. M. Gupta**

*Centre for Marine Living Resources and Ecology, Ministry of Earth Sciences,  
Cochin*

The development of oxygen-deficient zones along the coastal seas and their impacts on marine life forms an important issue as it has been largely attributed to the marine pollution through terrestrial activities. The coastal anoxia not only adversely affects the marine ecosystem especially fishery production/distribution causing a wide-spread social issue but also multi-fold enhances the greenhouse gases fluxes contributing to global warming. Being an agriculturally driven developing country, increasing fertilizer consumption and their runoff along with other anthropogenic discharges through estuaries have been projected earlier as root-cause for intensification of coastal oxygen-deficiency (anoxia) along the western India during southwest monsoon (June-September). However, the modern findings do not endorse human activities as significantly responsible for coastal anoxia but found it augmented primarily as a 'natural origin' of oxygen depleted offshore waters advection onto the shelf through a process called upwelling over which the effects of terrestrial nutrients supply acts in unison. Despite large-scale developmental activities, the impact of anthropogenic discharges is seen confined mostly to the nearshore regions (few kilometers away from the coast) only. This is due to the efficient turnover of nitrogen in the Cochin backwaters, as well as in most of the tropical monsoonal estuaries of India, before reaching coastal sea. The unaltered present dissolved oxygen concentrations compared to five decades ago over the southwestern shelf chiefly supports insignificant anthropogenic effect. Nevertheless, the degree of coastal anoxia due to natural origin from offshore is severe along the Karnataka and Goa coasts and fishes avoid these regions and concentrate over the bordering zones along Kerala and Maharashtra coasts, thereby influencing their migration and stocks distribution across the coastal states of western India. The acute oxygen deficiency has also adversely affected the marine nitrogen and carbon cycles and enhanced the greenhouse gases production.

## **SMC-IL-03 : Triple isotopic composition of oxygen in nitrate to identify atmospheric borne nitrogen in the seawater**

**V. V. S. S. Sarma**

*CSIR-National Institute of Oceanography, Regional Center, 176 Lawsons Bay Colony, Visakhapatnam - 530 017*

Nitrate is an important compound in healthy natural, agricultural, urban and marine ecosystems but it can have negative impacts at elevated levels. Excess nitrate can lead to eutrophication in the aquatic environments, such as river, estuary, and coastal waters, which can result in hypoxia and the destruction of fisheries and other aquatic life. Nitrate is a major component of acid rain and harmful, respirable particulate matter in urban areas. Therefore, understanding the sources of nitrate is important from ecological, economic, and human health perspectives. The atmospheric pollutants over the Bay of Bengal are rapidly increasing, than elsewhere in the world, due to extensive industrial growth. The anthropogenic processes release nitrogen oxides ( $\text{NO}_x$ ) to the atmosphere through fossil fuel combustion and its oxidation by photochemical radical chemistry forms nitrate in the atmosphere.

The oxygen has three isotopes, namely 16, 17 and 18O and they fractionate in mass dependent (MDF) manner in the troposphere whereas mass-independent fractionation (MIF) occurs in the stratosphere. Due to significant exchange between stratosphere and troposphere, significant amount of stratospheric MIF oxygen remains in the troposphere. When this MIF oxygen is reacted with  $\text{NO}_x$  through photochemical reactions, the MIF signature is transferred to nitrate. The measurement of triple oxygen isotopes of nitrate and oxygen-17 anomaly ( $^{17}\text{D}$ ) is a good tracer to identify atmospheric nitrate in the marine waters. The  $^{17}\text{D}$  anomaly of organic fertilizers ranged from 18 and 21 per mil whereas commercial fertilizers varied between -0.15 and -0.25 per mil. The  $^{17}\text{D}$  anomaly in the atmospheric nitrate varied from 5 to 10 per mil. Based on the distinct characteristics of the  $^{17}\text{D}$  anomaly, it is possible to separate their sources in the seawater using  $^{17}\text{D}$  anomaly of seawater nitrate. It was noticed that 20-40% of surface water nitrate in the coastal Bay of Bengal is contributed by atmospheric borne nitrate and suggests that atmospheric deposition of pollutants have significant impact on coastal ecosystem.

## **SMC-IL-04 : Monitoring Seawater Quality and Restoration of Coastal System**

**P. Madeswaran**

*Scientist F, Integrated Coastal and Marine Management Project, Chennai*

Coastal regions are playing a vital role in development of any maritime nation, as it provides huge economical support towards urbanization, industrialization, transportation, tourism, etc. Consequently, due to discharge of domestic waste and industrial effluents, the coastal seawater remains the most disturbed ecosystem all over the world. The developmental activities along Indian coast are constantly growing with rapid speed; mainly agricultural activities, urbanisation, industries, construction of ports and harbours, etc. The rapid developmental activities along the coastal areas prompted the Ministry of Earth Sciences (MoES), erstwhile called, "Department of Ocean Development (DOD)" for implementing a nationally coordinated Research and Development programme on, "Coastal Ocean Monitoring and Prediction System (COMAPS), since 1990, to assess the status of seawater quality, whether these anthropogenic activities make any adverse impact to the coastal system and its biota. During XII Plan period, this programme has been renamed as, "Seawater Quality Monitoring (SWQM)". Presently, the SWQM is being coordinated by "Integrated Coastal Marine Area Management - Project Directorate (ICMAM-PD), an attached office of MoES, Chennai. The primary objective of SWQM is to monitor seawater quality systematically at selected locations along Indian coast. Based on the two and a-half decadal observations, the concentrations of dissolved inorganic nitrogen (DIN) and dissolved inorganic phosphorus (DIP) were found to be high in all the sampling locations. Since, the anthropogenic pressures differ from each sampling sites, spatial variations are much stronger than the temporal variations. Discharge of untreated sewage was found to be a major threat to the Indian coastal waters, as it brings higher organic load and leads to the higher bacterial remineralization processes, which ultimately triggers release of inorganic nutrients into the water column. Overall, the intra-annual variation in the water quality was found less when compared to the inter-annual or the long-term changes. The upward trends of all the measured nutrients, over the years in most of the locations are of major concern, as this will increase the incidences of eutrophication, fuelling algal blooms causing increasing anoxia and hypoxia in the coastal waters. Having understood that our seawater is getting deteriorated, mainly due to discharge of untreated sewage, the Government have initiated actions for restoration of coastal systems.

## **ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION**

### **Sectional President's Address**

#### **Flame Retardant Technology : Designing the Synthesis of Polymer-clay Nanocomposite Flame Retardant**

**Prafulla Kumar Sahoo**

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Fire Protection Technology requires the basic knowledge on Fire Science. Fire Science deals with the four basic components of a fire, known as 'Fire Tetrahedron', i.e., Fuel, Source of Ignition, Oxygen and Combustion (chemical chain reaction). Fire develops and spreads widely by the presence of combustible & flammable materials. Combustible material has a flash point of 100 F or above, whereas flammable material has a flash point below 100 F (NFPA 96).

One of the aspects of Fire Protection Technology involves the use of fire retardants. Therefore, we are interested in designing the synthesis of polymer-clay nanocomposite fire retardants. The present paper/work depicts the significant outcome in the development of different polymer nanocomposites via the application of nanotechnology and their application as fire retardants. The formation of the polymer nanocomposite was confirmed by infrared spectra (IR). Furthermore, as evidenced by transmission electron microscopy (TEM), the composite so obtained was found to have nanoscale structure. X-ray diffraction (XRD) was used to characterize the nanoscale dispersion of the layer silicate and useful for measurement of d-spacing in interlayer system. It was found from thermogravimetric analysis that the nanocomposites had more thermal stability as compared to the virgin polymer due to intercalation. Burning test of the nanocomposites performance exhibited a flame retardant property, which was also verified from cone calorimeter analysis. For its commercialization, the ecological friendly nature was studied via biodegradation and was found to have better biodegradability than the virgin polymer.

## **AIL-01 : A Study on Effects of Fog on Aerosol Chemistry**

**Pratima Gupta, Rohini Singh and Ranjit Kumar\***

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Atmospheric aerosol carries various ionic species which are detrimental to the human health and ecosystems. The ionic species such as ammonia, nitrate, and sulfate in the aerosol can change the chemical properties of the aerosols and may also influence cloud formation, visibility, acidification of the aerosols and climate change. This paper deals with measurements of aerosols and their chemical properties at Agra in the Indo-Gangetic plain during winter season. The measurements were performed during the foggy and non-foggy conditions, separately. The mean SPM load for the entire campaign period at Agra was  $441.2 \mu\text{g m}^{-3}$  and it ranged between  $60.47 \mu\text{g m}^{-3}$  and  $1004.6 \mu\text{g m}^{-3}$ . Mean TSP value at Agra is higher than the NAAQS (National Ambient Air Quality Standards) value for residential areas. SPM load was higher during initial foggy days and lower during post foggy days. Higher value during initial foggy days may be probably due to decrease in the height of boundary layer and temperature inversion so suspended particulates gets trapped while lower value during post foggy days may be due to scavenging by fog. The aerosol chemical analysis revealed that  $\text{NH}_4^+$  concentration is highest followed by  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{Cl}^-$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Mg}^{2+}$  and  $\text{F}^-$ . The highest concentration of  $\text{NH}_4^+$  at present site may be due to nearby cattle yard, and frequent use of fertilizer in the agriculture field. The concentration of  $\text{Ca}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Mg}^{2+}$ ,  $\text{Cl}^-$  and  $\text{F}^-$  were higher during the pre-foggy days while the concentration of  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$  and  $\text{NH}_4^+$  were higher during post foggy days. The fog influences the removal of the pollutants from the atmosphere and hence, alters the aerosol chemistry.

## **AIL-02 : First Assessment of Heavy Metals Contamination in Road Dust and Roadside Soil of Suva City, Fiji**

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Studies have claimed the road dust and the roadside soil as potential banks of pollutants generally in urban areas. Thus, quantifying the concentrations of the heavy metals in urban area is a prerequisite for assessing pollution and their health effects. Hence,

this study reports the concentration of the heavy metals such as Cd, Co, Cr, Ni, Cu, Pb, Zn and Fe in the road dust and the roadside soil of Suva city. The samples were collected at eighteen different locations around the Suva city with potential traffic influence and analysed. The respective heavy metals concentration in the road dust and the roadside soil samples of Suva city were: Cd (3.7 and 3.1 mg/kg), Co (35.0 and 33.2 mg/kg), Cr (40.0 and 34.0 mg/kg), Ni (54.3 and 32.4 mg/kg), Cu (172.3 and 265.7 mg/kg), Pb (71.0 and 59.3 mg/kg), Zn (685.0 and 507.0mg/kg) and Fe (41,010.4 and 39,525.5 mg/kg), and showed the decreasing order as Fe>Zn>Cu>Pb>Ni>Cr>Co>Cd and Fe>Zn>Cu>Pb>Cr>Co>Ni>Cd for the road dust and the roadside soil, respectively. Furthermore, the mean values of the heavy metals surpassed their normal concentrations which confirmed anthropogenic influence while the concentrations of Zn, Cu and Cd in the road dust and the roadside soil of Suva exceeded their permissible limits. The geo-accumulation index ( $I_{geo}$ ) assessment of Suva city road dust indicated a non-polluted to moderate pollution by Cr, Ni, Cu and Pb while moderate pollution by Zn. The  $I_{geo}$  assessment of the roadside soil showed moderately polluted by Cu and Zn but no pollution due to rest of the studied heavy metals. Overall, the study indicated that the sampling locations at an industrial site of Suva city is highly predominated with almost all the studied heavy metals and is a concern to the general public who live and work within the vicinity of Walu Bay industrial area.

### **AIL-03 : Catalytic Hydrocracking of Biomass Derived High FFA Vegetable Oils to Green Hydrocarbons**

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Multiple concerns over fossil derived liquid fuels such as, vertical ascending of crude oil prices, diminishing oil reserves, unstable market and the detrimental environmental concerns linked with its exploration and use have compelled the researcher to search for sustainable green fuels and chemicals in the recent years. In this regard, fuels derived from the lipid fractions of biomass are considered as a feasible alternative for carbon neutral substitution of fossil fuels in industrial and transport sectors.

Mesua ferrea L. and Jatropha curcas, the two wild non edible plants, containing high free fatty acid (FFA) were catalytically hydro cracked using biomass derived heterogeneous catalysts viz. Musa

balbisiana Colla underground stem (MBCUS) nanomaterial and biomass based thermal power plant fly ash (BBTPFS). Reactions were carried out in a batch mode in a bench scale reactor at 400 °C under variable initial H<sub>2</sub> pressure (1-75 bar) for 1-4 h using 1-5 wt. % catalysts loading.

Our results confirm that the reaction network consisted of multiple pathways leading to a product mixture rich in hydrocarbons, non-polar oxygenates and organic acids commonly known as biocrude. Decarboxylation, hydrolysis, hydrocracking and thermocatalytic cracking appeared to be the dominating reactions subsequently leading to the production of hydrocarbon mixture of chain length C8-C19.

The resultant biocrude was fractionated into fractions within the boiling range 35-140 °C, 140-180 °C, 180-370 °C and 370-482 °C as per ASTM D2892 and ASTM D5236 specifications. Further, the recovery in each fraction was directly affected by biocrude quality which in-turn was dependent catalyst properties and reaction conditions. The reaction network also varied significantly with respect to reaction atmosphere and as well as for the two catalysts which directly affected the yield and quality of product (higher heating value, acidity index, liquid distillate recovery, overall efficiency in IC engine and reduction of emission profile).

## **AIL-04 : Recent Developments in Advanced Materials for CO<sub>2</sub> Uptake : A Solution to Reduce the Global Warming**

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Ever increasing scientific evidence underline the fact that CO<sub>2</sub> emission from fossil fuel is leading to global warming and climate change. Hence selective removal of CO<sub>2</sub> from the gaseous mixture is of utmost importance for protecting the environment. Large dependence of world population on fossil fuels will still remain to be 65% by 2050. Copenhagen accord has laid down that the global temperature increase be limited to 2°C above the pre-industrial level by 2100. According to International Energy Agency (IEA), Carbon capture and sequestration (or storage)—known as CCS—is a physical process that involves capturing man made carbon dioxide (CO<sub>2</sub>) at its source and storing it before its release to the atmosphere. Among the number of technologies available for CO<sub>2</sub> capture using various porous metal-organic frameworks, zeolitic imidazolate frameworks (ZIFs) with close resemblance to metal-organic frameworks have attracted the

attention of researchers as an alternative to other microporous materials because of their promising properties such as large surface area, facile synthesis, and controllable pore size.

### **AIL-05 : Synthesis, Characterization of Nano Materials and their Application in Removal of Organic Pollutants**

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Nanomaterials have been synthesized by several methods such as bottom up and top down approach. The construal of bottom up approach is to synthesize nanomaterial from basic things such as atoms or molecules. Top down method is not more precise, but bottom up method gives elevate to uniform size and shape nanomaterial. Top down method is sub divided in to physical and chemical method. Especially chemical method is used for the synthesis of such nanomaterials. These nonmaterial's were characterized for morphological properties by using X-ray diffractometry (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FT-IR). The utilization of such material for adsorptive removal of organic pollutant and photocatalytic degradation of dye is important application. For removal of such organic pollutant, many conventional methods are available, but these are not much more effective. Hence several alternatives are developed for removal of such harmful organic pollutants. The photocatalytic degradation is an efficient alternative for removal of such organic pollutants. The usage of thin films for such purpose is an effective way for it.

### **AIL-06 : Road-Map to Anticancer-Activity of Coordination Compounds : A Strategic Planning**

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A coordination compound possesses quite different properties compared to organic molecules. A number of drug molecules which were previously very useful are now almost useless (e.g. penicillin, sulpham drugs) More and more new molecules are required to act as more effective drugs as well as less toxic to human body. In today's practice, treatment of cancer is still carried out as removal of cancerous tissues, radiation therapy or chemotherapy or a combination of them. Looking to the importance of chemotherapy, it is obvious that organic

as well as inorganic molecules have their own significance and none of them can be ignored although amidst the fact that majority of drug substance being organic molecules. Another significant matter is that normal tendency of majority of researchers to prepare compounds and then to test their activity. Rather rational approach would be to test probable activity as In-silico analysis as early as possible and then to ascertain the theoretical predictions. Today's practice of new drug formation is to make collaboration with several international agencies giving weightage to their fields of expertise rather than to carry out things alone. This is an era where several softwares or programs like PASS, GOLD, DOCK, ICM, Auto Dock, FlexX, Glide, Surflex etc. are available and are highly recommended to use along with the regular studies. This presentation is about giving an insight into detailed application of selected programs.

### **AIL-07 : Chemistry of Fog Water**

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Acidification of the atmosphere and long range transport of acidifying pollutants have been an important environmental issue due to the rapid industrialization and the dramatic increase in fuel consumption. Fog consist visible cloud water droplets or ice crystals suspended in the air at or near the earth's surface. It can be considered as a type of low-lying cloud and is heavily influenced by nearby bodies of water, topography, and wind conditions. Fog is one of the important mechanisms of removal of pollutants from the atmosphere to earth surfaces. Fog water collection depends on several factors: the composition of incoming fog water, the material of collection and the chemical composition of the dry deposition on the collection, which increases with length of time between foggy days. This talk will focus on fog water collection and chemical characterization of fog water. pH, major cations ( $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{NH}_4^+$ ), major anions ( $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ ), elemental carbon, organic carbon, inorganic nitrogen and organic nitrogen of fog water will be discussed. This talk will also highlight the possible sources of fog and change in chemistry.

### **AO-CYSA-01 : DRS-FTIR Spectroscopy: A Tool for Quantitative Analysis of Growth Promoter Medicine in Poultry Set**

**Ramsingh Kurrey**

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A rapid, simple and sensitive quantitative method for determination

of fluoroquinolone class of antibiotics e.g. ciprofloxacin, norfloxacin, ofloxacin and gemifloxacin from egg-yolk by direct combination of diffuse reflectance-Fourier transforms infrared (DRS-FTIR) spectroscopic has been successfully established. The Ciprofloxacin was analyzed using DRS-FTIR, the most steady and strongest vibrational IR peak at  $1627\text{ cm}^{-1}$  was selected for the quantification of fluoroquinolone class of antibiotics. This present method was found to give a linear calibration curve in the concentration range from 0.05 to 0.50 ng/mL ciprofloxacin with a limit of detection (LOD) and limit of quantification (LOQ) of 0.032 ng/mL and 0.065 ng/mL, respectively. The precision in terms of standard deviation (SD) and relative standard deviation (RSD) for six replicate measurements was found to be 0.0148 ng/mL and 2.2%, respectively at a level of 0.20 ng/mL.

### **AO-CYSA-02 : A Selective Spectrophotometric Method for Determination of Azoxystrobin Pesticide in Different Environmental Samples**

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A new spectrophotometric method for determination of fungicide azoxystrobin was developed. The method is based on the bromination of azoxystrobin to form dibromoazoxystrobin which react with Potassium iodide-Potassium iodate mixture in the presence of leucomalachite green (LMG) to form a blue colored complex. The complex shows maximum absorbance at 615 nm. Beer's law obeyed over the concentration range of 0.5-4.0  $\mu\text{g}$  in final solution volume of 25 mL. The reproducibility assessed by carrying out seven days replicate analysis of a solution containing 2  $\mu\text{g}$  of azoxystrobin in a final solution of 25mL. The molar absorptivity of the coloured system is  $1.936 \times 10^6\text{ L mol}^{-1}\text{cm}^{-1}$  and sandell's sensitivity is  $0.800 \times 10^{-4}\text{ }\mu\text{g cm}^{-2}$ . The standard deviation and relative standard deviation for the absorbance value were found to be  $1.957 \times 10^{-3}$  and 0.509% respectively. The proposed method is free from the interference of other toxicants. The analytical parameters were optimized and the method was applied to the determination of azoxystrobin in water, soil and food samples.

### **AO-CYSA-03 : Development of Electrochemical Immunosensor as Prostate Cancer Diagnostic Tool**

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In this study, we have developed an electrochemical immunosensor

for the detection of prostate-specific antigen (PSA) based on gold nanoparticles (AuNPs) and a chitosan (CHI) nanocomposite film coated on a screen printed electrode (SPE). The modified SPE was characterized using scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The immunosensor was fabricated by sequential immobilization of anti-PSA primary antibody, PSA antigen and HRP-tagged secondary antibody on the surface of AuNPs/CHI/SPE. When this immunosensor was placed in 2.5mM H<sub>2</sub>O<sub>2</sub>, as HRP substrate, and 1mM methylene blue (MB), as redox mediator, greatly amplified immunosensing signals were observed. Immunosensing signals for the reduction of H<sub>2</sub>O<sub>2</sub> were monitored in phosphate buffer (pH 7.0) by CV and square wave voltammetry (SWV). Under optimized conditions steady state current increased linearly with PSA concentration over the range 1-18ng/ml with a detection limit of 0.001ng/ml. The fabricated immunosensor demonstrated excellent sensitivity, stability and reproducibility and therefore was successfully applied to analyse PSA in biological samples. Finally, the results indicate that the proposed immunosensor has potential in clinical screening of cancer biomarkers.

### **AO-CYSA-04 : Ternary M<sub>x</sub>Ag<sub>1-x</sub>S (M = Zn, Cd and Cu; X = 0, 0.5 and 1.0) Nanoparticles: Synthesis, Characterization And Photocatalytic Degradation of Organophosphorous Pesticides For Environmental Applications**

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In this work, we have successfully synthesized ternary M<sub>x</sub>Ag<sub>1-x</sub>S (M = Zn, Cd and Cu; x = 0, 0.5, and 1.0) nanoparticles, using hydrothermal method without any surfactant. In particular, we have the synthesis of ZnS, Zn<sub>0.5</sub>Ag<sub>0.5</sub>S (ZnAgS), CdS, Cd<sub>0.5</sub>Ag<sub>0.5</sub>S (CdAgS), CuS, Cu<sub>0.5</sub>Ag<sub>0.5</sub>S (CuAgS) and Ag<sub>2</sub>S NPs without any surfactant. The samples were fully characterized by UV-VIS DRS, photoluminescence, FTIR, XRD, SEM and TEM. Particle size was observed to be in the range of 10-30 nm. We have accessed the photocatalytic ability of prepared nanoparticles in the photodegradation of three types of organophosphorous pesticides (malathion, chlorpyrifos and monocrotophos) under sunlight irradiation. The superior photocatalytic ability of ZnAgS, CdAgS and CuAgS compared to bare ZnS, CdS, CuS and Ag<sub>2</sub>S NPs were ascribed to an efficient charge transfer from ZnS, CdS and CuS to Ag<sub>2</sub>S. The experiment demonstrated that the pesticides

were effectively degraded by prepared NPs more than 90% with 3 h irradiation time. The recyclability results also demonstrated the excellent stability and reliability of the prepared nanoparticles. This system showed high activity even after five photocatalytic cycles. It provides new insights into the synthesis and characterizations of prepared ZnS, ZnAgS, CdS, CdAgS, CuS, CuAgS and Ag<sub>2</sub>S NPs and its wide applications in the environmental protection issues.

## **AO-CYSA-05 : Spatiotemporal Variation of Atmospheric Carbonaceous Aerosols During A Year-long Measurement in Rural and Urban Environments**

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Air pollution, has become a serious health issue in many developing countries including India and could generate adverse effects on human beings. This study describes a year-long Particulate Matter (PM<sub>2.5</sub>: aerodynamic diameter of less than 2.5 μm) sampling campaigns which were conducted (gravimetrically) during October 2015 to September 2016 (once in a week) using a set of two parallel PM<sub>2.5</sub> cut-off impactor consisted MiniVol air samplers in urban, Industrial and rural environment of Raipur, Bhilai and Kosmarra (a village of Dhamtari District), Chhattisgarh, India, respectively. Weekly PM<sub>2.5</sub> sampling in urban site was carried out, separately, for day and night time to evaluate the impact of selected meteorological parameters on occurrences of PM<sub>2.5</sub> masses. Filter deposited ambient PM<sub>2.5</sub> samples, collected during the sampling period, were analyzed for carbonaceous aerosols using DRI Thermal/Optical carbon analyzer and operated on IMPROVE-A Protocol. The annual average PM<sub>2.5</sub> mass concentrations were found to be ~2 to 5 folds higher than the Indian National Ambient Air Quality Standard (NAAQS) value. Average concentrations of organic carbon (OC) and elemental carbon (EC) were higher during the night time and winter season. On comparing reported studies of other Indian locations, highest percentage of Total Carbonaceous Aerosols (TCA) in ambient PM<sub>2.5</sub> of Bhilai and Raipur has been observed. The OC/EC and char/soot ratios, evaluated in this study, have shown significantly higher variation in spatial and temporal scale for all three sites. The high percent contribution of the secondary organic aerosol (SOA) is also observed which is greater than 50% to total organic carbon. The highest concentration of SOA was at Bhilai area which is due to impact of industrial activity. Bhilai is a well-known major Industrial

area of Chhattisgarh, more than 350 major and minor industrial units are located here.

### **AO-01 : Bio-Adsorbent Column of Activated Carbon for Removal of Coliform Bacteria and Escherichia Coli from Water**

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New bio-adsorbent carbon materials were synthesized from the leaves and veins of *Mucuna pruriens* plant, which are locally available in abundance. The synthesized carbon was activated using  $\text{HNO}_3$  and found to be having high surface area of  $918 \text{ m}^2/\text{g}$ . Scanning electron microscopy analysis of the carbons reflects open pore sizes, shapes and dimensions having complex disorganized surface structures. A sand-supported carbon has been developed using this synthesized activated carbon for its possible use in the removal of coliform bacteria and *Escherichia coli* (E. Coli) from raw water samples. The removal percentage of E. coli was found to be 100% as confirmed from the McCarty most probable number table. Similarly, the removal percentage of coliform bacteria was found to be 99 %. This activated carbon synthesized from locally available plant possesses the characteristics of good low cost adsorbents which can be easily used for the removal of bacteria from water by adsorption method.

### **AO-02 : Method Development and Validation for Simultaneous Determination of Amlodipine Besylate and Atorvastatin Calcium By RP - HPLC**

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The present study describes a simple, accurate and precise RP-HPLC Technique for the simultaneous determination of Amlodipine besylate and Atorvastatin calcium in pharmaceutical dosage form. The method involves an isocratic elution of drug in a stationary phase of Waters X-Terra, C18 (150mm  $\times$  4.6mm, 5 $\mu\text{m}$ ) column using a mobile phase composition of methanol and 10mM Sodium acetate buffered to pH 4 in the composition ratio of 70:30 v/v with a flow rate of 1.0 mL/min at 240 nm of detection. The injection volume is 20  $\mu\text{L}$ . the method has been validated for specificity, linearity, range, precision, accuracy, limit of detection, limit of quantification, ruggedness and

robustness.

The retention times for Amlodipine besylate and Atorvastatin calcium are about 2.28 and 7.71 minutes respectively. Quantitative linearity was observed over the concentration range of 2.51 to 50.18 µg/mL for Amlodipine besylate and 5.02 to 100.33 µg/mL for Atorvastatin calcium respectively. The regression equations of concentration of Amlodipine besylate and Atorvastatin calcium are found to be  $y = 41001x + 39729$ ,  $y = 52986x + 12518$  respectively where y is the peak area and x is the concentration of drug (µg/mL). The % recovery of Amlodipine besylate and Atorvastatin calcium are found to be in the range of 97% to 100%. All the validation parameters are within the acceptance range.

### **AO-03 : Phytochemistry of Some Ferns & Fern Allies of Sitamata Wildlife Sanctuary of Rajasthan**

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Rajasthan lies in the north western part of India. The Sitamata wildlife sanctuary has an area of 423 sq. km falling in Pratapgarh and Chittorgarh districts of Rajasthan. Ferns and fern allies grow luxuriantly in this sanctuary. Phytochemical investigations such as total soluble sugars, soluble proteins and phenols from the entire plant have been taken up in *Ampelopteris proliferata*, *Christella dentata* and *Selaginella ciliaris*. Among the investigated species maximum sugar content for the entire plant was recorded in *Christella dentata*. Maximum protein content for the entire plant was recorded in *Selaginella ciliaris* and Maximum phenols in entire plant was recorded in *Ampelopteris proliferata*.

### **AO-04 : Physico-Chemical Study of Effluents of Orient Paper Mill and Son River Water Near Amalai, District Shahdol M.P.**

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The water quality of Son river get changed in the region of Shahdol district near Orient Paper Mill (OPM), Amalai due to presence of various chemicals in its effluent. These chemicals are used for the pulping and bleaching process of woods in OPM. The total discharge of OPM and Soda factory, Amalai is being received by Son river. During the study 10 sampling stations were selected, out which 6

sampling stations were in downstream of effluents running toward Son river and 4 sampling stations were in Son river nearby village area. The study was carried out during January to June, 2015. Effluent was found acidic in nature at sampling stations SS-01 and 02 near OPM. The higher mean values of TSS were  $183.8 \pm 19.0$  and  $143.8 \pm 1.5$  mg/L at sampling stations SS-01 and SS-02 respectively. The high mean value of alkalinity  $239.5 \pm 20.7$  mg/L was observed at sampling station SS-05. It was observed that the value of total suspended solids and odour was fluctuated widely from station to a station which was an indication of pollution by paper mill effluent. The magnesium was found below to its permissible limit (BIS, 2012) at all sampling stations in effluent of OPM and Son river water during the study.

### **AO-05 : Amperometric Sensor for the Detection of Mercury Metal as an Environment Pollutant**

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It is very essential to develop a simple, effective, sensible, reliable and accurate technique to detect different metals present as an environment pollutant in the atmosphere. For this, we have fabricated graphite, Carbon Nano Tube (CNT) and conducting polymer (polyaniline) based electrochemical sensor for the detection of Mercury metal as an environment pollutant. The electrochemical performance of amperometric sensor was tested by Cyclic Voltammetry, Amperometry and Linear Sweep Voltammetry experiments. The developed amperometric sensor displays good electrochemical activity towards the detection of mercury metal as an environment pollutant. Storage and stability condition of working electrode was also tested. Fabricated amperometric sensor was successfully used for the precise, sensitive and specific detection of different environment pollutant present in the atmosphere.

### **AO-06 : Removal of Basic Dye from Aqueous Solution using Activated Carbon Prepared from Bombax Malabaricum**

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Activated carbon adsorbent was prepared from Bombax Malabaricum waste and named as BMC. Batch sorption experiments

were carried out with BMC for the removal of cationic dye Basic Blue 9(BB9) from its aqueous solution. The effect of adsorbent mass, particle size, solution, pH, contact time and initial dye concentration were studied. It has been found that, solution pH greatly influence sorption process. BMC was characterized by BET, SEM and FTIR analysis. The BET surface area of BMC was found to be 958m<sup>2</sup>g<sup>-1</sup>. The Freundlich, Langmuir, Tempkin and Dubinin-Radushkerich (D-R) Isotherms were used to describe adsorption equilibrium. The results indicated that Langmuir Isotherm was best suited. The kinetics of adsorption process was examined using pseudo-first order, Pseudo- second order, Intra particle diffusion, pore distribution and Elovich models. The adsorption process can be best described by pseudo-second order model.

### **AO-07 : Solvent Extraction of Chromium (III) Using Triphenylphosphine Oxide**

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Solvent extraction of chromium (III) from hydrochloric, sulphuric, nitric and perchloric acid solutions has been investigated by using triphenylphosphine oxide (TPPO) and as extractant in chloroform. Detailed investigations on the effects of different parameters (pH, shaking period, concentration of metal ion, extractant Tetrabutylammonium iodide, anion, various diluents and thermodynamic parameters on the extraction) on the extraction of Cr (III) by TPPO were then carried out. Stripping of the extracted metal species using different stripping agents was investigated and the selective removal of Cr (III) was done. Thermodynamic parameters including  $\Delta G$ ,  $\Delta H$  and  $\Delta S$  for the Cr (III) -TPPO extraction system were determined from the distribution ratio values obtained at different temperatures. Based on the experimental results, extraction mechanism was explained and the extracted species were identified as follows:  $CrX_3 \cdot 3TPPO_{(org)}$ , Where X = Cl<sup>-</sup>, HSO<sub>4</sub><sup>-</sup>, NO<sub>3</sub><sup>-</sup> and ClO<sub>4</sub><sup>-</sup>.

### **AO-08 : Seasonal Analysis of Ganga River Sediments in the District of Vaishali, Bihar**

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River or lagoon beds which are ideal habitat for several species of organisms usually serve as a sink for both domestic and industrial wastes from anthropogenic activities. Dumping of such wastes could

alter the ecological states of these ecosystems. Hence baseline studies are required to determine the status of sediments and quality to give complementary data on the physicochemical characteristics of the habitats. The present study aims to implement master variables, best characterising the sediment stability. Certain chemical characteristics of sediments of river Ganga at Vaishali district were evaluated during the year 2016-17 in different stations. Organic carbon was higher in rainy season. Available nitrogen was lower in rainy season. The analysis among the sediments characteristics of the river proves the common sources of nitrogen in agriculture run-off during rainy season. However, their different sources of enrichment is marked during winter season. During rainy season the dissolved constituents is responsible for increasing electrical conductivity. During summer the sources of nitrogen is mainly from dead decomposed and decay of living organisms. Salinity was higher in summer and low in monsoon season indicating that during summer it could be attributed to faster evaporation. Salinity could reduce in monsoon. PH was slightly alkaline in pre monsoon. DO (Dissolved oxygen) indicates higher value during monsoon which could be due to the cumulative effect of higher wind velocity coupled with heavy rainfall and resulting in mixing with fresh water. Conductivity slightly decreases in the post monsoon season and TDS slightly increases in the post monsoon.

### **AO-09 : Adsorption of Malachite Green by Polyaniline-Nickel Ferrite Magnetic Nanocomposite: Isotherm and Kinetic Study**

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This work deals with the development of an efficient method for the removal of aMG (malachite green) dye from aqueous solution by using polyaniline (PANI)-Nickel ferrite ( $\text{NiFe}_2\text{O}_4$ ) magnetic nanocomposite. It is successfully synthesised in situ through self polymerisation of monomer aniline. Adsorptive removal studies are carried out for water soluble MG dye by using PANI-Nickel ferrite magnetic Nano-composite in aqueous solution. Different parameters like dose of adsorbent, contact time, different initial conc., and pH have been studied to optimise reaction condition. It is concluded that adsorptive removal by PANI-Nickel ferrite magnetic Nano-composite is efficient method for removing a MG dye from aqueous solution than work done before. The optimum conditions for the removal of the dye are initial concentration  $30 \text{ mg lt}^{-1}$ , adsorbent dose  $5 \text{ gm lt}^{-1}$  and pH 7. The adsorption capacity is found  $4.09 \text{ mgg}^{-1}$  at optimum

condition 30 mg/lit. The adsorption followed pseudo 2<sup>nd</sup> order kinetics. The experimental isotherm is found to fit with Langmuir equation. The prepared adsorbent is characterised by techniques SEM, EDS, XRD and VSM.

## **AO-10 : A New Era in Photocatalysis (Organic Catalyst 6,13 Pentacenequinone (PQ))**

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A serious problem of industrial waste water treatment has troubled the mankind because of globalization. Dyes and pigments are the vital waste which damages the human health as well as aquatic life. Researches are working to overcome this serious issue from many years, but to develop cost-effective and ecofriendly method is unsolved challenge. Of late, inorganic based photocatalysis helps to treat industrial waste water upto some extent. Various inorganic semiconductor photocatalysts with high efficiency have been reported with different dyes degradation.

In this regard, we have synthesized PQ an intermediate require to synthesize Pentacene which is well known organic semiconductor. After complete characterization we explored PQ for Industrial Dye degradation and photocatalytical H<sub>2</sub>S splitting for the first time. We also synthesized composite system of PQ-TiO<sub>2</sub> with inorganic semiconductor photocatalyst. Recently a report of PQ-MoS<sub>2</sub> photocatalyst also covers the water splitting area. This organic PQ photocatalyst have high potential in photocatalysis field which can be utilized for the water treatment and for clean environment.

## **AO-11 : Modern Life Style and Environment**

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The Population has increased tremendously over the years. This over population has created a wide gap between haves and have-nots in the society. Due to this it has become necessary to overuse land, soil and other resources through chemicals and pesticides. Several problems have thus emerged like land degradation, soil erosion and air pollution. Increase in population has also put tremendous pressure on water. Our modern life style have made us use the resources lavishly and ruthlessly. The availability of resources is limited but

due to increase in population the per head availability has started declining. All human activities have serious implications on land, water, forest, air etc. The top most layer of soil creates the most important resources of the world. Our modern life style affects this vital layer adversely. Water is precious resources which is cyclic in nature. Industrial and domestic waste disposal into water bodies are polluting them. Deforestation and industrialization causes air pollution. Energy resources (coal, petroleum and natural gas) are depleting day by day due to over consumption of it. It may be depleted in coming future. Plastics, paints and detergents are some other important elements which determining our modern life styles and environment.

### **AO-12 : Estimation of Calorific Value and Analysis of Municipal Solid Waste Collected from Bangalore Urban**

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High Net Calorific values of 9013 cal/g and 8818 cal/g have been obtained by the waste composites and plastics than the other waste material like textiles etc., collected from the various sources in Bangalore urban when all these wastes are being subjected to calorific determination. It assists to recover heat content in calorific values from the waste materials. Also, reduction in volume or mass of waste is being achieved around 75% - 90% in present project work. Besides, the concentration of heavy metals leached from the different organic waste materials into the soil, have been estimated as Zn > Cu > Pb ≈ Cr (ppm) and Hg (PPB) as a pollutants and TOC of the different wastes is analysed as plastics > Textiles > Composites > Liquids > Organics > papers.

### **AO-13 : Effective Removal of Fluoride in Drinking Water Using Biosorbent : Brachiaria Distachya**

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Fluoride is present in low to high concentrations in water. Both the higher and lower levels of fluoride effects the human health. Excess fluoride in drinking water are currently found in all regions of the country. The only choice to reduce fluoride in drinking water is the treatment of contaminated water. Several defluoridation methods

have been adopted but adsorption process is widely used. Adsorption process using plant species is advantageous and eco-friendly. So, biosorption process have been done using plant species i.e., *Brachiaria distachya*.

*Brachiaria distachya* is an annual grass weed produces large volume of biomass grown in tropical regions and easily available. It was used as biosorbent in the powdered form for defluoridation. The efficiency of the plant to remove fluoride from water has been investigated under varying parameters such as contact time, pH, adsorbent dosage, temperature and initial fluoride concentration. The maximum fluoride removal has been observed at pH-6 with adsorbent dosage of 8.5 g for the removal of 40 ppm fluoride in 100 mL of water in 120 minutes. Under these conditions, temperature variation studies were also carried out from 30-60° C and the removal efficiency of fluoride was found to be 92.5 % at pH-6 and temperature 60° C. The biosorption process is exothermic and spontaneous following both Langmuir and Freundlich isotherms. The fluoride biosorption process obeyed pseudo-second order kinetics. The results showed that the biosorbent used was cost- effective for treating fluoride contaminated water.

## **AO-14 : A New Analytical Reagent for the Determination of Sulpha Drugs**

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Metol in the presence of an oxidizing agent is proposed as new, versatile analytical reagent for the spectrophotometric determination of microgram amounts of pharmaceutically important sulpha drugs. When Metol (para-N-methylaminophenol sulphate) in the presence of an oxidizing agent is mixed with any sulpha drug under acidic buffer conditions has developed purple – red colour with wavelength maximum at 530 nm. The intensity of colour is directly proportional to the concentration of drug added. Beer's law limits, molar absorptivity, reagent concentrations and interference studies are made. The method can be extended to other dosage forms like tablets, injections and eye drops after preliminary treatment of the preparation. The colour is developed within 15 minutes and is stable for about 2 hours. The coloured complex is cationic in nature which is indicated by the retention of the purple – red colour on treatment with IR – 50 cation exchange resin. The charge transfer complex formation is suggested as a model to explain the colour formation, where sulpha drug acting

as donor and PMBQI (formed insitu when metal is treated with oxidizing agent) acting as acceptor. The complex is not extractable by organic solvents but is adsorbed by cation exchange resin. The method is simple, accurate and economical for the estimation of sulphadiazine.

## **AO-15 : Removal of Heavy Metals From Contaminated Water Samples Using Nano Materials**

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Now day's nano adsorbents are used to removal the heavy metals from the polluted water. In the present study, activated carbon and nano particles of pennisetum glaucum cobs and zea mays cobs are used to remove the Cd, Cr and Pd. The prepared nanoparticale were studied in terms of size morphology, surface area using different techniques such as TEM, SEM, XRD, FTIR and EDAX. The nano particles are more efficient removal of heavy metals than activated carbon.

## **AO-16 : Decolorization Textile Effluents by Using Activated Carbon Prepared from Cornhusk**

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The control of water pollution has become of increasing importance in recent years. Textile effluents sewage directly enters water streams without any treatment. The color and the non-biodegradable nature of the spent dyebaths constitute serious environmental problems and various deleterious effects caused by them. In this research work activated carbons were prepared with corn husk, those were characterized. The pore structures of the resulting carbons were analyzed using N<sub>2</sub> adsorption, X-ray diffraction (XRD) and scanning electron microscope (SEM). Surface area was calculated by Brunauer–Emmett–Teller (BET) equation. Thermal stability of carbons was analyzed by thermogravimetric analysis (TGA) and temperature programmed desorption (TPD) studies. The nature of functional groups present on surface of activated carbons was analyzed by FTIR and XPS techniques. The effluents are collected from three different places

of their disposal. The efficiency of prepared carbon adsorbents in decolorizing these textile effluents was studied.

### **AO-17 : N-doped ZnO and Graphene Oxide Dispersed N-Doped ZnO : Potential Candidate for Anti-Corrosion and Battery Application**

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Application and synthesis of N-doped zinc oxide have been reported by many. But most of them have discussed about the problem in producing the N-doped zinc oxide for optoelectronic application as a p-type semiconductor. This paper deals with the synthesis of N-doped zinc oxide starting from a imidazole derivative. The synthesized zinc oxide nano particles are of the size of the order of 20nm. The N-doped zinc oxide nano particles have significant anti-corrosion effect on mild steel. With doping of graphene into it lowers the anti-corrosion activity. On the other hand, the graphene dispersed N-doped zinc oxide nano particles possess lower contact and charge transfer impedances as per the Nyquist plot and thus be a promising candidate for battery.

### **AO-18 : Comparative Study of Assessment of Ground Water Quality of Rural and Urban Area of Muzaffarpur District, Bihar**

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Water is the most important and precious natural resources not only to humanity but to the entire living community of the globe as a whole. Water quality assessment comprises all activities to obtain information with respect to the water system. Muzaffarpur district is today, faced with serious problems of pollution and falling ground water level in urban as well as in rural areas. The steady fall ground water table is seriously impairing the original productive power of state. It is highly disastrous for stable and sustainable development. So, basic monitoring on water quality has been necessitated to observe the demand and pollution level of ground water. Assessment of Water quality is an important to evaluate the nature and extent of pollution control required and also the effectiveness of pollution control measures already in existence. Under this study a systematic and scientific study of the quality of supply drinking water in different localities of

Muzaffarpur has been analysed in different seasons for their physico-chemical characteristics such as pH, temperature of water, chloride, carbonates and bicarbonates, dissolved oxygen and hardness by standard analytical techniques at laboratories. Special emphasis will be laid out in analyzing and estimating prevalence of water borne disease organisms in these water samples. By analyzing the data founded after the physico-chemical and bacteriological examination has been co-related with the reported cases of health hazards and illness. Based on the observations suitable recommendations has been drawn from the study for planning environmental health programme for the city.

### **AO-19 : $\text{Ni}_{0.6}\text{Zn}_{0.4}\text{Cu}_{0.2}\text{Cd}_x\text{Fe}_{1.8-x}\text{O}_4$ ( $0.2 \leq x \leq 0.8$ ) Magnetic Ferrite Nanoparticles: Synthesis, Characterization and Photocatalytic Activity Towards Degradation of Methylene Blue.**

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Nanocrystalline magnetically separable solar light active  $\text{Ni}_{0.6}\text{Zn}_{0.4}\text{Cu}_{0.2}\text{Cd}_x\text{Fe}_{1.8-x}\text{O}_4$  ( $0.2 \leq x \leq 0.8$ ) photocatalyst with different cadmium content were synthesized by tartarate coprecipitation method. These tartarate complexes were monitored by FTIR and thermal studies (TG-DTA) and were decomposed at 600°C to obtain respective magnetic ferrites. The obtained ferrites were characterized by XRD, TEM, D.C. electrical conductivity measurement and UV-vis spectroscopy. From TEM images it was found that the particle sizes of all ferrite particles are in the range of 23 to 51 nm. The photocatalytic activity of these ferrites in the degradation of methylene blue (MB) was studied under solar light irradiation. It was observed that the cadmium substitution dramatically enhances the photocatalytic activity of nickel-zinc ferrites. This means that cadmium substituted nickel-zinc ferrites utilize the possibility of solar energy in the solar spectrum.

### **AO-20 : Heavy Metal Analysis of Ground Water in Chitrakoot Region, District Satna**

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The Chitrakoot is geographically located at coordinated -25.00°N latitude 7-80.83°Elongitude. It borders the Chitrakoot District in Uttar Pradesh, whose headquarters chitrakoot Dham (Karwi) is located nearby. The town lies in the historical chitrakoot region, which is

divided between the present-day Indian states of Madhya Pradesh and Uttar Pradesh. The Procedures followed to analyze the Heavy metal concentration were from Standard Methods All the water sample are leaving very little concentration of Iron and showing good quality of water as for as Iron is concerned.

### **AO-21 : Hydrothermally Modified Nanocrystalline Nb<sub>2</sub>O<sub>5</sub> and its Visible-light Photocatalytic Activity for the Degradation of Congo Red and Methylene Blue**

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In this work, photocatalytic degradation of dyes in aqueous suspension was studied using modified nanocrystalline Nb<sub>2</sub>O<sub>5</sub> by the hydrothermal method as a photocatalyst in the presence of visible light in a photocatalytic reactor. The modified Nb<sub>2</sub>O<sub>5</sub> characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), EDX. The photocatalytic experiments of modified Nb<sub>2</sub>O<sub>5</sub> on dyes were carried out to optimize the various parameters like effect of catalyst dose, initial dye concentration, contact time, and pH. The nanocrystalline Nb<sub>2</sub>O<sub>5</sub> photocatalyst shows enhanced photocatalytic activity. The degradation of Congo red (CR) is reached up to 90% and for methylene blue (MB) 87% in 150 minutes. Also beside this kinetic study of CR and MB degradation was carried out.

### **AO-22 : Hydrochemical Analysis and Evaluation of Groundwater Quality in Andhra University, Visakhapatnam, Andhra Pradesh State, India**

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Water plays an important role for the survival and existence of life on earth. An attempt is made in the present study to assess the ground water quality in Andhra university of Visakhapatnam which is a part of coastal region in Andhra Pradesh. The samples of ground water are collected from 11 different sampling locations in the surroundings of Andhra University and samples were analysed for physical characteristics like Electrical Conductivity (EC), Total Dissolved Solids (TDS), P<sup>H</sup>, salinity, Dissolved Oxygen (DO) and Temperature,

chemical parameters like Calcium ( $\text{Ca}^{2+}$ ), Magnesium ( $\text{Mg}^{2+}$ ), Sodium ( $\text{Na}^+$ ), Potassium ( $\text{K}^+$ ), Nitrate ( $\text{NO}_3^-$ ), Chloride ( $\text{Cl}^-$ ), Sulphate ( $\text{SO}_4^{2-}$ ) and Total alkalinity (TA) were determined using standard procedures and interprets the data with scientific softwares like Wateq and Surfer. These results declare that the collected water samples are in permissible limits and used for drinking purpose.

### **AO-23 : Study of Physico-Chemical and Growth Parameters of *E.foetida* During Vermicomposting**

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Earthworm as one of the best means of abating organic population and also to minimize indiscriminate use of inorganic fertilizers. Earthworms have important functions by virtue of their feeding and general behavioral activities like burrowing, digestion, excreting with micro-organisms and supporting further decomposition of biodegradable matters. The growth and reproductive efficiency of locally available earthworm species, *Eisenia foetida* was accessed in various urban wastes such as vegetable wastes found in market. Maximum weight and length of *Eisenia foetida* was noted in 90days. Similarly the maximum biomass of 1234 (+0.04)g of earthworm in the VMW was also noted in 90 days. The worms when introduced into wastes into wastes thus showed an increased growth rate and reproduction activities.

### **AO-24 : Synthesis and Ion Exchange Studies of Pectin Based TIN (IV) Phosphate : A New Hybrid Ion Exchange Material**

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Hybrid ion exchange materials are of recent interest as they exhibit outstanding chemical, mechanical and thermal stability, in addition to metal ion selectivity. It has been observed that the introduction of organic species into an inorganic material enhances its reproducibility in ion-exchange behavior and its chemical stability to some extent. In these laboratories, a large number of hybrid ion exchange materials have been synthesized by incorporating both organic substances and inorganic substances. The potential of these materials has been demonstrated by achieving separations of several metal

ions. In continuation of such a work, we have synthesized pectin based tin (IV) phosphate as a new phase of hybrid ion exchange material. It has been characterized by its ion exchange, elution, concentration and thermal behavior. Adsorption studies have been done with different alkaline earths and heavy metal ions in different acidic media. On this basis, the material has been found selective for Hg (II), a toxic heavy metal. Some binary separations have been performed in order to explore its analytical applications in environmental and pollution chemistry where a separation of Hg (II) ions from other ionic species is needed.

### **AO-25 : Study of Physico-Chemical Parameters of Ground Water in Agra**

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Today, due to massive increase in population and human activities, the demand of pure water is increasing continuously. Different samples of groundwater have been collected from the various places of Agra (UP) for this study. The results of this study were compared with the water quality standards of WHO and ISI. In this study, various physico-chemical parameters like conductance, turbidity, pH, temperature, color, odour, chemical oxygen demand, total dissolved solids and concentrations of ions like Nitrate, Nitrite, Sulphate, Phosphate, Magnesium, Calcium, Cl<sup>-</sup>, F<sup>-</sup>, CN<sup>-</sup>, Na<sup>+</sup>, K<sup>+</sup>, etc. were determined by using standard parameters. The results were compared with drinking water standards of ICMR and EU (1998). The values of mean, standard deviations and correlation co-efficients (r) were also calculated for these water odour, quality characteristics.

### **AO-26 : Chemical Composition of Egg Shell Membrane of Pigeon (Columba Livia) and its Therapeutic Applications**

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In this study, chemical composition of some external and internal egg shell membrane of pigeon were compared. The egg shell membranes are connective tissue. The organic matter of egg shell membrane contain protein as a major constituents with small amounts of carbohydrates and lipids. Calcium is the chief mineral element in the outer and inner shell membrane. Outer shell membrane contain

slightly more calcium than the inner shell membrane and their mineral oxide. Mineral magnesium, phosphorus, sodium and their corresponding oxides are found in traces in the outer and inner shell membranes.

Moisture content is found in less amount but ash content is slightly greater amount in the outer shell membrane than the inner shell membrane. Crude fat of outer shell membrane is found in greater amount than the inner shell membrane of egg whereas total nitrogen and crude protein of outer and inner shell membranes are found in the same amount. This can be attributed to the greater absorption of fat in the outer shell membrane. Obviously supply of the fat to the inner shell membrane will be less as the inner shell membrane itself deposit less fat than the outer shell membrane. Total amino acid present in egg shell membranes are eighteen. Amino Acid contents of the outer shell membrane of egg is higher than the inner shell membrane of egg. That is why outer shell membrane appears to be strongly developed than the inner shell membrane.

### **AO-27 : Assessment of Physico-chemical and Microbiological Analysis in Drinking Water of Chitrakoot Nagar Panchayat Area (M.P)**

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A study was conducted to evaluate the quality of drinking water samples from the four types drinking water sources namely, Public Health Engineering (Water Supply), handpump, river Mandakini and dug wells. Total sampling stations were 17 all from Chitrakoot nagar panchayat area, M.P. parameters investigated were physico-chemical and microbial parameters i.e pH, temperature, turbidity, conductivity, TDS, dissolved oxygen (DO), biochemical oxygen demand (BOD) and chemical oxygen demand. The pH, temperature and conductivity ranged from 7.0-7.6, 209-295 mg/l, 27-30°C and 372-789 mg/l. respectively. TDS, turbidity, dissolved oxygen (DO), biochemical oxygen demand (BOD) and chemical oxygen demand ranged from 252-660 mg/l, 2.4-3.5 NTU, 4.4-5.6mg/l, 4.6-5.3 mg/l and 21-45 mg/l respectively. All the physicochemical parameters analyzed were within the WHO guideline values except EC, TDS, DO, BOD and COD which exceeded the WHO limits at sampling sites. However, the pH, temperature and turbidity values of all the water samples were below the WHO permissible limit which was within the permissible limit. Microbial analysis revealed that all water samples were not free from pathogens and thereby were not suitable for drinking.

## **AO-28 : Environment Sustainability through Environment Audit of Manufacturing Unit**

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**Concept :** This study aims to give information about the effect of green manufacturing practices by manufacturing unit for environment sustainability. First of all, environment and environmental problems, one of the reason why the environment audit emerged, as the new buzzword/concepts focused on issues as explained.

**Methodology :** Literature review has been continued and studies conducted on this subject leads to together with the hypothesis development. Green practices are evaluated by manufacturing unit evaluated critically.

**Observations :** Adoption of new concepts like Five Star Buildings, ISO 14000 certification has great impact on the issues so studied. Concept of Reverse logistics for effective use of resources is few highlighting features of organizations showing concern for environment. According to the results of the analysis environment vision and mission is a guiding force for focused approach for environment conservation. Environment Management system is at its place for environment sensitive organizations.

**End Notes :** Environmental awareness, Green product features, green promotion activities affect in positive way, and sharing of technical know-how of leading units on green initiative affect sustainability of environment to great extent.

## **AO-29 : Adsorption Studies of (Cr (VI), Cd (II), and Cu (II)) Metal Ions from Aqueous Solutions by Synthesized Fe<sup>3+</sup> and Ag<sup>+</sup> Co-Doped TiO<sub>2</sub> Nanoparticles**

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The present communication has been addressed to the removal of Cr (VI), Cd (II) and Cu (II) from aqueous solutions by Fe<sup>3+</sup>-Ag<sup>+</sup>/TiO<sub>2</sub> nano metal oxide synthesized by Sol-Gel technique and characterization was done by XRD, SEM, TEM, EDS, and FTIR. Batch equilibrium experiments were performed for various concentrations of 0.1 mg/L to 1 mg/L and the effect of contact time, pH and adsorbate dosage was

investigated. The adsorption kinetics was well fitted to pseudo-second order kinetic model, Weber-Morris & Reichenberg Kinetic equations. Langmuir and Temkin isotherms were found well fitted with the data.

### **AP-CYSA-01 : Microwave Assisted Synthesis : A Footstep towards Sustainable Development**

**Anshul Singh and Ashu Chaudhary**

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Chemistry has improved our quality of life, and made thousands of products possible. Unfortunately, this achievement has come at a price: our collective human health and the global environment are threatened. The excessive and unconsidered use of some toxic compounds, without proper safety measures; has led to a highly polluted environment. With the world facing hostile consequences due to this pollution, green chemistry is increasingly being viewed as a means to address this concern. Microwave technology is emerging as an alternative energy source powerful enough to accomplish chemical transformations in minutes, instead of hours or even days. For this reason, microwave irradiation is presently seeing an exponential increase as compared to conventional methods which require more reaction time, and drastic conditions of temperature. Within this frame, we have synthesized new series of heterobimetallic complexes via a microwave-assisted method and then characterized these complexes by physicochemical and spectroscopic techniques such as IR, mass and ESR. These complexes have been screened for their antifungal, antibacterial and anti-inflammatory effects and the results are compared with the starting materials.

### **AP-CYSA-02 : Analytical and Biochemically Characterization of Some Lanthanide Complexes**

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The compound of lanthanide ions with complexing or chelating biologically important kynurenic acid ligand to form coordination compound is an important area of current research. Less explored biologically important kynurenic acid ligand is allowed to react with solution of lanthanides perchlorates and attempt has been made to synthesize solid kynurenic acid complexes. These complexes are subjected to U.V visible spectroscopy, IR spectroscopy, TGA analysis, Mass Spectroscopy, Elemental analysis and antimicrobial activity of these compounds has been evaluated by standard methods and attempts

have been made to correlate structural characteristic with properties of these complexes.

### **AP-CYSA-03 : Determination of Fenpropathrin Pesticide in Different Environmental Samples Using A Sensitive Non-extractive Spectrophotometric Method**

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An efficient, effective, simple and sensitive non-extractive spectrophotometric method has been developed for the quantification of pesticide fenpropathrin in different environmental samples. This method is based on the simple multistep reactions of fenpropathrin to form a yellow dye. In this method fenpropathrin was firstly hydrolysed by NaOH to form cyanohydrin intermediate product. This cyanohydrin intermediate molecule was further treated with bromine and pyridine to form glutaconic aldehyde, which is finally coupled with p-Aminodimethyl benzaldehyde to give a yellow colored dye with resulting  $\lambda_{\max}$  at 440 nm. Under optimised experimental conditions, calibration graph was linear over the range 0.5 - 4.0  $\mu\text{g mL}^{-1}$ . The molar absorptivity and sandell's sensitivity values were found to be  $9.83 \times 10^5 \text{ L mol}^{-1} \text{ cm}^{-1}$  and  $0.20 \times 10^{-3} \mu\text{g cm}^2$ , respectively. The detection limit and RSD was calculated as  $0.0268 \mu\text{g mL}^{-1}$  and 0.28%, respectively. The applicability of developed method has been successfully examined for the detection and quantification of minor concentration of fenpropathrin in different environmental samples.

### **AP-CYSA-04 : Screening of Naphthylhydroxamic Acids Through Bio-mimetic Membrane Evaluated by RP-HPLC and Octanol-Water System**

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Lipophilicity is an important Qualitative Structural Activity Relationship (QSAR) parameter to reveal the drug likeliness of compound. In the present investigation, lipophilicity of five naphthyl derivatives of hydroxamic acids i.e. N-N-1-naphthyllaurohydroxamic acid (N-NLHA), N-1-naphthylphenylacetohydroxamic acid (N-NPAHA), N-1-naphthyl-o-ethoxybenzohydroxamic acid (N-NEBHA) N-1-naphthyl-o-methylbenzohydroxamic acid (N-N-o-MBHA) and N-1-naphthyl-p

methylbenzohydroxamic acid (N-N-p-MBHA) have been described. Lipophilicity of five compounds has been evaluated from Reverse Phase Liquid Chromatographic Method (RP-HPLC) and by octanol-water system. Organic modifier concentration indices ( $\delta_o$ ), constituent contribution factor ( $\delta_x$ ), separation efficiency (N), resolution, separation time ( $R_s$ ), height equivalent of a theoretical plate (H), polarizability, distribution coefficient ( $\log D_{7.4}$ ), total polar surface area (TPSA) and calculated molar refraction (CMR) parameters are also experimented and computed for all the compounds. The lipophilicity values by RP-HPLC method ( $\log k_w$ ) are in the range of 1.228 to 2.624 and by octanol-water system ( $\log P$ ) the values ranges from 0.625 to 1.452. Lipophilic values of all the molecules are within the range of "Lipinski Rule of 5" which suggests that these are drug like molecules.

### **AP-CYSA-05 : Particulate Size Distribution Concentration in Urban, Semi Urban and Rural Traffic Junction**

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Size segregated Particulate matter concentration was determined by Grimm Aerosol Spectrometer (1.109) at urban, semi-urban and rural traffic junctions in Agra region. The average mass concentrations of  $PM_{10}$  were  $137.09\mu g/m^3$ ,  $270.14\mu g/m^3$  and  $71.3\mu g/m^3$  at the urban, semi-urban and rural traffic junction, respectively, which were significantly higher than the threshold limit of  $100\mu g/m^3$  given by CPCB, India and of  $50\mu g/m^3$  given by the WHO. Average mass concentrations of  $PM_{2.5}$  were  $41.45\mu g/m^3$ ,  $48.88\mu g/m^3$  and  $23.28\mu g/m^3$  at the urban, semi-urban and rural traffic junction, respectively which was significantly higher than WHO standard of  $10\mu g/m^3$ . The average mass concentration of  $PM_{1.0}$  were found  $30.35\mu g/m^3$ ,  $12.56\mu g/m^3$ ,  $14.13\mu g/m^3$  and the  $PM_{0.25}$  were  $0.06\mu g/m^3$ ,  $0.17\mu g/m^3$ ,  $0.14\mu g/m^3$  at urban, semi-urban and rural site respectively.  $PM_{10}$ ,  $PM_{2.5}$  and  $PM_{0.25}$  values were found higher in semi-urban site in comparison to urban and rural traffic junction whereas values of  $PM_{1.0}$  was found higher in urban areas. The values were found to be higher during morning time for all size fractions. The surface morphology of  $PM_{2.5}$  was also analyzed by Scanning Electron Microscopy (SEM). The results indicate flaky, branched chain like aggregates of carbon bearing spheres at the urban site and cluster, branched, spherical and fluffy appearance at semi-urban site.

## **AP-CYSA-06 : The Role of Human Biomonitoring in Accessing Human Exposure and Managing Risks**

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No matter where we live, we are exposed to the variety of chemicals present in the surrounding. They are present in the air we breathe, present in the water we drink, present in the food we consume and the products we use. Most of these substances occur naturally in the environment, but others are the result of anthropogenic activities. Human Biomonitoring (HBM) is a scientific procedure that allows us to estimate whether and to what magnitude these environmental pollutants have entered our bodies and how exposure may be changing over time. Measuring the concentration of natural and synthetic compounds in body fluids (blood, urine, and breast milk) or tissues (hair, nails, adipose, placenta and bone), biomonitoring can postulate valuable evidence on environmental exposures and, in some cases, help, identifying potential health risks. The importance of HBM is that it can give very precise information on the total internal exposure of an individual at a given time, as it adds together exposure from various sources and routes (e.g. air, water, food). When combined with information on possible sources, the way chemicals enter our bodies, and how they are metabolised this is vital information for the authorities who have a role to play in reducing human exposure to toxic chemicals. During my presentation, I will discuss the environmental chemicals which needs to pay attention in recent time and how human biomonitoring can be helpful in environmental medicine.

## **AP-CYSA-07 : Hydrogen Uptake by Composites of Metal-Organic Frameworks and Metal (Ni, Pd) Decorated Multi-Walled Carbon Nanotubes : A Green Energy Approach**

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Hydrogen is regarded as one of the most promising green energy carrier alternative to the existing fossil fuels for transport sector because of its high abundance, light weight, and eco-friendliness. Metal Organic Frameworks (MOFs) and carbon nanotubes (CNTs) are the

suitable candidates for adsorption of hydrogen at non-cryogenic temperatures for on-board vehicle applications. MOFs have open metal sites that are built into the pore walls in a repeating, regular fashion. HKUST-1 is one of the interesting MOFs build from Cu and BTC has large surface area and pore volume ( $1721 \text{ m}^2\text{g}^{-1}$  and  $0.7424 \text{ cm}^3\text{g}^{-1}$ ). So we have attempted to synthesize the composites from metal-doped MWCNTs and MOFs for better hydrogen uptake. In this direction we have prepared Ni@f-MWCNTs@Cu<sub>3</sub>(BTC)<sub>2</sub> and Pd@f-MWCNTs@Cu<sub>3</sub>(BTC)<sub>2</sub>. It is found that Ni@f-MWCNTs@Cu<sub>3</sub>(BTC)<sub>2</sub> and Pd@f-MWCNTs@Cu<sub>3</sub>(BTC)<sub>2</sub> adsorb 4.68, 5.31 wt% of hydrogen, respectively, at 77 K and 70 bar pressure. At 298 K and 70 bar pressure both materials adsorb 1.29 and 1.67 wt% of hydrogen, respectively.

## **AP-01 : Development of Greener Synthesis Routes for Nanoporous Silica from Biomass : A Review**

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Nanostructured silica materials have an unprecedented foothold in the field of material synthesis owing to the exploitation of their superior surface properties. Consequently, they have been extensively used in various fields ranging from catalysis, adsorption, sensors, nano-casting, chromatography and medicine. Moreover, due to their high surface area and availability in various forms viz., fumed silica, silica gel and mesoporous silica, silica nanoparticles are now even being used in nano-electronics, photonics, energy harvesting, energy storage and biotechnology as food additives, drug carrier, bio-sensing and tissue engineering etc. Different approaches have been developed to synthesize nanostructured silica materials using silicon alkoxide (silicon tetraethoxysilane) as the typical silicon source. However, in view of the credentials of the green chemistry, high cost, harsh synthetic conditions and sustainability issues associated with the silica precursors, limit their manufacture at an industrial scale. What aggravates the problem is the use of expensive structuring agents (surfactants) that are eliminated during the last step of mesoporous silica synthesis. So, there has been an emergent need to develop more environment-friendly and economical procedures for synthesizing mesoporous silica nanostructures. In consideration with the sustainable and greener aspects of mesoporous material synthesis, nowadays ordered mesoporous silica (OMS) materials have been synthesized using the agricultural wastes like rice straw, corn cob and bagasse etc. So, a review on recent advances on the eco-friendly synthesis of

mesoporous silica nanostructures (from biomass) and their use for various industrial applications will be presented.

### **AP-02 : ZnO Assisted Photocatalytic Degradation of Explosive Metal Picrate in the Presence of UV Light**

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The Photocatalytic degradation of metal - picrate in aqueous solution using ZnO photocatalyst has been carried out. The absorbance of photocatalytic reaction at different time intervals has been observed by spectrophotometrically. Rate of reaction was observed at different parameters like concentration, effect of photocatalyst, pH, light intensity and band gap.

### **AP-03 : Assessment of Major and Trace Elements in Groundwater of Sandur Area and its Surroundings, Bellary District Karnataka, India**

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The present paper deals with major and trace elements geochemistry from the groundwater of Sandur taluk and its surrounding area, Bellary district, Karnataka, India. Geologically, The Sandur schist belt is predominantly characterized by greenschist facies of regional metamorphism, which increases to amphibolite facies near the periphery of the schist belt. The higher facies rocks are marked by the appearance of metamorphic index minerals like garnet, andalusite, staurolite and cordierite. The main objectives of this paper is review and the determination of some of physical and chemical parameters along with six trace metals namely Iron, Zinc, Copper, Nickel, Chromium, Cadmium and Lead in the underground water at 50 selected locations of Sandur taluka and its surroundings of Bellary District of Karnataka State. Concentrations of magnesium, sodium and potassium are generally within the permissible limits. The concentration of anions are characterized by  $SO_4^{2-} > Cl^- > NO_3^- > F^-$ . Nitrate and sulphate concentrations exceed the permissible limits in a few samples; elevated concentrations appear to be related to the aquifer lithology. The fluoride concentration exceeds the desirable limit in some areas; the elevated fluoride values are attributed to the application of chemical fertilizers in agriculture

and to the occurrence of fluoride bearing minerals in shale formation. Six trace elements (Fe, Cu, Ni, Pb, Mn, Cd) were also analysed. The iron concentration exceeding the permissible limit in drinking water. The nickel and cadmium concentrations are well within the permissible limits. The elevated concentrations of trace elements are combined effects of geogenic sources as well as of mining activities and excessive use of chemical fertilizers. It is recommended to control anthropogenic activities adequately in order to minimize the pollution problems.

## **AP-04 : The Social Cost and the Impact of Carbon Emissions**

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Climate change is a classic market failure and pollution a negative externality, it is thus important to have a parameter that would optimally allocate assets. The social cost of carbon emission is a monetary measure in dollars of the damages done to the ecosystems and the environment by a tonne of CO<sub>2</sub> in a year. This measure is basically a cost benefit analysis that determines the cost of emitting more CO<sub>2</sub> and the benefit of reducing it. The SC-CO<sub>2</sub> is meant to be a comprehensive estimate of climate change damages and includes changes in net agricultural productivity, human health, property damages from increased flood risk, and the increased costs for air conditioning. However, it is quite difficult to measure all the damages done to the environment by measuring every emission in a given year. The paper analyses the impact of this parameter on policy formulation and the efficiency it would bring to the market by optimally allocating the assets. The costs of these emissions are borne by the society whereas the benefits are accrued by the creators of this externality. Since no market can ever operate in equilibrium the main idea behind this parameter is to quantify the damages and reduce the emissions accordingly. Since SC-CO<sub>2</sub> is a future measure it is difficult to find the exact measure in monetary terms by discounting as there are socio economic projections, climate modules, future damages done to the environment and the combined effect of these factors. Integrated assessment models (IAMs) calculate the effects on GDP but this is not the only factor that needs to be measured other important factors such as mortality rates too need to be assessed. The study reveals that the non-linear negative climatic impact will be higher if SC is higher and vice versa. Thus the paper analyses the different models to estimate SC and various ways of discounting to predict the future damages.

## **AP-05 : Thermo-Acoustic and Ftir Studies on Binary Liquids Mixture of Ethyl Oleate and Benzaldehyde at 303.15 to 318.15k**

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Ultrasonic velocity, density and viscosity of two liquid mixtures ethyl oleate with benzaldehyde have been determined at various temperatures in the range of 303.15 to 318.15K. The ultrasonic velocity, viscosity and density data are used to estimate adiabatic compressibility, free length, molar volume and free volume along with their excess values. The observed variations of the said parameters with concentration and temperature, are discussed in terms of the intermolecular interactions between the unlike molecules of the binary mixtures. FT-IR spectra confirm the expected interactions.

## **AP-06 : Evaluation of La Doped ZnO Nanospheres for Catalytic Thermal Decomposition of Ammonium Perchlorate**

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Ammonium perchlorate (AP) oxidizer is one of the major ingredients used in propellant and explosive formulations. Lower thermal decomposition temperature (TDT) and higher calorific output is always desired from an ideal AP oxidizer energetic composition. The metal oxide catalysts are often used as a catalyst for reduction of TDT of AP. In present study the synthesis and catalytic application of pure and lanthanum-doped ZnO (La-doped ZnO) was studied towards the thermal decomposition of the ammonium perchlorate. The pure and La-doped ZnO nanocrystallites with 0.1 to 1.0 % of La were successfully synthesized by simple co-precipitation method. The microstructures of synthesized materials were characterized by UV, IR, Photoluminescence, XRD spectroscopic techniques. The spherical morphology and elemental composition of the catalytic materials was ascertained by SEM-EDS analysis. The presence of La in doped form is ascertained by higher Bragg's angle shift of two theta value in accordance with the increase in La % in doped materials. The TG-

DSC analysis of AP samples associated with 1 % amount of catalysts revealed that the added catalyst plays a crucial role to facilitate early decomposition of AP. It is also found that as the amount of La in catalytic composition increases the TDT of AP decreases by lowering the required energy of activation.

### **AP-07 : Spectrophotometric Determination of Piperazine with 4 - Aminobenzoic Acid in the Presence of N - Bromosuccinimide**

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A sensitive spectrophotometric method has been developed for the assay of piperazine (PPZ) in bulk and their pharmaceutical preparations. The method is based on the formation of coloured species with 4-aminobenzoic acid. The reaction involves oxidation of the piperazine by N-bromosuccinimide, when oxidized product (light red coloured) is coupled with 4-aminobenzoic results violet coloured product. Beer's law of the coloured species is obeyed in the range of PPZ concentrations of 8 to 20 µg / ml at the maximum absorption of 560 nm. The optimum reaction conditions and other analytical parameters are evaluated. The proposed method has been successfully applied to the analysis of the bulk drugs and their dosage forms tablets and, syrup. No interference was observed from talc, dextrose or magnesium stearate in the proposed method. The reliability of these methods is established by parallel determination with the reported and official methods.

### **AP-08 : Synthesis, Characterization and Applications of Zinc Oxide Nanostructures**

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Oflate, nanostructured Zinc Oxide (ZnO) is well discussed inorganic semiconductor material which is used in various fields. Due to its fascinating properties like eco-friendly, anti-bacterial, anti-fungal and high surface area ZnO have wide range of applications. These applications includes photocatalysis, organic conversions, gas and humidity sensing, solar cell and anti-bacterial applications. Mainly, ZnO can be synthesized by using hydrothermal/ solvothermal, sol-gel

and precipitation methods. With specific reaction conditions ZnO can be synthesized with different morphologies like spherical particles, rods, plate and hexagonal shape.

Herein, ZnO synthesized by sol-gel and hydrothermal method and after complete morphological and spectroscopic characterization we have employed ZnO nanostructures for photocatalytic dye degradation. Also, the anti-bacterial properties were also checked for these as synthesized ZnO nanostructures.

### **AP-09 : Methylene Blue Dye Degradation Using Novel Organo-Inorganic (6, 13-pentacenequinone-tio<sub>2</sub>) Nanocomposite**

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The coupled semiconductor photocatalyst of 6, 13-Pentacenequinone/TiO<sub>2</sub> (PQ/Ti) with different weight ratios were prepared. The PQ was loaded on anatase TiO<sub>2</sub> by simple wet impregnation method. The prepared catalyst was characterized with various spectroscopic methods. XRD confirms the monoclinic and anatase phase of PQ and TiO<sub>2</sub>, respectively. The presence of both phases was observed in the prepared coupled catalyst. FE-SEM showed the sheet like morphology of PQ, whereas the coupled catalyst depicts the formation of homogeneous layer on TiO<sub>2</sub> surface in all three compositions. Optical study by Diffuse reflectance UV-Visible absorbance spectra (DRS) indicate the band gap of PQ and TiO<sub>2</sub> around 2.8 and 3.2 eV respectively. The absorbance in the range of 450 nm was also observed in case of prepared coupled catalyst confirming the loading of PQ on TiO<sub>2</sub>. Photocatalytic activity of coupled catalyst was studied by observing the degradation of methylene blue (MB) dye under visible light irradiation. As compare to individual the coupled organo-inorganic catalyst showed higher photocatalytic activity towards MB degradation. TiO<sub>2</sub> loaded with 0.2 wt% PQ showed highest rate of MB degradation i.e.  $K_{app} = 5.2 \times 10^{-2} \text{ min}^{-1}$ .

### **AP-10 : Synthesis, Characterization and Applications of Polyindole-Meatal Oxide Composites**

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Polyindole have gained immense importance because of its

fascinating properties These applications includes photocatalysis, organic conversions, gas and humidity sensing, solar cell and anti-bacterial applications. Herein, the chemical oxidative polymerization of Indole was carried out at optimized reaction conditions using varied ratios of citric acid as a dopant and copper chloride as oxidant. The as synthesized polymer is well characterized using IR, XRD and FESEM techniques. After characterization we also synthesized various metal oxide and polymer composite systems for gas sensing. Also, the anti-bacterial properties were also checked for these as synthesized polymer-inorganic composite material.

### **AP-11 : Physico - Chemical Analysis of Water from Various Sources in Anakapalli City, Visakhapatnam District, Andhrapradesh**

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Water is essential to life. The provision of water of adequate quantity for human use and consumption is not only a pre-requisite for development but also a major contribution towards the improvement of health, hygiene and welfare of people. They added that access to safe water reduces water-borne and water-washed diseases. In ordered to assess the quality of water we have determined Physico- chemical analysis in some areas of Anakapalli city, Visakhapatnam District, of Andhrapradesh. In Physico-chemical analysis, various quality parameters are measured including pH, Specific Conductivity, Turbidity, Total hardness, Alkalinity, Acidity, Calcium, Magnesium, Chloride, compared with WHO standards of water quality. The assessment of these parameters is essential to identify magnitude and source of any pollution load. These characteristics can identify certain condition for the ecology of living organisms and suggest appropriate conservation and management strategies.

### **AP-12 : Silver Nanoparticles based Optical Fiber Transmission Sensor for the Detection Of Mercury**

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Exploring the biological materials as a reducing/capping agent for the

synthesis of metal nanoparticles has set a new trend in green nanotechnology with improved environmental quality. Herein, a facile, one pot and “Green” synthesis of silver nanoparticles (AgNPs) was achieved using gum acacia as a cost effective and eco-friendly biomaterial. Synthesized AgNPs were characterized using UV-VIS spectroscopy, FTIR, TEM and AFM analysis. The solution of AgNPs was found decolorized owing to the dissolution of AgNPs and the formation of an Ag-Hg amalgam. In this context, a simple and easy to miniaturized optical fiber transmission sensor was developed for the detection of  $\text{Hg}^{2+}$  based on the decolorization of AgNPs. The sensor was found to show linear response in the range of  $10^{-5}\text{M}$  to  $10^{-3}\text{M}$   $\text{Hg}^{2+}$ . The present method for the detection of  $\text{Hg}^{2+}$  is simple, rapid and can be miniaturized into a portable system for the routine onsite sample analysis.

### **AP-13 : Adsorption Studies Of (Cr (VI), Cd (II), And Cu (II)) Metal Ions from Aqueous Solutions by Synthesized $\text{Fe}^{3+}$ and $\text{Ag}^+$ Co-doped $\text{TiO}_2$ Nanoparticles**

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The present communication has been addressed to the removal of Cr (VI), Cd (II) and Cu (II) from aqueous solutions by  $\text{Fe}^{3+}$ - $\text{Ag}^+$  / $\text{TiO}_2$  nano metal oxide synthesized by Sol-Gel technique and characterization was done by XRD, SEM, TEM, EDS, and FTIR. Batch equilibrium experiments were performed for various concentrations of 0.1 mg/L to 1 mg/L and the effect of contact time, pH and adsorbate dosage was investigated. The adsorption kinetics was well fitted to pseudo-second order kinetic model, Weber-Morris & Reichenberg Kinetic equations. Langmuir and Temkin isotherms were found well fitted with the data.

### **AP-14 : Microwave Assisted Synthesis and Characterization of Carboxymethyl Lignin from Lignin Bio-polymer Obtained from Biomass of Bagasse Pulping**

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In the present study, a simple and efficient method is described

for the synthesis of biodegradable soluble Carboxymethyl lignin (CML) using insoluble Kraft lignin bio-polymer which was isolated from bio mass of bagasse pulping under microwave irradiation. The present work revealed that rapid synthesis of CML and CML's degree of substitution (D.S.) was studied with respect to reaction time, microwave power and concentration of reactants. Further the characterization like FTIR, and PSD studies were carried out to evidence the changes observed in the CML.

### **AP-15 : Estimation of Iron (III) in Natural Food Samples by Tetra Butyl Ammonium Bromide from Aqueous Acid Solutions**

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Solvent extraction of iron (III) has been carried out with Tetra butyl ammonium bromide (TBAB) in chloroform from hydrochloric, sulphuric, nitric and perchloric acid media. Stripping of iron from the organic phase was done with 2M hydrochloric acid. The extractions were nearly quantitative with all the acid systems employed in the study. Based on the results obtained, estimation of iron in natural food samples has been attempted.

### **AP-16 : Synthesis and Characterisation of Chitosan-Guar Gum-G-Poly(Methyl Methacrylate)/Silica (Gg-G-mma/Silica) and its Use as Bio-sorbents of Heavy Metal Ions In Water**

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Utilization of raw materials available in nature and their applications to synthesize useful bio nanocomposites without any adverse impact on the environment has long been a desired goal. Recently, a lot of work has been done in the development of low-cost sorbents for water remediation. Bio-based polymers have greater impacts on the human being by reducing the dependence on fossil fuels and through the related positive environmental impacts such as reduced carbon dioxide emissions. In this work, cross-linked super adsorbent bionanocomposite has been synthesized using two biopolymers such as chitosan, guar gum and monomer methyl methacrylate by graft copolymerization via emulsifier-free emulsion polymerisation reaction in presence of potassium persulfate (KPS) as an initiator and silica as cross linking agent in aqueous solution.

FTIR analysis was carried out to confirm chemical structure of the so formed composite and SEM was used for morphological study. The composite was also characterized by XRD to study its crystalline nature. The effect of the various reaction parameters such as guar gum, chitosan concentration, monomer concentration, initiator concentration, cross-linker concentration and pH on adsorption of metal ions were investigated to achieve improved methods for water remediation. The main application of the so prepared composites could be for the removal of micro quantities of heavy metal ions such as V (V), Mo (VI), Cr (VI) from the water for the betterment of our environment.

### **AP-17 : Synthesis and Study of Thermal, Mechanical and Biodegradation Properties of Chitosan-G-PMMA with Chicken Egg Shell (Nano-Cao ) as A Novel Bio-filler**

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The important objective of this study is to evaluate the effect of chicken eggshell (nano-Cao) as a functionalized bio-filler on the mechanical strength and thermal stability of acrylic based bionanocomposite of chitosan grafted with poly (methyl methacrylate) (PMMA). The chitosan grafted PMMA adsorbed with functionalized biofiller was prepared via emulsion polymerisation technique and physicochemically characterized as bone graft substitute. The so prepared grafted bioactive bone cement (BBC) bionanocomposite (BNC), Chitosan-g-PMMA/ nano-CaO was characterised by FTIR, XRD, FESEM and TGA. The water uptake, retention ability, their biodegradability and the nanosize particle arrangement in the polymeric BBC-BNCs were undertaken. These preliminary investigations of the BNCs will open the door for their use in bioadhesive bone cement implants in future.

### **AP-18 : Development of Biodegradable Cellulose-G-Poly (Butyl Acrylate)/Kaolin Nanocomposite with Improved Fire Retardancy and Mechanical Properties**

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The main aim of the work is to convert a low cost renewable biopolymer to a high performance fire retardant biomaterial by modification via grafting. Cellulose, a linear and most abundant

biomacromolecule, has gained increasing attention for its interesting properties and potential applications in the synthesis of polymer nanocomposites. Cellulose has been grafted with butyl acrylate via emulsifier free emulsion polymerisation using in situ developed transition metal complex initiating system:  $\text{CuSO}_4$ /glycine/ammonium persulfate (APS) with and without additive kaolin to prepare nanocomposites and copolymer respectively. The morphology of so prepared grafted nanocomposites was characterised by fourier transform-Infrared (FTIR) spectroscopy, X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). The enhancement in thermal behaviour and mechanical properties of nanocomposites over copolymer were outstanding. The fire retardant properties were evaluated by limiting oxygen index (LOI) and cone calorimetry test. The biodegradation and water absorbency of the fire retardant nanocomposites have been carried out for better commercialisation and environmental concern.

### **AP-19 : Studies on Molecular Interactions of 2-Aminothiazole at Different Temperatures**

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Measurements of physicochemical properties such as density and ultrasonic velocity of pure components and mixtures have been used for investigations of thermo-acoustical parameters. In present study physicochemical properties of ternary liquids mixtures namely; 2-Aminothiazole + 1, 4-Dioxane (Dx)-water have been estimated at T= (303.15, 308.15 and 313.15) K for the entire range of molar concentrations. From the experimental data viz. adiabatic compressibility ( $\beta_s$ ), intermolecular free length ( $L_p$ ), specific acoustic impedance (Z) and relative association ( $R_A$ ), have also been calculated using standard relations. The result suggests presence of molecular interactions in components. The effect of different temperatures on strength of molecular interaction has also been studied.

### **AP-20 : Acoustical Studies of 2-Mercapto-benzothiazole at Different Temperatures**

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This paper report measurements of densities and ultrasonic

velocities for ternary mixture 2-mercaptobenzothiazole + acetonitrile + distilled water as a function of composition at T=(303.15, 308.15, 313.15, 318.15 and 323.15) K. Densities and ultrasonic velocities were measured using densitometer and ultrasonic interferometer respectively. The experimental results compared with data published in the literatures.

## **AP-21 : Physicochemical Characteristics of Groundwater in Different Sites of Agra City, Uttar Pradesh**

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A systematic study has been carried out to evaluate the physicochemical characteristics of groundwater in Agra city. Six groundwater samples were collected from various locations during April 2015 to May 2015 and analysed for pH, turbidity, electrical conductivity, total dissolved solids, total alkalinity, total hardness, calcium, magnesium, fluoride and chloride following the standard methods and procedures. Present work revealed that groundwater is comparatively very hard and slightly alkaline. Fluoride contents vary from place to place. The sampling sites showed that the physicochemical parameters were not within the water quality standard and was not found fit for drinking.

## **AP-22 : Health Risk Assessment of Exposure to Fine Particulate Matter in Different Types of Small Scale Industries in Agra**

**Prerna Arya and Ajay Taneja**

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Small scale industry is a potential source of air pollution and responsible for number of health effects in both indoor and outdoor environment. Present study is carried out to evaluate health risk assessment on occupational workers. Sampling was done for three days (two days indoor and one day outdoor) in each industry in the month of August to September 2016 in three small scale industries in Agra which are respectively: vehicle servicing centre (S1), engineering unit (S2), and foundry (S3). In these industries PM<sub>2.5</sub> samples were collected on PTFT filter paper by using Particulate Sampler (APM550 Envirotech). Further, elements (Fe, Cr, Pb, Ni, Cd, Zn, Na, Ca, Mg) in PM<sub>2.5</sub> was analysed with the help of ICP-AES (Inductive Coupled Plasma- Atomic Emission Spectroscopy). Results revealed the I/O and

ratio of  $PM_{2.5}$  and elements were maximum observed at S1 and S2 sites respectively. Percentage bioavailability for the elements followed the trend as  $Pb > Zn > Fe > Ni > Cr$  in indoor while for outdoor followed the trend as  $Fe > Cr > Pb > Zn > Ni$ . A calculated value of HQ for Cr is equal to (1.7400) through inhalation pathway in indoor of S2 sampling site further posing non carcinogenic risk. The ECR calculated value for the metals Cr, Ni, and Pb for indoor exposure, ranged from 0.012- $8.36 \times 10^{-7}$  among which Cr was found to pose maximum cancer risk to workers at all industrial sites.

### **AP-23 : Effect of Furfuraldehyde on the Polymerization of Acrylonitrile Initiated by Benzoyl Peroxide**

**Gyan Singh and R.K.S. Dhakarey**

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PAN (polyacrylonitrile) is a synthetic, semicrystalline organic polymer resin, with the linear formula  $(C_3H_3N)_n$ . In the present study, effect of Furfuraldehyde on the polymerization of acrylonitrile initiated by benzoyl peroxide has been studied. The different techniques like, FT-IR and UV-VIS were used for characterization. The UV-VIS study showed that the rate of polymerization of acrylonitrile decreases with increase in the concentration of furfuraldehyde. The FT-IR study proves the successful interaction of polyacrylonitrile with furfuraldehyde.

### **AP-24 : One-pot Green Synthesis of Magnetite/Reduced Graphene Oxide Composite using Aqueous Pod Extract of Dolichos Lablab L. for Selective Adsorption of Crystal Violet**

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A facile one-pot green synthesis using low cost and eco-friendly pod extract of Dolichos lablab as reducing agent has been developed to prepare magnetite/reduced graphene oxide ( $Fe_3O_4$ -RGO) composite for removal of crystal violet dye pollutant from aqueous solution. The synthesized  $Fe_3O_4$ -RGO composite was characterized by Ultraviolet-visible spectroscopy (UV-Vis), Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Field emission scanning electron microscopy (FE-SEM), Energy dispersive X-ray spectroscopy (EDX), Transmission electron microscopy (TEM) and vibrating sample

magnetometer (VSM). The presence of RGO enhanced the performance of dye removal efficiency of  $\text{Fe}_3\text{O}_4$ -RGO composite compared to  $\text{Fe}_3\text{O}_4$  NPs alone. The crystal violet dye adsorption capacity of  $\text{Fe}_3\text{O}_4$  NPs and  $\text{Fe}_3\text{O}_4$ -RGO composite were 55.56 mg/g and 79.03 mg/g, respectively. The adsorption behavior of  $\text{Fe}_3\text{O}_4$ -RGO composite adsorbent fits well with the Freundlich isotherm and its kinetic model was pseudo second order.  $\text{Fe}_3\text{O}_4$ -RGO composite can be used as excellent adsorbent in water treatments.

### **AP-25 : Water Effect of crops at District Firozabad (U.P.)**

**Prem Prabhaker**

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The prehistoric man, after exhaustion of his food resources at one place, used to migrate to other places. No one exactly knows when men learnt about agriculture, the science of preparing the land, sowing the seeds, taking care of their irrigation and manure and fertilizers need and to reaping the harvest. It has been a great step in the history of mankind towards civilization. It was due to this that they started living at a place and came nearer to each other. The improvement of this particular science of agriculture has always been a concern of mankind. With the increasing population and comparatively low supply of agricultural goods from the farmer's side, it has always been an interest among the scientists to find out new means of improving it. Now a days, the farmers have started using the underground water of wells, ponds, tubewells etc. for irrigation. Ground water mainly comes from the seepage of surface water and is held in the subsoil and pervious rocks<sup>1</sup>. This water is never (without exception) pure. It always contains some amount of chemical salts dissolved in it. The presence of these salts alters the pH of water from the normal. Different crops and even the different varieties of some crops need different proportions of these salts. Slight deviations from the required optimum values affect the crop and the harvest qualitatively as well as quantitatively. This is, therefore, an attempt to study the suitability of irrigation waters for different crops.

### **AP-26 : Study of Physico-Chemical Parameters and Heavy Metals in Sainger River a Tributary of District Etawah, U.P.**

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Water samples from selected point of Sainger river in distt. Etawah

were collected and physico-chemical parameters and heavy metals were determined using standard analytical procedure. For the physico-chemical analysis the results were obtained as follows. pH gave the range (8.00-8.7), temperature was found between 22°C to 31°C and turbidity gave the range 8-9.8 N.T.U. The Chloride and Sulphate contents of all the water samples were found between 18-23 mg/l and 18-48 mg/l, total hardness gave range 135-180 mg/l, total dissolved gave range 302-480 mg/l and alkalinity gave range 189-225 mg/l, zinc and Iron were found in the range 140-175 µg/l and 430-540 µg/l respectively. Fluoride level was also high in Sainger river, which was found in the range 1.4-2.3 mg/l. Copper and Chromium were found in the range 10.75-13 µg/l and 5.2-6.0 µg/l. These results were said to have agreed with the limits set by WHO for drinking water except Fluoride concentration.

## INORGANIC CHEMISTRY SECTION

### Sectional President's Address

#### Development of New Generation Aromatic Dithiophosphate Ligands and their Metal Complexes

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Dithiolate complexes are well known for their technical applications as waste water aerofloate, superconductors, pesticides, resins, Q-switching dyes for IR spectroscopy, biocatalysts and are also used in both metal extraction and analytical chemistry. Recent years have witnessed a new beginning in the area resulting from the use of metal dithiolates as single-source precursors (SSPs) to metal sulfide materials. These sulfur rich ligands are very interesting from the viewpoint of their electrical conductivity, molecular magnetism, electrochemical properties, biological processes and optoelectronic properties. Metal dithiolates and their adducts with variety of Lewis bases such as amine, imine and phosphine are extensively investigated, not only for their wide applications in various fields but also due to coordination ability of dithiolates (dithiophosphate) anions, which bind in mono- or bidentate fashion or may also lie outside the coordination sphere of central atom. Dialkyl and alkylene dithiophosphates of metals and metalloids have already been received the attention owing to their versatile applications in several fields. We have recently reported for the first time new dithiophosphate ligands containing disubstituted phenyl ring instead of alkyl or alkylene moiety. Several new complexes of transition and non-transition metals have been synthesized with newly isolated disubstituted diphenyldithiophosphate ligands corresponding to  $[\{(RO)_2PS_2\}_nSn(^nBu)_xCl_{4-x-n}]$ ,  $[\{(R)_2PS_2\}_3M]$  and  $[\{(RO)_2PS_2\}_2ML_2]$  [R = o-, m-, p-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>, p-Cl-m-CH<sub>3</sub>C<sub>6</sub>H<sub>3</sub>, 2,4-

(CH<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 2,5-(CH<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 3,4-S(CH<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 3,5-(CH<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>3</sub> and 4-Cl-3-(CH<sub>3</sub>)C<sub>6</sub>H<sub>3</sub>; M = V, Mn, Cr, Fe, Co, Ni, Cd and Bi; L = C<sub>5</sub>H<sub>5</sub>N, 3,4-(CH<sub>3</sub>)<sub>2</sub>C<sub>5</sub>H<sub>3</sub>N and 4-(C<sub>2</sub>H<sub>5</sub>)C<sub>5</sub>H<sub>4</sub>N]. These were characterized by elemental analyses, magnetic moment, IR, heteronuclear NMR (<sup>1</sup>H, <sup>13</sup>C and <sup>31</sup>P) spectroscopy and single crystal X-ray analysis. Single crystal X-ray analysis of several complexes reveals the square planar and octahedral geometry around the metal centre. The dithio ligands are coordinated to the metal ion as a bidentate fashion via thiolate sulfur atoms. Cyclic voltammetry experiment was carried out to probe the redox capabilities of these complexes. The thermal properties of the complexes have also been examined by combined DTA/DTG thermal analyses which displayed the end product as metal sulfide or sulfate. The theoretical studies of dimethyl diphenyldithiophosphate ligands and few complexes have been also carried to correlate the experimental and theoretical data. Theoretically calculated frontier molecular orbitals (HOMO–LUMO) and their energies suggest that charge transfer occurs within the compounds. The cytotoxicity of the complexes has also been measured in vitro using the cultivated human cell lines. The biological activities of the ligands and complexes against specific bacteria and fungus have shown potential activity.

## **IIL-01 : Medicinal Inorganic Chemistry : Existing Scenario and Emerging Prospects**

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Medicinal inorganic chemistry and Biomedical Inorganic chemistry are fairly recent offshoot of bioinorganic chemistry, which itself is a science still with much to learn. It includes metal-based drugs, metal sequestering or mobilizing agents, metal containing diagnostic aids and the medicinal recruitment of endogenous metal ions. It offers the potential for the design of novel therapeutic and diagnostic agents and hence for the treatment and understanding of diseases which are currently inter-actable. Inorganic elements play crucial role in biological and biomedical processes and it is evident that many organic compounds used in medicine do not have a purely organic mode of action; some are activated or biotransformed by metal ions including metalloenzymes, other have a direct or indirect effect on metal ion metabolism.

The unique properties of metal complexes tend to offer advantages in the discovery and development of new drugs. Metal centers are capable of organizing surrounding atoms to achieve pharmacophore geometries that are not readily achieved by other means. Additionally, the effects of metals can be highly specific and can be modulated by recruiting cellular processes that recognize specific types of metal-macromolecule interactions. Metals can be useful probes of cellular functions. Understanding these interactions can lead the way towards rational design of metallopharmaceuticals/metallo-drugs implementations of new co-therapies. Metal based agents can modify both DNA and RNA with high degree of regiochemical, sequential and conformational specificity.

The related issues will be discussed with special reference to antidiabetic and insulinomimetic functional models of vanadium-chelates.

## **IIL-02 : Advances in Nano-Chemistry : Hazards with Benefits with Special Context to Inorganic Nano-Particles**

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Research in the nano-particles (NP) and nanotechnology field is growing at a breathtaking pace. The reason is simple: the unique

properties of NP will allow the development of products with unprecedented characteristics and opportunities in every field of human activity, and with tremendous economic impacts. It is currently anticipated that the number of exposed Quebec workers, not only in manufacturing these products but also in using and processing them, will increase over the next few years. Several products are already available commercially and some Quebec companies now have large-scale NP production capacity. While technological research is already well established, with many transfers to industrial production, research on occupational health and safety (OHS) risk assessment has lagged behind significantly. Fortunately, the latter has shown strong growth in the scientific community over the last 10-15 years. Among the inorganic nano-particles, TiO<sub>2</sub> has been studied abundantly. NIOSH published a preliminary version of its assessment of the health risks related to occupational TiO<sub>2</sub> exposure. The details of the assessment can be consulted in the NIOSH document. To summarize, NIOSH recommends an exposure limit of 0.1 mg/m<sup>3</sup> for ultrafine TiO<sub>2</sub> particles, while the recommended limit for fine TiO<sub>2</sub> particles is 1.5 mg/m<sup>3</sup> (for exposure up to 10 h per day during a 40 h work week). This difference reflects the influence of specific surface in the toxicity of ultrafine particles. These recommendations should reduce the lung cancer risk to less than 1 in 1000 among workers exposed to TiO<sub>2</sub>. Health effects of other nano-particles will also be presented in the talk.

### **III-03 : Graphene Oxide and its Composites as Novel Heterogeneous Catalysts in Organic Synthesis**

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The whole world is grappling with energy crisis. Catalysis is one of the core areas of contemporary research since it plays a crucial role in the conversion of renewable and non-renewable sources to useful products such as fuels, fine chemicals, and pharmaceuticals etc. Presently, there is a great need for development of new, green, cheap, and sustainable materials that could act as catalysts in industrial sector to mitigate the energy crisis all over the world.

The Graphene, after Carbon Nanotubes (CNT's), has become a new super star in the carbon world. Graphene oxide (GO) is one of the most important derivatives and oxidized form of graphene. By virtue of its remarkable structure and physicochemical properties, GO alone and its composites have recently been used as heterogeneous catalysts in several organic reactions.

During the talk, the synthesis and characterization of GO and its several composites with  $\text{TiO}_2$  (GO- $\text{TiO}_2$ ),  $\text{MnO}_2$  (Go- $\text{MnO}_2$ ) and Cu(II) Schiff base complex (GO-Cu) will be discussed. The results of characterization of these new composites by FT-IR, FT-Raman, XRD, UV, TEM, FE-SEM, EDAX, TGA,  $\text{N}_2$  adsorption-desorption and AAS analysis will be revealed. The catalytic potential of these new emerging heterogeneous catalysts will be elaborated in the synthesis of amides, azo-derivatives, heterocyclic compounds and in the -C-H activation reactions.

### **III-04 : Mixed Sulfur Donor Ligand Complexes of Antimony(III) : Synthesis, Structural Investigation, characterization, Power XRD, FAB<sup>+</sup> Mass, Supramolecular Association, Single Crystal X-ray, Thermal (TGA, DTA, DSC) and Antimicrobial Activities**

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The 1,1 dithiolato, 1,2 dithiolato and other sulfur donor ligands and their antimony(III) complexes have found their applications in a number of ways like in analytical methods, in production of petroleum derivatives, for regeneration of cracking catalysts, lubricants oil additives and as antiviral agents, antidotes, antimicrobial as well as antitumor drugs. These complexes have wide range of structural possibilities: Ligands can behave as monodentate, bidentate (bridging and chelating) and bimetallic- triconnective and small ligand bite, substituents organic groups as well as antimony(III) has a stereochemically active lone pair of electrons. Polymeric supramolecular assemblies also play important role in deciding the geometry of the molecules.

In view of the above antimony(III) compounds with sulfur donor ligands have been synthesized by the reactions of antimony(III) precursors with 1,1 dithiolato, 1,2 dithiolato and other sulfur donor ligands, in different suitable molar ratios in anhydrous organic solvents with different sets of yellow solids or semisolids are soluble common organic solvents. These compounds have been characterized by physicochemical, spectral [UV-Vis, FTIR, Far IR, NMR ( $^1\text{H}$  and  $^{13}\text{C}$ )], Power XRD, FAB<sup>+</sup> Mass and Thermal (TGA, DTA and DSC) studies. Thermal studies have been carried out in inert atmosphere and the last thermal decomposition product was formed to be pure  $\text{Sb}_2\text{S}_3$  which be used in a number of ways.

The single crystal studies of tris(N,N'-dimethyldithiocarbamato-S,S') antimony(III) found to be a dimer with Sb...S and C-H...S interaction as well as chlorobis(N,N'-dimethyldithiocarbamato-S,S') antimony(III) also found it to be a dimer with C-H...Cl interaction as in supramolecular structure.

Some of these compounds have been screened in vitro against four human pathogenic bacterial species, two Gram-positive [Staphylococcus aureus (ATCC 9144) (G+) and Bacillus subtilis (ATCC 6051) (G+)] and two Gram-negative [Escherichia coli (ATCC 9637) (G-) and Pseudomonas aeruginosa (ATCC 25619) (G-)] and two fungal species [Aspergillus niger (ATCC 9029) and Penicillium chrysogenum (ATCC 10106)].

### **III-05 : Facile Synthesis, Structural Evaluation, Antimicrobial Activity and Synergistic Effects of Novel Imidazo[1,2-a]Pyridine based Organoselenium Compounds**

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In continuation of our long-standing interest in the design of synthetic methodologies for the generation of biologically active organochalcogens,<sup>1-3</sup> we have exploited a potentially active imidazo[1,2-a]pyridine moiety as a core template for the synthesis of a number of hitherto unknown imidazo[1,2-a]pyridine selenides by reaction of 2-chloroimidazo[1,2-a]pyridines with aryl/heteroarylselenols, generated in situ by reduction of various diselenides with hypophosphorous acid. The crystal structures of 3-nitro-2-(phenylselanyl)-imidazo[1,2-a]pyridine, 2-(mesitylseyanyl)-3-nitro-imidazo[1,2-a]pyridine and 3-nitro-2-(pyridin-2-ylselanyl)-imidazo[1,2-a]pyridine were confirmed by X-ray crystallography, and the DFT calculations were performed to determine various structural parameters which were correlated with the X-ray crystal structures. The synthesized compounds were subjected to antimicrobial evaluation and it was found that compounds 5a and 5j were active against gram negative bacterium Escherichia coli whereas compound 5e was active against different fungal strains. Time kill assay was performed to understand the microbial activity of synthesized organoselenium compounds and the toxicity of these compounds was evaluated against human cell lines. Synergistic effects of active compounds 5a and 5e were tested with existing antibiotic drugs which exhibited that the antibiotic combination with synthesized organoselenium compounds efficiently enhanced the antimicrobial activity.

### **IIL-06 : Syntheses, Single Crystal Structures, DFT Studies and Antioxidant Superoxide Dismutase Studies of Some New Pyrazine Bridged Copper(II) Complexes**

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A series of pyrazine bridged copper(II) complexes  $[\text{Cu}_2(\text{L}^1)_2(\text{pyrazine})](\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$  1,  $[\text{Cu}_2(\text{L}^2)_2(\text{pyrazine})(\text{NO}_3)(\text{H}_2\text{O})]\text{ClO}_4$  2 and  $[\text{Cu}_2(\text{L}^3)_2(\text{NO}_3)_2(2\text{-aminopyrazine})] \cdot 2\text{H}_2\text{O}$  3 have been synthesized using tridentate monoanionic Schiff bases  $\text{HL}^1$ ,  $\text{HL}^2$  and  $\text{HL}^3$  [ $\text{HL}^1$  = 4-chloro-2-[(E)-[2-(pyridin-2-yl)hydrazinylidene]methyl]phenol,  $\text{HL}^2$  = N'-[(E)-phenyl(pyridin-2-yl)methylidene]thiophene-2-carbohydrazide and  $\text{HL}^3$  = N'-[(E)-phenyl(pyridin-2-yl)methylidene]benzohydrazide and pyrazine] by a one pot synthesis. These complexes were characterized by routine physico-chemical techniques. The single crystal X-ray structures of 1, 2 and 3 were determined. X-ray single crystal analyses reveal that complex 1 is four coordinated square planar while complexes 2 and 3 are penta coordinated complex with square pyramidal geometry around each copper centre. Variable temperature magnetic susceptibility data display antiferromagnetic couplings in 1–3. The X-band epr spectra for polycrystalline samples of 1–3 exhibit copper(II) hyperfine structures as well as zero-field splitting which are appropriate for the triplet state of such a dimer. Epr data also indicate antiferromagnetic behavior for binuclear complexes 1–3. These complexes were also studied using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The conproportion constant ( $K_{\text{con}}$ ) of complexes 1–3 have been evaluated and discussed. Modelling by DFT and TD-DFT are done to elucidate the nature and location of the excited state in superoxide dismutase (SOD) mimics. In addition, antioxidant SOD activity showed that copper(II) complexes 1-3 possess significant scavenging effect against  $\text{O}_2^{\bullet-}$  free radicals.

### **IIL-07 : Development of Heterogeneous Catalysts and their Applications in Organic Synthesis**

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Heterogeneous catalysis, particularly based on biomaterial derived composites is an attractive area of research playing a crucial role in the chemical industry with significant economic and environmental impact. The preparation of porous materials from renewable resources such as starch, cellulose, chitosan etc is particularly attractive as

they are renewable, biodegradable and have broad chemical-modifying capacity. The combination of high surface area inorganic mesoporous materials like silica with organic polymer systems provides further strength and it is an emerging class of hybrid materials with numerous potential applications. Moreover, an appropriate surface modification for these inorganic/organic composites can be done to prevent the aggregation of metal nanoparticles, leading to stable, finely dispersed active species. The surface modification can be done by introducing amines, substituted amines, imines, thiols, carboxyl groups. These groups bind the metal nanoparticles and hence stabilize them. These heterogeneous catalysts proved to be highly efficient for carrying out industrially important organic transformations. The development of some active and stable heterogeneous catalysts based on organic-inorganic hybrid composites and their applications in organic synthesis would be discussed in the 36<sup>th</sup> Annual Conference of the Indian Council of Chemists.

### **III-08 : Synthesis of Newer Chalcone and Flavones Tethered 1,2,4 Triazole Hybrids as Potent Antimicrobial Agents**

**Alka Agarwal**

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Chalcones and flavones containing compounds showed a wide spectrum of biological activities such as antimicrobial, antimalarial, anticancer, antiinflammatory, antileishmanial, antiprotozoal, anti-HIV, antioxidant, and activities. Due to its remarkable bioactivities and structural novelty, much more effort has been devoted to the synthesis of chalcone and flavone analogues.

In recent years, 1,2,3-triazoles have gained special attention in the drug discovery because several drug molecules contain 1,2,3-triazole group such as Tazobactam, Cephalosporin and Cefatrizine which are clinically used for the treatment of bacterial infections. A series of 1,2,3-triazole bearing chalcone showed notable antimalarial activity against the D10, Dd2 and W2 strains of Plasmodium falciparum, a family of 1,2,3-triazole tethered b-lactam-chalcone bifunctional hybrids exhibited moderate to good cytotoxic activity. 1,2,3-triazole analogues of flavone displayed antimicrobial activity and are estrogen receptor alpha-positive breast cancer inhibitors.

On basis of above facts and a part of ongoing research work in our laboratory, we synthesised a small library of 25 compounds of 1,4-disubstituted-1,2,3-triazole derivatives of chalcones and flavones. Some of synthesized Compounds showed promising antibacterial activity while

other compounds showed good antifungal activity as compared to the corresponding standard drugs. Compound 10 b was found to be the most active against Plasmodium falciparum while the remaining compounds showed moderate to weak antiplasmodial activity. However, cytotoxic activities of all compounds were found ineffective against Huh-7 cells. More details of study will be discussed in conference.

### **IIL-09 : Newer Approach for Antimalarial Drug Discovery**

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The chemistry is the most fascinating areas to develop newer drugs for human welfare. Heterocyclic compounds have immense application in the area of biology, in drug discovery, chemical transformations, nanotechnology and material science etc. Sincere efforts have been made in the last two decades to optimize synthetic procedure and produce diversified newer molecules for drug discovery. Malaria has plagued man since ancient times and now threatens approximately half of the world's population. Over one million people die annually due to malaria, especially young children and women of resource poor families in Africa. Malaria remains the most cause of mortality and morbidity in the developing world and is caused by Plasmodium falciparum, P. vivax, P.ovale, and P. malariae. Chloroquine, a synthetic 4-aminoquinoline, is an affordable antimalarial drug which has been the mainstay for the treatment of malaria for decades. Artemisinin (and its derivatives), extracted from Artemisia annua, is now the only drug which cures all forms of malaria and drug resistance has not been found so far. Significant progress has been made to eradicate malaria globally, still more research is needed. We have developed few series of tetraoxane analogs with nanomolar activity. We will discuss the results in details.

### **IO-CYSA-01 : Synthesis, Structural Characterization and DFT Studies of New Mixed Ligand Oxovanadium(IV) Complex with NNO Donor Schiff Base**

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The mixed ligand oxovanadium(IV) complex  $[VO(L_1)(L_2)]$  [ $L_1 = N'$ -[(E)-phenyl(pyridin-2-yl)methylidene]benzohydrazide and  $L_2 =$

Benzhydrazide] has been synthesized in aerobic condition. The complex was characterized by elemental analysis spectroscopic (UV-vis, IR, epr) and electrochemical methods. X-ray diffraction pattern was also used to characterize this complex, which has a distorted octahedral structure. Single crystal diffraction analysis reveals that C-H... $\delta$  (aryl/metal chelate rings) interactions contribute to the stabilization of the crystal structure in given dimension.

## **IO-CYSA-02 : Synthesis, Structure, photophysical and DFT Studies of Eu(III) and Tb(III) Complexes with Remarkably Narrow Emission**

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The present study describes synthesis, characterization, photophysical study and density function study of europium(III) and terbium(III) complexes of a new C<sub>3</sub>-symmetric polydentate ligand, 1,4,7-tris-{(5-methyl-8hydroxyquinoline)-1,4,7-triazacyclononane}, (9N3Me5Ox). The characterization was done by elemental analysis, FT-IR, FT-NMR, and ESI-mass spectrometry techniques. The analytical data confirm the formulation of the complexes as [Ln(9N3Me5Ox)(H<sub>2</sub>O)<sub>3</sub>].xH<sub>2</sub>O (x= 3 for Eu complex and x= 2 for Tb complex). The experimental data obtained in the present study were successfully assigned based on the quantum chemical calculations like DFT (GGA/B3LY), performed for the monomer [Ln(9N3Me5Ox)(H<sub>2</sub>O)<sub>3</sub>].xH<sub>2</sub>O molecule. The molecular modeling studies suggest that the metal ion can be easily encapsulated in its central cavity without altering the basic metal-ligand coordination sphere. The nature of the bonding between the lanthanide ions and the 9N3Me5Ox<sup>3-</sup>, elucidated by means of the natural bond orbital (NBO), Morokuma Ziegler energy decomposition analysis (ETS-NOCV) scheme, suggest that the Ln-L bonds are more electrostatic (~82%) than covalent (~18%). The photoluminescence spectral studies of the metal complexes revealed that the luminescent properties of the compounds in the solid state and solution are of different origin. In solid state, complexes show the characteristic narrow emission bands of corresponding lanthanide ions with ligand related emission peaks. Lanthanide-centered emission of the complexes overlapped with the ligand emission in solution. An antenna effect of 8-hydroxyquinoline based ligand was observed in powder form of the complexes only, whereas in solution, no effect was noticed. The excitation and emission

behaviour of the ligand and the complexes were established by molecular orbital analysis of the ground state DFT geometry as well as on the excited state optimized geometry using TD-DFT, excitation and emission properties.

### **IO-01 : Synthesis, Spectroscopic and Biological Studies of Novel Heterobimetallic Complexes of Copper**

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The rational design and synthesis of bimetallic complexes is of significant interest to many different areas of chemistry. Originally motivated by biology, the preparation of bimetallic complexes allowed scientists to explore the coordination environments of various metal centers at biologically active sites. In recent years, studies of heteronuclear bimetallic complexes have been of cumulative importance in inorganic and bioinorganic chemistry. The presence of two metals in the same molecule largely affects both the physical properties and the reactivity of the complexes. In this context we have made an attempt to synthesize heterobimetallic complexes of copper. These synthesized complexes are characterized by physicochemical and spectroscopic techniques such as IR, mass and ESR spectra. These complexes have been further screened for their antifungal, antibacterial and anti-inflammatory effects and the results are then compared with the starting materials.

### **IO-02 : Study of Coordination Complexes of Cobalt, Nickel and Copper with Bidentate Schiff Base Ligand their Non-isothermal Degradation and Kinetic Parameters**

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Three mononuclear Co(II), Ni(II) and Cu(II) coordination complexes of a new bidentate 2-chloro-6-[(2,3-dimethoxy-benzylidene)-amino]-4-nitro-phenol ligand derived from 2,3-di methoxy benzaldehyde and 2-amino-4nitro 6-chlorophenol have been synthesized and characterized by elemental; FT-IR, UV-Vis, molar conductance and thermal analysis studies. Thermal properties of the complexes show degradation of complexes under a nitrogen atmosphere up to 1073K. Non-isothermal kinetic parameters, such as activation energy ( $E^*$ ), entropy of activation ( $\Delta S^*$ ), enthalpy of activation ( $\Delta H^*$ ), frequency factor ( $Z$ ) and free energy

change ( $\Delta G$ ) have been calculated using Coats-Redfern (C-R), Piloyan-Novikova (P-N) and Horowitz-Metzger (H-M) methods for the different steps in the decomposition sequence. The theoretical investigations of molecular structures of the synthesized ligand and its metal complexes have been carried out using density functional theory at B3LYP level with standard 6-31G and LANL2DZ basis sets to access reliable results to the experimental values. The calculations were performed to obtain the optimized molecular geometry, HOMO-LUMO, energy gap ( $\Delta E$ ), ionization potential (I), electron affinity (A), absolute electronegativity ( $\chi$ ), chemical hardness ( $\eta$ ), softness (S), electrophilicity index ( $\omega$ ), Molecular electrostatic potential map (MEP) and spin-density.

### **IO-03 : Nanoparticulate Metal Complex Drugs : Synthesis and Spectroscopic Characterization**

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Synthesis and characterization of biologically active nanoparticulate metal complex drugs are of great interest due to the special properties and their potential applications in chemistry, physics and biology. In the past two decades, these fascinating properties have prompted special studies on bioactivity. Synthetic analogs of nano particulate drugs have been studied by different spectroscopic techniques to determine their structure and chemistry, and relate these to their novel chemical properties, physical behavior and pharmacological investigations.

### **IO-04 : Spin Transport Studies of Nitrogen Functionalised Graphene**

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We report on spin transport characteristic of graphene and its nitrogen functionalised counterpart. Initially graphene is synthesized by root chemical method and is functionalised with by adding, spin polarized donor; tetrakis (dimethyl amino) ethylene (TDAE,  $(\text{CH}_3)_2\text{N}_2\text{C}=\text{CN}_2(\text{CH}_3)_2$ ). The presence of nitrogen was confirmed by Fourier Transformed Infra-red (FTIR) Spectroscopy. The analysis

revealed that nitrogen is present in the form of amine functional group. Following this graphene and functionalised graphene was subjected to investigate electron spin resonance (ESR) spectroscopy and cyclic voltammetry (CV) measurement. ESR measurement were performed over 123–473K and CV at room temperature. Analyses of ESR revealed that inter spin and spin lattice relaxation were reduced due to presence of nitrogen. Moreover, this is consistent with electrochemical behaviour for the systems. We underlined the fundamental fact that swift charge transfer of itinerant electron of nitrogen played crucial role on spin transport and charge dynamics.

### **IO-05 : Green Reduction of 2-Nitrophenol by Magnetically Separable Cobalt Substituted Barium Ferrite ( $\text{Ba}_{1-x}\text{Co}_x\text{Fe}_2\text{O}_4$ ; $x=0.0, 0.2, 0.4, 0.6, 0.8, 1.0$ ) Catalyst Synthesized by Citric Acid Auto Combustion Method**

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Cobalt Substituted Barium ferrite  $\text{Ba}_{1-x}\text{Co}_x\text{Fe}_2\text{O}_4$  ( $x=0.0, 0.2, 0.4, 0.6, 0.8, 1.0$ ) samples with uniform particle size are synthesized by using the citric acid auto combustion technique. Cobalt Barium iron citrate precursors by using TG-DTA, revealed the calcination temperature 800 °C. The phase purity and crystal structure was determined by Powder X-ray diffraction, it demonstrated the single phase formation of synthesized catalyst. The synthesized ferrites are used as catalysts for the reduction of 2-nitrophenol to 2-aminophenol by  $\text{NaBH}_4$  as a reducing agent. The reduction of 2-nitrophenol is carried out in water. The catalyst is separated from the reaction mixture by using external magnet. The effect of varying ratio of amount of catalyst and 2-nitrophenol is studied. The enhanced reduction was observed with the introduction of  $\text{Co}^{2+}$  in to the Barium ferrite lattice.

### **IO-06 : Speciation Studies of Ternary Complexes of Pb(II), Cd(II), Hg(II) with L-dopa and Phenanthroline in Dimethylformamide–Water Mixtures**

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Formation of ternary complexes of Pb(II), Cd(II) and Hg(II) ions with L-dopa and 1,10-Phenanthroline was studied pH metrically in

the concentration range of 0–60% v/v Dimethylformamide-water mixtures maintaining an ionic strength of 0.16 mol L<sup>-1</sup> at 303.0 K. Alkalimetric titrations were carried out in different concentrations of metal (M = Pb(II), Cd(II) and Hg(II) to Dopa (L) to Phen (X). Stability constants of ternary complexes were calculated and various models were refined with MINIQUAD75. The best fit chemical models were selected based on statistical parameters and residual analysis. The species detected are MLXH, and ML<sub>2</sub>X for Pb(II) and Cd(II), and Hg(II). The chemical speciation, metal bioavailability and transportation are explained based on the stability constants.

### **IO-07 : Coordination Chemistry, Crystal Structure, Anti-Microbial and Anti-Tuberculosis Screening of Copper (II) Complexes of Tautomeric Azine Schiff's Base : 3,5-di-tert-butyl-2-hydroxybenzoylhydrazone of 2-Acetylpyridine**

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Schiff base L<sup>1</sup> was synthesized by the condensation of 3,5-Di-tert-butyl-2-hydroxybenzoylhydrazide with 2-acetylpyridine. The resulting carboxyhydrazone with R1HC=N-NH-COR2 type of core functional group was found to have tautomerized to the more stable azino enol or diimino enol form i.e. R1HC=N-N=COHR2 type, during complexation. This is nothing but the derivative of the versatile azine group, which gives the main functionality to the ligand while complexing with the transition metal ions. The azines are receiving increasing attention in recent years because of their utility in many interesting chemical, physical and biological applications. The ligand was complexed with copper (II) chloride and acetate salts which resulted into square pyramidal dichlorido-bridged dinuclear complex, with the [Cu<sub>2</sub>(μ-Cl)<sub>2</sub>] core unit and z-in compressed mononuclear octahedral complex for acetate salt. The complexes were characterized based on various physico-chemical and spectral analyses like melting point, molar conductance, elemental analysis, FTIR, C<sup>13</sup> and H<sup>1</sup>NMR, UV-Visible, EPR, Thermo-Gravimetric and single crystal XRD analyses. The ligand and its complexes were screened for the antimicrobial and anti tuberculosis properties.

## **IO-08 : Effect of Glycine on Optical, Dielectrics and Second Harmonic Generation (SHG) Efficiency of Bis-Thiourea Copper Malonates : Semiorganic Non-Linear Optical Materials**

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A new class of semiorganic nonlinear optical materials viz. pure and glycine doped bithiourea copper malonates (BTCuM, BTCuM-Gly) have been synthesized by solvent free mechanochemical method. Chemical composition was confirmed by CHNS and chemical analysis. Incorporation of glycine in the pure compound was confirmed by FTIR and EDAX. FTIR studies also ascertained the coordination of metal ions to thiourea through sulphur atom. SEM images show BTCuM is porous and agglomerated while BTCuM-Gly is crystalline in nature. Thermal behavior has been investigated by TG and DTA showing BTCuM is more stable. Transmittance spectra reveal that lower UV cut-off wavelength of these compounds ranges between 324nm to 321nm indicating good optical transmission in entire visible region. This improves the NLO property of materials and can be used in opto-electronic devices. The dielectric measurements with varying frequencies at room temperature were studied. Dielectric constant and dielectric loss of glycine doped compound shows lower values than that of values shown by pure, which enhance SHG coefficient. SHG measured by Kurtz-Perry powder technique was found to be 1.014 times higher for BTCuM-Gly than that of pure compound which defines nonlinear optical nature of materials and their suitability for NLO applications.

## **IO-09 : Improved Photocatalytic Properties of NiS Nanocomposites Prepared by Displacement Method for Degrading Rose Bengal**

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The present work describes NiS nanoparticles are prepared by chemical displacement method using CTAB as a stabilizer or Surfactant. For the source of Sulphur ion, we used thioacetamide as fuel and metal salt like nickel nitrate. The structural, morphological, metal percentage and optical properties of as synthesized nanoparticles are investigated by using x-ray diffraction (XRD), UV-Visible Spectra; field

emission gun Scanning electron microscopy (FEG-SEM) with EDAX, Fourier transforms infrared spectroscopy (FTIR) and High-resolution Transmission electron microscopy (HR-TEM). The x-ray diffraction patterns revealed that the particles exhibited a crystal structure at the suitable temperature. The average particle size of the nanoparticles from the x-ray diffraction is about 20-40 nm and also field emission gun Scanning electron microscopy shows good morphology and exhibited clearly hexagonal shape. The Transmission electron microscopy (HR-TEM) shows the crystalline size of structures is 22 nm. Further, the Photocatalytic activity of Synthesized NiS nanoparticles was investigated by photo degradation of Rose Bengal as a model of organic pollutant.

### **IO-10 : Structures and Biological Evaluation of Copper(II) Complexes with Isoxazole Schiff bases**

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Copper(II) binary complexes of the type  $[\text{Cu}(\text{L}^{1-3})_2]$ , where  $\text{L}^1 = 2$ -((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-6-methylphenol (1),  $\text{L}^2 = 2$ -((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-6-ethoxyphenol (2),  $\text{L}^3 = 2$ -((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-4,6-di-tert-butylphenol (3) have been synthesized and characterized by analytical, structural, and spectral methods. The X-ray crystal structure analysis shows that the complexes adopted distorted square planar geometry. The interaction of calf thymus (CT) DNA with the copper(II) complexes was explored using absorption, emission spectral methods and viscometry. Spectral evidence showed the intercalative mode of DNA binding with the complexes. Agarose gel electrophoresis results revealed that all these complexes induced double strand breaks of pBR 322 plasmid DNA in the presence of  $\text{H}_2\text{O}_2$  through an oxidative pathway and in the presence of UV light as photolytic path way. Moreover, the synthesized compounds were monitored for antimicrobial activities and the results of these studies indicated that the complexes exhibit a stronger antimicrobial efficiency compared to their corresponding ligands.

### **IO-11 : Chemical Speciation of Ternary Complexes of Mercaptosuccinic Acid and 1,10-phenanthroline in Acetonitrile-Water Mixtures**

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Formation of ternary complexes of Pb(II), Cd(II) and Hg(II) ions

with Mercaptosuccinic acid and 1,10-Phenanthroline was studied pH metrically in the concentration range of 0–60% v/v acetonitrile-water mixtures maintaining an ionic strength of 0.16 mol L<sup>-1</sup> at 303.0 K. Alkalimetric titrations were carried out in different concentrations of metal (M = Pb(II), Cd(II) and Hg(II) to MSA (L) Phen (X). Stability constants of ternary complexes were calculated and various models were refined with MINIQUAD75. The best fit chemical models were selected based on statistical parameters and residual analysis. The species detected are MLXH, MLX for Pb(II) and Cd(II), and Hg(II). The chemical speciation, metal bioavailability and transportation are explained based on the stability constants.

### **IO-12 : DNA Binding, Cleavage and Antimicrobial Studies on Co(II), Ni(II) and Cu(II) Complexes of 4-Trifluoromethoxy Aniline Schiff Base**

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Three mononuclear complexes, 1[Co(L)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>], 2[Ni(L)<sub>2</sub>] and 3[Cu(L)<sub>2</sub>] with Schiff base ligand, LH (2-((E)-(4-(trifluoromethoxy) phenylimino)methyl)-6-tert-butylphenol, C<sub>18</sub>H<sub>18</sub>F<sub>3</sub>NO<sub>2</sub>) have been synthesized and characterized by elemental analysis, ESI mass, FT-IR, ESR, UV-visible, magnetic susceptibility and TGA studies. The spectral and analytical data suggested that, complexes 1 adopted an octahedral geometry whereas complexes 2 and 3 owned a square planar geometry. DNA binding and cleavage studies of all complexes have also been investigated against calf thymus (CT-DNA) and supercoiled pBR322 DNA respectively. The experimental results revealed that the complexes bound effectively to CT-DNA through an intercalation mode and also cleaved pBR322 DNA in an efficient manner. The complexes along with ligand have been screened for antimicrobial activity against bacterial species *Bacillus amylo-liquefaciens* and *Escherichia coli* as well as fungal species *Macrophomina phaseolina* and *Sclerotium rolfsii*, and it is found that all complexes are more potent than ligand.

### **IO-13 : A Selective Fluorogenic Probe for Detection of Al<sup>3+</sup> in Aqueous Medium**

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A Schiff-base compound, 2-((E)-1-(2-(dimethylamino) ethylimino)

ethyl) phenol (HL), has been synthesized and characterized by different spectroscopic methods. The chemosensor shows selective “turn-on” cyan color fluorescence response to  $\text{Al}^{3+}$  ion over a wide variety of other competing metal ions such as  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Hg}^{2+}$ ,  $\text{Mn}^{2+}$  and  $\text{Ca}^{2+}$ . The fluorescence emission intensity at 462 nm displayed by the chemosensor increases progressively during the addition of  $\text{Al}^{3+}$  ion until saturation point, with over 27 fold intensity enhancement. Similar fluorescence behavior is also observed in a variety of solvents/solvent mixtures in the presence of  $\text{Al}^{3+}$  ion. UV-visible titration experiment has established that the chemosensor, HL, binds to  $\text{Al}^{3+}$  in 2:1 ratio. The fluorescent emission can be observed when a sample solution of HL containing  $\text{Al}^{3+}$  is irradiated by UV light. The effect of emission intensity of  $\text{Al}^{3+}$ -chemosensor complex, in the presence of other interfering metal ions was also monitored to check the effectiveness of the sensor. The detection limit of the  $\text{Al}^{3+}$ -chemosensor is found to be  $4.32 \times 10^{-6}$  M and the stability constant is obtained as  $1 \times 10^4 \text{ M}^{-1}$ . The DFT and TD-DFT calculations performed on HL, L and its aluminium complex, give insight into the geometric, electronic, thermodynamic and optical properties of chemosensor- $\text{Al}^{3+}$  interactions.

#### **IO-14 : Selective Epoxidation of Styrene using Alkali and $\text{Sr}_x\text{Ca}_{1-x}\text{Fe}_2\text{O}_4$ ( $0.0 \leq x \leq 1.0$ ) Catalyst**

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Spinel type strontium substituted calcium (SSC) ferrite  $\text{Sr}_x\text{Ca}_{1-x}\text{Fe}_2\text{O}_4$  ( $0.0 \leq x \leq 1.0$ ) catalyst synthesized by citrate-gel combustion method are well characterized by various techniques such as TG-DTG, FT-IR, XRD, SEM, EDS and BET. The crystallization temperature of the spinel SSC ferrite particle prepared by citrate gel is 600 °C, which is lower than that prepared by other methods. Among this series of catalysts,  $\text{Sr}_{0.2}\text{Ca}_{0.8}\text{Fe}_2\text{O}_4$  has highest surface area, shows the best catalytic efficiency. GCMS analysis revealed that, the insertion of oxygen takes place selectively than the oxidative cleavage of C=C bonds; to give epoxide as major product, while addition of NaOH suppress further isomerization of the styrene epoxide, thereby increasing the selectivity remarkably to give epoxide as major product. The catalyst containing both  $\text{Sr}^{2+}$  and  $\text{Ca}^{2+}$  ions are more active than pure  $\text{SrFe}_2\text{O}_4$  and  $\text{CaFe}_2\text{O}_4$ . The synergistic effect of  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$  ions and greater site preference energy of  $\text{Sr}^{2+}$  than  $\text{Fe}^{3+}$  favors the selective epoxidation of styrene in presence of 30%  $\text{H}_2\text{O}_2$  as oxidant. The optimization of various reaction conditions like reaction time,

temperature, solvents, substrate to oxidant molar ratio, oxidant, amount of catalyst and of NaOH on the conversion of styrene and product distribution were also studied.

### **IO-15 : Synthesis, characterization and biological studies of binary metal complexes derived from Schiff base ligand**

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A series of new binary metal complexes of Cu(II), Co(II) and Ni(II) complexes were synthesized from Schiff base derived from 2-hydroxy-1-naphthaldehyde and substituted aromatic amine. The synthesized compounds were well characterized by I.R., U.V., Proton-NMR, <sup>13</sup>C-NMR and Mass spectral data and SEM-EDX analysis. Compounds so prepared have been subjected to interactions with calf thymus DNA (CT-DNA). These studies revealed that these complexes have good interacting property. All the newly synthesized compounds have been screened for their in-vitro antibacterial activities against E.coli, B. subtilis, Staph. aureus, P.aeruginosa, E. coli and antifungal activities against Candida parapsilosis and Rizopus and the results showed that the complexes exhibited good activity against various pathogens.

### **IO-16 : Synthesis, Characterization and Crystal Structure of Cu(II) Complex of Trans-Cyclohexane-1,2-Diamine : Application in Synthesis of Symmetrical Biaryls**

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The C-C bond formation has emerged as an important synthetic methodology for generating more complicated organic compounds from simpler ones. Symmetrical biaryls are synthesized by various methods reported in literature such as Suzuki reaction, Ullmann reaction, and Kumada-Corriu-Tamao reaction etc. Suzuki coupling reaction is one of the most important methodologies for the synthesis of symmetrical biaryls from a single aryl precursor. Copper has emerged as cheap catalysts for obtaining symmetrical biaryls by the homocoupling reaction of arylboronic acids. Therefore, in continuation of our research interest on the synthesis, structural characterization and catalytic applications of transition metal complexes, we herein, describe the synthesis of a new Cu(II) complex  $[\text{Cu}(\text{cyhxn})_2(\text{H}_2\text{O})_2][\text{OTf}]_2$  by the reaction of ligand cyhxn (cyhxn = trans-cyclohexane-1,2-diamine) with  $\text{Cu}(\text{OTf})_2$  in

methanol at room temperature. The complex was fully characterized by elemental analysis (CHN), FT-IR, UV-Vis and EPR spectroscopic techniques. The structure of the complex was confirmed by single crystal X-ray diffraction study. The EPR spectrum is isotropic type having  $g_{\text{iso}} = 2.078$ , which indicates a distorted octahedral geometry of the complex. The complex was found to be an active homogeneous catalyst for the homocoupling reactions of arylboronic acid to obtain symmetrical biaryls at room temperature in methanol at a low catalyst loading (2 mol %) without the use of any additives such as a base and or an oxidant.

### **IO-17 : Copper(II) and Nickel(II) Mono/Binuclear Complexes with N'-(Z)-Phenyl(Pyridin-2-yl)Methylidene]acetohydrazide : Single Crystal Structures, DFT Studies and Antioxidant Activity**

**Yogendra Singh**

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Using N'-(Z)-phenyl(pyridin-2-yl)methylidene]acetohydrazide ligand and metal(II) salts, three new mononuclear and one binuclear  $[\text{Ni}(\text{HL})(\text{NO}_3)(\text{H}_2\text{O})]\text{NO}_3$  1,  $[\text{Cu}(\text{HL})(\text{H}_2\text{O})_2]2\text{NO}_3$  2,  $[\text{Ni}(\text{HL})_2]2\text{ClO}_4$  3 and one end to end thiocynato bridged complex  $[\text{Cu}_2(\mu)(\text{SCN})_2(\text{L})_2]$  4 have been synthesized and characterized by routine physico-chemical techniques. All complexes were structurally characterized using single crystal X-ray diffraction. Complexes 1 and 2 have penta coordinated environment around metal(II) centre whereas complex 3 has distorted hexa coordinated geometry. In complex 4 two symmetry related, adjacent copper(II) coordination entities are unprecedented end to end thiocynato bridged, yielding a dicopper entity. The presence of two "symmetric" thiocynato bridges with Cu-SCN and Cu-NCS distances 2.832 and 1.925 Å, respectively results in a Cu...Cu distance of 5.503 Å. The binuclear complex 4 shows weak antiferromagnetic interaction between adjacent copper(II) centres. Copper(II) mononuclear and binuclear complexes have also been studied by X-band epr spectroscopy. The crystal packing of the structure of these new complexes is stabilized by H-bonding,  $\text{lp} \dots \pi$ ,  $\text{CH} \dots \pi$  and  $\pi \dots \pi$  interactions. The electrochemical data (CV and DPV) of the complexes shows  $\text{M}^{\text{I}}/\text{M}^{\text{0}}$  reduction. Electronic structures and spectral features are explained by DFT studies. Finally the antioxidant superoxide dismutase activity measurements show that the complexes behave as superoxide dismutase mimics.

## **IO-18 : Computer Augmented Speciation of 5-Sulfosalicylic Acid Complexes of Co(II), Ni(II) and Cu(II) in DMF-Water mixtures**

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Speciation of Co(II), Ni(II) and Cu(II) complexes with 5-Sulfosalicylic acid (5-SSA) in the presence of N, N'- Dimethyl formamide-water mixtures (0.0-60% v/v) at an ionic strength of 0.16 mol dm<sup>-3</sup> and temperature 303 K were investigated pH metrically. The existence of different binary complex species was established from modeling studies using the computer program MINIQUAD75. The increased stability of the complexes with increasing DMF was explained by electrostatic forces. The influence of the DMF on the chemical speciation is discussed based on the dielectric constant of the medium. Distribution diagrams of various species of the complexes in relation to pH are presented.

## **IO-19 : Synthesis, Characterization and DFT Studies of Copper Phene Complexes**

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Two new mononuclear [Cu(2,9-dimethylphen)<sub>2</sub>]ClO<sub>4</sub> 1 and [Cu(1,10-phen)<sub>3</sub>] 2ClO<sub>4</sub> 2 have been synthesized and characterized by various physico-chemical techniques. Both complexes were structurally characterized by single crystal X-ray diffraction. Complex 1 has tetra coordinated and Complex 2 hexacoordinated environment around copper centre. Both mononuclear complexes have been studied by UV-vis and electrochemical techniques. The crystal packing of the structure of these new complexes is stabilized by H-bonding interactions. Electronic structures and spectral features are explained by DFT studies. Additionally, the antioxidant superoxide dismutase activities of these complexes have also been studied.

## **IO-20 : Improved Photocatalytic Properties of NiS Nanocomposites Prepared by Displacement Method for Degrading Rose Bengal**

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The present work describes NiS nanoparticles are prepared by chemical displacement method using CTAB as a stabilizer or Surfactant. For the source of Sulphur ion, we used thioacetamide as fuel and metal salt like nickel nitrate. The structural, morphological, metal percentage and optical properties of as synthesized nanoparticles are investigated by using x-ray diffraction (XRD), UV - Visible Spectra; field emission gun Scanning electron microscopy (FEG- SEM) with EDAX, Fourier transforms infrared spectroscopy (FTIR) and High-resolution Transmission electron microscopy (HR-TEM). The x-ray diffraction patterns revealed that the particles exhibited a crystal structure at the suitable temperature. The average particle size of the nanoparticles from the x-ray diffraction is about 20-40 nm and also field emission gun Scanning electron microscopy shows good morphology and exhibited clearly hexagonal shape. The Transmission electron microscopy (HR-TEM) shows the crystalline size of structures is 22 nm. Further, the Photocatalytic activity of Synthesized NiS nanoparticles was investigated by photo degradation of Rose Bengal as a model of organic pollutant.

## **IO-21 : Antimicrobial, Spectral, Fluorescence and Thermal studies of Co(II) and Ni(II) Complexes of Schiff base Derived from 2-chloro-5-nitrobenzaldehyde with 4-Amino-5-mercapto-3-propyl-1,2,4-triazole**

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The cobalt(II) and Nickel(II) metal complexes have been synthesized from the Schiff base derived from 4-Amino-5-mercapto-3-propyl-1,2,4-triazole with 2-chloro-5-nitrobenzaldehyde. The Schiff base and its metal complexes were further characterized by various physicochemical techniques (IR, <sup>1</sup>H-NMR, Visible, Fluorescence, thermal analysis, elemental analysis and magnetic moment measurements. IR spectra and thermal studies supported the coordinated water molecules in metal complexes. On the basis of these studies octahedral geometry for Co(II) and Ni(II) complexes have been proposed. Further,

synthesized complexes have been checked for their biological properties against the bacteria (*E. coli*, *P. aeruginosa*, *B. subtilis* and *S. aureus*) and two fungi (*S. cerevisiae* and *C. albicans*).

### **IP-CYSA-01 : Synthesis, Structural Characterization, DNA Binding, Cleavage, Antioxidant and Antimicrobial Studies on Copper(II) and Cobalt(II) Complexes of Benzothiazole Cored Schiff base Ligands**

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Three Schiff base ligands,  $L^1H = (2-((benzo[d]thiazol-6-ylimino)methyl)-6-nitrophenol)$ ,  $L^2H = (2-((benzo[d]thiazol-6-ylimino)methyl)-4,6-diiodophenol)$ ,  $L^3H = (2-((benzo[d]thiazol-6-ylimino)methyl)-4bromo-6-methoxyphenol)$  and their binary metal complexes, 1  $[Cu(L^1)_2]$ , 2  $[Co(L^1)_2]$ , 3  $[Cu(L^2)_2]$ , 4  $[Co(L^2)_2]$ , 5  $[Cu(L^3)_2]$  and 6  $[Co(L^3)_2]$  have been synthesized and characterized by elemental analysis, NMR, ESI mass, FT-IR, ESR, UV-Visible, magnetic susceptibility, TGA, SEM and powder XRD studies. The analytical and various spectral data suggested a square planar geometry for all complexes with  $N_2O_2$  donor atoms from the Schiff base ligands. Antimicrobial study revealed that metal complexes show more potent activity than free ligands. The free-radical scavenging ability of the complexes was evaluated by ABTS and DPPH assay methods using ascorbic acid as a standard antioxidant. DNA binding titrations indicated that all complexes bind to CT-DNA via an intercalation mode. Additionally, the metal complexes exhibit good cleavage ability against the pBR322 DNA even at low concentrations in the presence of activators,  $H_2O_2$  as well as UV light.

### **IP-CYSA-02 : Gamma Ray Enhanced Vis-NIR Photoluminescence of Biocompatible Silica Coated $Nd^{3+}$ Doped $GdPO_4$ Nanophosphors**

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Near infrared (NIR) emitting nanophosphors have great potential for biomedical and LED applications. The crystal structure, morphology and luminescence were investigated by X-ray diffraction, Scanning

electron microscopy, Transmission electron microscopy, and Photoluminescence spectra. This phosphor emits red luminescence at 681 nm and NIR luminescence at 797 nm corresponds to  ${}^4G_{7/2} \rightarrow {}^4I_{9/2}$  and  ${}^4F_{3/2} \rightarrow {}^4I_{9/2}$  transitions, respectively. Further the luminescence intensity of  $GdPO_4:Nd^{3+}@SiO_2$  phosphor was enhanced 10 fold after exposed to 150 and 300 kGy  $\gamma$ -radiation.

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## **IP-01 : X-ray Structures, Spectroscopic, Electrochemical and SOD Activities of Copper(II) Complexes with $N_2O$ Donor Schiff Base**

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The synthesis, structural, spectral and electrochemical characterization of  $[Cu(L)(acpy)]ClO_4$  1 and  $[Cu(L)(NO_3)]$  2 [where L = N'-(E)-phenyl(pyridin-2-yl)methylidene]thiophene-2-carbohydrazone and acpy = 2,6-Diacetylpyridine] have been done by elemental analysis, UV-vis, FTIR, electrochemical techniques (CV and DPV) and electron paramagnetic resonance (epr) spectroscopy. The geometry of copper(II) complexes are distorted octahedral for 1 and distorted square planar for 2. On the basis of density functional theory (DFT) calculation, the electronic excitations involve transitions mainly from metal ligand bonding mostly the  $\alpha$ -LUMO within the dominant Cu  $d_{xy}$  character and to  $\alpha$ -LUMO+1. Epr spectra for polycrystalline samples showed the copper(II) hyperfine features as well as half-field signal which are appropriate for  $\Delta M_s = \pm 2$  of dimmers. Presence of half-field signal in 1 is due to solid-solid interaction (intra-molecular) whereas in 2 the nature of interaction is intra-molecular. The superoxide dismutase activity measurements show that the both complexes 1 and 2 behave as superoxide mimic in alkaline nitro blue tetrazolium chloride assay.

## **IP-02 : Solid State Kinetics of Cu(II) Complex with Ligand 5- Anilino – 1,2,3,4- Thiatriazole**

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The Cu (II) complex was prepared by mixing legand i.e. 5- Anilino – 1,2,3,4- thiatriazole and Cu (II) acetate in 2:1 molar ratio in minimum quantity of ethanol. Dirty green precipitate of complex was obtained after refluxing. The themogram exhibits almost horizontal extending

up to 200C shows the pyrolytic stability of the complex. The first stage of decomposition was selected to evaluate the order of reaction and activation energy using graphical method of Freeman and Corroll. The values obtained have been corroborated by Doyle's procedure as modified by Zsako. The values of order of reaction and activation energy were found 0.9 and 18.703 k cal/ mol respectively. The apparent entropy of activation and apparent frequency factor were  $-176.240$  e.u and  $6.555 \times 10^8 \text{ sec}^{-1}$  respectively. These values are in good agreement with each other, hence may be utilized in the study of solid state reaction mechanism.

### **IP-03 : Graphene Oxide-Supported Cu(II) Schiff base Complexes as Recyclable Heterogeneous Catalysts for N-Arylation Reaction of Amines**

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Graphene oxide is one of the most promising support for a variety of metal oxides, nanoparticles, inorganic and organic complexes due to its remarkable thermal and chemical stability, high surface area, good accessibility, unique nanostructure and functional groups present on its surface and basal planes.

Bearing this in mind, we have synthesized copper(II) Schiff base complexes immobilized on the surface of the Graphene oxide and characterized them by FT-IR, XPS, FESEM, EDX and AAS analysis. The resultant supported complexes have been successfully used as recycle catalysts for the N-arylation of a series of amines. The catalyst could be easily recovered from the reaction mixture by using simple filtration and recycled up to five times without significant loss in catalytic activity and change in morphology as indicated by FESEM and other analytical studies.

### **IP-04 : Characterization and Biological Aspects of Co(II), Ni(II) and Cu(II) Metal Complexes Synthesized Using 2-Chloro-6-[(E)-(3-Hydroxy-4-Methoxyphenyl)Methylidene] Amino}-4-Nitrophenol Moiety**

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Schiff base metal complexes of Co(II), Ni(II) and Cu(II) derived from 3-hydroxy 4-methoxy benzaldehyde and 2-amino-6-chloro-4-nitro

phenol (HL) have been synthesized. The characterization of the compounds have been done by elemental analysis, FT-IR, molar conductance, electronic spectra,  $^1\text{H-NMR}$ , and thermal analysis. Analytical data reveal that all the complexes exhibit 1:2 (metal:ligand) ratio. IR data show that the coordination of ligand to metal is bidentate (donation from N, O sites). Thermal data shows the degradation pattern of the complexes which gives the idea about their stability. The Schiff base and their metal complexes show good activity against the E.coli, S. xylosus and F. bacterium bacterial strains. The antibacterial results also indicate that the metal complexes are better antibacterial agents as compared to the Schiff base.

### **IP-05 : A Potentiometric Study of Ternary Complexes of some Transition Metals with Iminodiacetic Acid and Piconolic Acid**

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Mixed ligand complexes of some transition metal viz.,  $\text{Cu}(\text{II})$ ,  $\text{Ni}(\text{II})$ ,  $\text{Co}(\text{II})$  and  $\text{Zn}(\text{II})$  have been investigated Potentiometrically with Iminodiacetic acid (IMDA) and Z Piconolic acid (PIW) in aqueous solution at temp.  $25\pm 1^\circ\text{C}$  and  $40\pm 1^\circ\text{C}$  at an ionic strength of  $0.1 \text{ mol dm}^{-3}$  ( $\text{KNO}_3$ ). The stability constants of these 1:1:1 ternary complexes have been evaluated by the computational method. The relative order of stability has been observed to be  $\text{Cu}(\text{II}) > \text{Ni}(\text{II}) > \text{Zn}(\text{II}) > \text{Co}(\text{II})$ . Which is in accordance with the increasing ( $\Phi$ ) charge/radius ratio. The change in thermodynamic Parameter (Free energy change  $\Delta G^0$ , Enthalpy  $\Delta H^0$  and Entropy  $\Delta S^0$ ) has also been calculated under the same conditions.

### **IP-06 : Metal Complexes of Substituted Quinolinyl Thiosemicarbazide with their Synthesis, Characterization and Biological Activity**

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Synthesis was carried out for Copper (II), Nickel (II) and Cobalt (II) complexes of quinolinyl thiosemicarbazide moiety. The characterization of the ligand and metal complexes were done by various Spectroscopic techniques like Mass, IR,  $^1\text{H}$  &  $^{13}\text{C}$  NMR, UV-Visible, Elemental analysis and Thermogravimetric analysis. The Data shows stoichiometry of 1:2 ratio of metal and ligand. Antimicrobial study was evaluated of these compounds with various stains using standard drugs as reference.

## **IP-07 : Synthesis, Characterization and Antimicrobial Activities of Cu(I), Ni(II) and Al(III) Complexes**

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Three complexes such as tris(thiourea) copper(I) chloride, tris(ethylenediamine) nickel(II) thiosulphate and potassium tris(oxalato)aluminate(III) trihydrate were synthesized by reflux method. These complexes were characterized by elemental analysis, atomic absorption spectroscopy, X-ray Fluorescence spectroscopy, FTIR, UV spectroscopy and magnetic susceptibility measurement. The antimicrobial potentials of these complexes were tested with *Bacillus subtilis*, *Pseudomonas aureogenosa* and *Escherichia coli*. The minimum inhibitory concentration was determined for these metal complexes, which ranges from 12–22 mm. These complexes have shown potential of being broad spectrum antimicrobial in nature.

## **IP-08 : Corrosion Study of Tin-Lead Alloy and Brass by Souring Substances**

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Souring substances are used as food additives in India. Souring substances contain organic acids as their components. Organic acids are corrosive to tinned brass vessels. Corrosion of tin-lead (50-50) alloy and brass (63/37) was studied in coupled and uncoupled systems at 30<sup>0</sup> C for 7 days duration. Different souring substances viz. lemon, tamarind, kokum, tomato, mango and curd were studied with and without sodium chloride. Films were formed over tin-lead specimens. In coupled system, tin-lead specimens underwent mostly pitting type corrosion.

## **IP-09 : Suzuki-Miyaura Cross-Coupling Reaction Catalysed by Different Ratio of Palladium Salt/ Ligands/Bases/Solvent**

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Tridentate ligands of 1-(Benzothiazole 2-yl) hydrazine were prepared by the condensation with substituted salicyldehydes or different

aromatic ketones. These ligands are thermally stable and neither air- nor moisture-sensitive. Suzuki–Miyaura cross-coupling reaction is carried out in presence of different ratio of palladium salts/ various ligands/ bases/solvent and studied effects on the performance of the coupling reaction.

### **IP-10 : Prediction of Chemical Speciation of Binary Complexes of Co(II), Ni(II) and Cu(II) with 5-Sulfosalicylic acid in Urea-Water Mixtures**

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Speciation of Co(II), Ni(II) and Cu(II) complexes with 5-Sulfosalicylic acid (5-SSA) in the presence of urea-water mixtures at an ionic strength of 0.16 mol dm<sup>-3</sup> and temperature 303 K were investigated pH metrically. The existence of different binary complex species was established from modeling studies using the computer program MINQUAD75. The increased stability of the complexes with increasing urea was explained by electrostatic forces. The influence of the urea on the chemical speciation is discussed based on the dielectric constant of the medium. Distribution diagrams of various species of the complexes in relation to pH are presented.

### **IP-11 : Synthesis and Antimicrobial Activity of Novel Schiff Bases and its Metal Complexes Derived from 5-amino Salicylic Acid**

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The field of Schiff base complexes has been first developing on account of the wide variety of possible structures for ligands depending upon the aldehydes and amines. Schiff bases are considered as a very important class of organic compounds, which have wide variety of

applications in many fields, including biological, industrial and analytical chemistry. In the field of heterocyclic chemistry, imidazoles are considered as an important pharmacophore in medicinal chemistry encompassing wide spectrum of biological activities such as antibacterial antirheumatoid arthritis, antituberculosis, antiviral, antiepileptic, anti-inflammatory and anticancer activities. Keeping the above literature in view, we prepared new Schiff base of (E)-5-((2-butyl-5-chloro-1H-imidazol-4-yl)methyleneamino)-2-hydroxybenzoic acid (BCIHB) from 2-n-butyl-5-chloroimidazol-4-carbaldehyde (BCI) and 5-amino salicylic acid (AS). Also metal complexes were prepared from chloride salts of Mg (II), Ni (II), Zn (II) and Pd (II) in an alcoholic medium. The chemical structures of the Schiff-base ligand and its metal complexes were confirmed by spectroscopic studies like IR, <sup>1</sup>H NMR, mass spectra, elemental analysis, molar conductance, thermo gravimetric analysis and also studied their antimicrobial activities.

## **IP-12 : Synthesis, Characterization and Electrical Properties of Halogen Doped ZnO Nano-Particles**

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ZnO is a semiconductor with a wide band gap (3.3 eV) and a large exciton binding energy and is abundant in nature; these characteristics make this material attractive for many applications, including solar cells, optical coatings, photocatalysts, and electrical devices. ZnO doped with halogen (such as Cl<sup>-</sup>, Br<sup>-</sup> and I<sup>-</sup>) were synthesized by annealing the mixture of ZnS and KX (X= Cl, Br, I) at 850 °C in air. The products were characterized by infrared spectra (Far IR), thermal analysis (TGA/DTA), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), Energy Dispersive X-ray Analysis (EDAX) and diffuse reflectance spectrum (DRS). The XRD studies of halogen doped ZnO exhibit the presence of hexagonal wurtzite type crystal structure similar to parent compound ZnO. The nanocrystalline nature of the sample and their crystallinity has been confirmed by SEM measurement. UV-DRS of rare earth doped ZnO nanoparticles shows a strong absorption peak at 388 nm due to ZnO band to band transitions. The UV-DRS absorption analysis reveals the decrease in energy band gap of halogen doped ZnO nanoparticles and creating defective sites on the ZnO surface. The variation of electrical conductivity (log $\sigma$ ) with reciprocal of temperature (T<sup>-1</sup>) is nonlinear. Two activation energies (E<sub>a</sub>) were calculated for two regions around break points.

## **IP-13 : Synthesis and Characterization of Pr<sup>3+</sup> Substituted Cobalt Ferrite Nanoparticles Prepared by Co-precipitation Method**

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Praseodymium substituted cobalt ferrite nanoparticles with composition of  $\text{CoPr}_x\text{Fe}_{2-x}\text{O}_4$  (where,  $x= 0.0 - 0.15$ ) have been prepared by tartarate co-precipitation method. The thermal studies were used to monitor the preparation process of these ferrites. The obtained ferrites were characterized by XRD, TEM, d.c. electrical conductivity, thermoelectric power and Magnetic hysteresis measurements. X-ray diffraction analysis reveals the formation of cubic spinel structure in all the ferrite samples. The lattice parameter increased with praseodymium content  $x$  d" 0.15. The TEM photographs of these compounds exhibited average particle size in the range of 70.8 to 89.12 nm. The temperature variation of the direct current electrical conductivity showed a definite breaks which corresponds to ferrimagnetic to paramagnetic transitions. The thermoelectric powers for all compounds are positive over the whole temperature range. The magnetic properties of praseodymium substituted cobalt ferrites showed a definite hysteresis loop at room temperature. The saturation magnetization (MS) and coercivity are found to decrease with increase in praseodymium content. The reduction of remanance to saturation magnetization ratio (MR/MS) and magnetic moments may be due to dilution of magnetic interaction. The high d.c. resistivity and low dielectric losses are desired characteristics of  $\text{CoPr}_x\text{Fe}_{2-x}\text{O}_4$  ferrites.

## **IP-14 : Synthesis, Characterization and Biological Activities of Tellurium(IV) Complexes of Bidentate Schiff base Derived from 5-Chlorosalicylaldehyde and 3-Aminopyridine**

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A series of tellurium(IV) complexes were synthesized from Schiff base i.e. 3-aminopyridine-5-chlorosalicylaldehyde Schiff base (3-APY-{5-ClSalH}). Obtained Schiff Base and their tellurium(IV) complexes have been characterized by elemental analyses, conductivity measurements, FT-IR and <sup>1</sup>HNMR spectral studies, suggests that Schiff

base ligand behave as monobasic ON-bidentate at tellurium metal centre. Also, the Schiff base and some of their tellurium(IV) complexes were tested for antifungal and antibacterial activities using Broth Dilution Method.

### **IP-15 : Investigation of New Disulfides of Aryldithiocarbonates Based on Spectroscopic, TGA, SEM and DFT Studies**

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Oxidation of sodium salt of 2-methyl-, 3-methyl-, 4-methyl- and 4-chloro-3-methylphenyldithiocarbonic acid by  $I_2$  affords the disulfides of respective dithiocarbonates  $[(ROCS_2)_2]$  ( $R = 2-CH_3C_6H_4$ ,  $3-CH_3C_6H_4$ ,  $4-CH_3C_6H_4$  and  $4-Cl-3-CH_3C_6H_3$ ). These compounds were characterized by elemental analyses, infrared, mass and heteronuclear NMR ( $^1H$  and  $^{13}C$ ) spectroscopic studies. Thermogravimetric analysis and scanning electron microscopic analyses were also carried out for deeper investigation of the structural features. Comprehensive theoretical investigation was performed by applying density functional theory (DFT) calculations on vanadium and niobium complexes by the DFT/B3LYP/LANL2DZ method to obtain the optimized molecular geometry, vibrational frequencies, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), thermodynamic properties and various other quantum-mechanical parameters. Furthermore, the compounds were examined through varied methods to find out biological activities for instance antioxidant and antimicrobial. The antimicrobial test of these complexes has also been conducted against the three bacterial strains (Gram-positive *Staphylococcus aureus* ATCC 25923; Gram-negative *Escherichia coli* ATCC 25922 and *Pseudomonas aeruginosa* ATCC 27853) and fungus *Fusarium oxysporium*, which indicated potential antimicrobial activity.

### **IP-16 : Removal of Malachite Green Dye from Aqueous Solution using Bentonite : Study of Some Physical Parameters**

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The adsorption of malachite green (MG) dye onto Bentonite was carried out in this work. The effects of different reaction parameters

such as the initial MG concentration, contact time, solution temperature and initial pH on MG adsorption were investigated. MG adsorption uptake was found to increase with increase in initial concentration, contact time and solution temperature. The adsorption equilibrium data were best represented by the Freundlich model. Adsorption kinetic was found to follow the pseudo-second-order kinetic model. Boyd plot indicated that the MG adsorption on the Bentonite was controlled by film diffusion. Thermodynamic parameters  $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta S^\circ$  and  $E_a$  were also determined.

### **IP-17 : Synthesis and Spectroscopic Characterization of Zn<sup>II</sup> Complexes of N<sub>2</sub>O<sub>2</sub> Macrocycles**

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Mononuclear macrocyclic complexes of Zn(II) of the type [ZnL] have been prepared by [1+1] cyclocondensation of  $\alpha$ -diketones such as 2,4-pentanedione, 1-phenyl-1,3-butanedione and 1,3-diphenyl-1,3-propanedione with 1,8-diamino-3,6-dioxaoctane in the presence of Zn(II) chloride. These complexes have been characterized by elemental analyses, molar conductivity data, magnetic measurements and infrared, electronic, <sup>1</sup>H NMR and mass spectral studies.

### **IP-18 : Synthesis, Spectral, Magnetic & Biological Screening Studies of Co (II) and Ni (II) metal complexes of Schiff Bases Derivatives of Heterocyclic Amines**

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The applications of metal chelates in bioinorganic field have been well established by their frequent use in medicine. A number of O, N and S containing Schiff bases have been found to be biologically active and exhibits anticancer, antiviral, antibacterial and antifungal activity. It has been observed that most of the metal complexes of these ligands are more effective than their parent ligand.

In view of the above applications, the synthesis and characterization of transition metal complexes with Schiff bases derived from some substituted p-hydroxy benzaldehyde promoted us to synthesize Co (II) and Ni (II) metal complexes of Schiff bases derived from p-hydroxy benzaldehyde-2-amino-6-methyl pyridine and p-hydroxy benzaldehyde-

2-aminothiazole were prepared and characterized and screened for their antimicrobial activities.

### **IP-19 : Divalent Transition Metal Complexes Co (II), Ni(II), Cu(II) and Zn(II) with N-donor Tetradentate [N<sub>4</sub>] Macrocyclic Ligand**

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The synthesis of macrocyclic metal complexes of Co(II), Ni(II), Cu(II), Zn(II) having a general formula : [M(L)X<sub>2</sub>] where L is C<sub>20</sub>H<sub>20</sub>N<sub>4</sub>; X = Cl<sup>-</sup>, NO<sub>3</sub><sup>-</sup>, CH<sub>3</sub>COO<sup>-</sup> was carried out with the condensation reaction of 4,5-dimethyl-1,2-phenylenediamine and glyoxal. These complexes have been structurally characterized with the support of elemental analyses, molar conductance measurements, magnetic susceptibility measurements, IR, and electronic mass spectra. All the complexes are non electrolyte in nature. Based on the studies, hexa-coordinated octahedral geometry was proposed for these complexes.

### **IP-20 : Philosophy of Science : Connection of Physics and Chemistry**

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The matter of how theories in science relate to each other is a key aspect of the unity of Science. For the philosophy of chemistry, this problem is of significant importance; chemistry and physics are binded so closely where it is sometimes difficult, if not impossible, to unimagined chemistry with the physics removed. Yet the widespread use of physical theories in chemistry is often not representatives of how these theories are used in physics.

This situation raises the question of how these two sciences are related. Nowadays, philosophers overall write as many publications per year as scientists do in four years. This shows the interest of philosophers into the science specially physics and chemistry.

Still an important topic in today's philosophy of chemistry is reduction – not of biology to chemistry but of chemistry to physics. Because of their narrow focus on theoretical physics, concepts of mainstream philosophy of science frequently require considerable revision before they help shed some light on chemistry. Context of justification and context of discovery binds physics and chemistry both.

The role of philosopher on these facts will be presented.

## IP-21 : Metal Interactions with Organic Secondary Metabolites in Herbal Plants with Respect to Cordia Dichotoma

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Metals from earth crust enter into plant via roots and they play an essential role in the biological system of the plants. They form metal chelates with plant secondary metabolites. Secondary metabolites are essential components of plant which play a vital role in plant's defence mechanism. Many Secondary metabolites of the plant show pharmacological activity. In this paper we are discussing about the metal chelation with secondary metabolites. These metal chelates further increase the activity of the original compound. Plants can help to remove the Heavy metals from earth by the process of phytoremediation. The plant Cordia dichotoma belongs to the family Boraginaceae is known for anti-fertility, anti-diabetic, anti-inflammatory, diuretic and so many other activities. The metal analysis report of the plant bark shows high concentrations of calcium and potassium, magnesium and sodium. These metals are cofactors of many enzymes involved in biological reactions, which are discussed in the paper.

## IP-22 : Synthesis, X-ray Structure and Spectroscopic Studies of Copper(II) Mono and Binuclear Complexes with NNO donor Schiff base

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Mono and binuclear copper(II) complexes namely  $[Cu(L^1)(L^2)]ClO_4$  1 and  $[Cu_2(L^1)_2(pyrazine)]ClO_4 \cdot 2H_2O$  2. Where  $L^1 = 5$ -bromo-2-[E]-(pyridine-2-ylhydrazone) methyl]phenol and  $L^2 = N,N$ -dimethyl formamide have been synthesized and characterized by elemental analysis, IR and single crystal X-ray diffraction. Copper(II) complexes have distorted square planer geometry. Both mono and binuclear copper(II) complexes shows epr spectra in 100% DMSO at 77K giving  $g_{\parallel} > g_{\perp} > 2.0023$  indicating ground state in a distorted square pyramidal geometry. Redox behaviour of both complexes has also been studied.

## **IP-23 : An Efficient Synthesis of New Pyrazine Based Polycyclic Aromatic Hydrocarbons through C-H Bond Activation: Pd(II) N4-Macrocyclic Complexes**

**Ramesh Gade, Suesh Kilaru and Someshwar Pola**

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The Schiff's base metal complexes have been concerned significantly due to their out-of-box applications in the field of C-H bond activation under visible-light irradiation. The Pd(II) complexes obtained from Na-marcocyclic ligands reacted with donor atoms N under solvothermal conditions. These complexes were characterized using the microanalysis, conductivity studies, and different spectral techniques. From these data reveals that the compound shows square planar geometry with ligands coordination via azomethine and amide nitrogen atoms. Oxidative cyclization of second position C-H bond of 3-phenyl pyrazine moiety has been examined the photocatalytic activity of [Pd(L)Cl<sub>2</sub>] under LED light (9 watts & 398 nm  $\lambda_{\text{max}}$ ). Due to the suitable of the bandgap energy for nature to the generation of ·Cl radicals during the catalytic reaction. For this reason, higher oxidation rate. [Pd(L)Cl<sub>2</sub>] as a very efficient photocatalyst for oxidative cyclization, due high surface area and very bandgap energy that supports to oxidative elimination mechanism.

## **IP-24 : Evaluation of Protonation Constants of 1,10-Phenanthroline in Aqua-Organic Mixtures**

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1,10-Phenanthroline (phen) or 4,5-diazaphenanthrene is a tricyclic compound. Phen is a metal chelator. As a bidentate ligand in coordination chemistry, it forms strong complexes with many metal ions through N-atoms. Due to hydrophobicity of aromatic rings of phen, the solubility of the neutral species is low in water which remarkably increases in organic solvents and also in aqua-organic mixtures. Protonation equilibria of 1,10 Phenanthroline have been studied in varying concentrations (0-60% v/v) of ACETONITRILE - water mixtures maintaining an ionic strength of 0.16 mol dm<sup>-3</sup> at 303 K using pH metric method. The protonation constants have been calculated with the computer program MINIQUAD75 and the best fit models are arrived at based on statistical grounds employing

crystallographic R factor,  $\chi^2$ , skewness and kurtosis. Phen has two dissociable protons. It exists as  $\text{LH}_2^{2+}$  at low pH and gets deprotonated with the formation of  $\text{LH}^+$ , L successively with increase in pH. The protonated species  $\text{Hphen}^+$  and  $\text{H}_2\text{phen}^{2+}$  were reported in the pH range 3.8-5.5 and  $< 1.0$ , respectively.

## **IP-25 : Compatibility Studies of Nanocomposites Polyacrylonitrile/CuO Nanoparticles on the Physical Properties for Fountain Pen Ink**

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Ink comprise of pigment or dyes dispersed in a solvent either aqueous or organic. Pigmented inks contain agents that ensure adhesion of the pigment to the surface and prevent it from being removed by mechanical abrasion. The manufacture of ink is associated with graphical arts, but it is classified as part of the chemical industry. Ink is easily definable as a fluid or viscous material used to write and to print.

The Nanocomposites were varied to 0.33 and 0.68gm with respect to prepared polyacrylonitrile and the effect on physical properties of ink such as, density, viscosity, surface tension, drying and smudging were observed to see the performance of it on polymer nanocomposites mixed in ink.

After adding the polymer nanocomposites in ink samples, it was observed that in pure blue ink samples viscosity is 2.156 which is increases after the adding of PNCs A and PNCs B is 3.156 and 3.656, black fountain pen ink viscosity is 1.750 which is increases after adding PNCs Y and PNCs Z is 2.750 and 3.250.

Surface tension is 30.454dyne/cm after adding the 1% polymer nanocomposites the surface tension is increased to 31.454 dyne/cm but in pure black ink samples surface tension is 28.165 dyne/cm but after adding the 1% polymer nanocomposites the surface tension is slightly decreases to 29.165.

In this study two types of fountain pen ink were analyzed by UV-Vis and FTIR spectroscopy to see the presence of individual component of nanocomposites. It was found that the solution with polymer nanocomposites shows, improved in the physical properties with variation of 2% with respect to ink solution. Finally the biological activities were performed to see the effect of it on the ink solution.

## ORGANIC CHEMISTRY SECTION

### Sectional President's Address

#### Chemistry of Selenoxopeptides and Selenoureido-peptidomimetics

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The field of peptide backbone modification has grown tremendously over the last decade owing to the improved biological and structural properties possessed by the resulting unnatural analogs. One of the major research interests of our group is to design and develop novel intermediates through C- or N-terminal modifications and demonstrate their utility for the synthesis of peptidomimetics. Selenium containing compounds have gained prominence with the identification of various selenoproteins where selenium is predominantly present as selenocysteine (Sec, U). Selenoamides have garnered considerable interest as pharmaceutical agents and as synthetic precursors for heterocycles. We have developed novel selenium building blocks namely isoselenocyanates at both N- & C- termini of amino acids and demonstrated their utility in selenoureido peptidomimetics. Further  $\text{PCl}_5/\text{LiAlSeH}$  reagent system has been employed for efficient synthesis of selenoxopeptides from native peptides. Thus obtained selenoxopeptides are used as units for N-terminal chain extension through  $\text{N}^\alpha$ -deprotection/ coupling to yield peptide-selenoxo peptide hybrids. Multiple selenation was demonstrated by conversion of two peptide bonds of tripeptides into selenoxo peptide bonds. Some of these results will be presented in this talk.

## **OIL-01 : Role of Chemical Structure and its Modifications on the Biological Activity of Curcumin**

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Curcumin, the active component of turmeric, known since ancient times for medicinal properties, is in advanced clinical trials for therapeutic purpose against a number of diseases including cancer. The unique biological activities of curcumin are attributed mainly to its chemical structure, and its three important functionalities: an aromatic o-methoxy phenolic group,  $\alpha$ ,  $\beta$  –unsaturated diketo moiety and a seven carbon linker. Extensive research in the last two decades has provided evidence for the role of these different functional groups in its crucial biological activities. However the properties limiting its potential are low bioavailability and fast degradation. To overcome these limitations, researchers have developed several new analogues are being developed with modifications on specific functional groups of curcumin. Modifications in both o-methoxy group and the diketo structures yielded new molecules with improvement in their in vivo performance. The work carried out from our group in the last one decade on some of these aspects will be discussed in the lecture.

## **OIL-02 : Opportunities and Challenges in Natural Products Research**

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The Indian subcontinent has a vast coastal belt along with the wide range of forest environment, which host large number of unexplored plant/marine species. This diversity has been the source of unique chemical compounds with the potential for industrial development as pharmaceuticals, cosmetics, nutritional supplements, molecular probes, fine chemicals and agrochemicals. In recent years, a significant number of novel metabolites with potent pharmacological properties have been discovered from the natural sources including marine and terrestrial plants. Recent move of society towards nature for the treatment of various diseases where there is no satisfactory cure in modern medicine has diverted the attention of natural/medicinal chemists and biologists to unravel their chemical characteristics and biological activities together in order to define their therapeutic potential in the light of modern pathobiological understandings. This move has led collectively to rediscover, design and refine the therapeutic application of medicinal plants/marine sources.

During last ten years, we have studied several medicinal plants and marine organisms guided by in vitro based bioassays to delineate the chemistry of natural products responsible for biological activities. This effort has led to identify several potent multiple active medicinal plants/marine sponges, their active fractions and synergistic molecular compositions. We have identified particularly, several free radical scavengers, xanthine oxidase and  $\alpha$ -glucosidase inhibitory, anti-cancer principles present in substantial yields. Presence of multiple active phytochemicals in rich concentrations in some of the medicinal plants therefore offers exciting opportunity for development of novel therapeutics and also provides scientific justification for their use in traditional medicines. Therefore, biologically activity based chemical characterization of these medicinal plants may provide scientific explanation for their use in traditional medicines and also redesign and develop preparations for novel therapeutic applications. The opportunities in the development of this therapeutics from natural sources are divided into three topics (terrestrial plant, marine sponges and Lichens). Each topic will be exemplified with suitable examples.

### **OIL-03 : PTs Entry Inhibitors of HIV-1: Bursting and Killing Virus**

**K. Kantharaju**

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Initial entry of human immunodeficiency virus-1 (HIV-1) into host cells remains a compelling and yet elusive target for developing agents to prevent infection. This step is mediated by a sequence of interactions of a trimeric gp120/gp41 envelope (Env) protein complex with host cells, including initial gp120 encounter with the cellular receptor CD4 and a chemokine co-receptor, usually CCR5 or CXCR4. A peptide triazole (PTs) class of entry inhibitor leads has been shown to be bind on to gp120 with close to nanomolar affinity, to suppress protein–ligand interactions of the Env-gp120 protein at both its CD4 and co-receptor binding sites, and to inhibit cell infection by a broad range of virus subtypes. The promising functional activity and unique mode of action of peptide triazoles as a HIV-1 entry inhibitors led us to seek potency enhancement by multivalent conjugation. For this study, synthesized the peptide triazole denoted KR-13, composed of 12-residue amino acid sequence of the previously identified high potency peptide triazole HNG-156 with a C-terminal extension containing a Cysteine-SH group. Serendipity observed that, the designed modified KR-13 that target HIV-1 gp120 to disrupt virus particles in the absence of host cells. Under conditions similar to those at which the peptide triazole KR-

13 inhibits HIV-1<sub>BaL</sub> pseudovirus infection of HOS.T4.R5 cells, it also causes release of HIV-1 p24 when incubated with virus alone. Both inhibition of cell infection and p24 release are enhanced substantially by multivalent display of KR13 on gold nanoparticles. Virucidal function of the modified peptide triazoles argues for their potential use as microbicidal and therapeutic agents to suppress the progression and spread of HIV-1 infection.

### **OIL-04 : Lewis Acid Mediated C-C And C-O/N Bond Forming Reactions Beyond Friedel-Crafts Reaction: Applications in Medicinal Chemistry**

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As a privileged class of heterocyclic compounds N-heterocyclic structures have found enormous applications in many areas including medicinal/pharmaceutical chemistry and drug discovery. Consequently, a wide variety of methods have been reported for their synthesis. While not free from their own limitations Lewis acid mediated reactions to form C-C and C-O/N bond forming reactions provides useful methodologies for the construction of various N-heterocyclic structures. These methodologies are operationally simple, efficient and can be performed in a cost effective manner. In this presentation, we wish to provide a comprehensive overview on various novel methodologies that have been developed by our group along with others.

### **OIL-05 : Intramolecular [3 + 2]-Cycloadditions of Azomethine Ylides Derived from Secondary Amines Via Redox-Neutral C-H Functionalization**

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Azomethine ylides are accessed under mild conditions via benzoic acid catalyzed condensations of 1,2,3,4-tetrahydroisoquinolines or tryptolines with aldehydes bearing a pendent dipolarophile. These intermediates undergo intramolecular [3 + 2]-cycloadditions in a highly diastereoselective fashion to form polycyclic amines with four new stereogenic centers. Challenging substrates such as piperidine, morpholine, and thiomorpholine undergo the corresponding reactions at elevated temperatures. Diastereoselective synthesis of oxazolo[2,3-c]isoquinoline was also achieved. A new approach for the synthesis of highly substituted 1H-pyrrolo[2,1-c][1,4]oxazine was carried out.

## **OIL-06 : Lewis Acid Catalyzed Synthesis of Highly Substituted Indoles and Indol-3-Carbinols**

**Alagesan Balasubramani and Sengodagounder Muthusamy**

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Propargylic alcohol is one of the most important and useful classes of substrate in organic synthesis. The  $\delta$ -nucleophilic character of the triple bond is a common functional group, which makes a versatile entity for further chemical transformations. Recently, the chemistry of propargylic alcohol and their derivatives has attracted much attention and extensively investigated. Indoles are among the most abundant structural components that occur ubiquitously in bioactive natural products, pharmaceuticals, and agrochemicals. In recent days, 3H-indole-N-oxides and their analogues are intriguing chemical entities as they may play important biological roles and serve as useful synthetic building blocks. Avrainvillamide is the natural product having anticancer properties and it possesses the key functional group of 3-alkylidene-3H-indole-N-oxides. However, there are only few reports available for the preparation of this inimitable structural moiety, 3-alkylidene-3H-indole-N-oxides. Therefore, the development of transition metal free, mild, and efficient methods to directly access various 3-alkylidene-3H-indole-N-oxides is highly desirable and of prime synthetic value. As a part of our continued efforts devoted to the exploitation of propargylic alcohols in organic synthesis, we herein report highly substituted indoles from propargylic alcohols and nitrosobenzenes and will be discussed in detail.

## **OIL-07 : Bond Formations between Two Nucleophiles: Sustainable Metal-Catalyzed Oxidative Annulation Reactions**

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The development of efficient methods for construction of C-C and C-X (X = N, O, S, etc) bonds under mild and green conditions is one of the great challenges in organic chemistry. Transition-metal catalyzed classical coupling reactions have been proven to be powerful tools for the construction of various C-C and C-X bonds, and reactions of this type have been widely applied in the areas of pharmaceuticals, agriculture, food industries, and so on. Normally, in those classical coupling reactions, bond formations occur between an electrophile and a nucleophile in the presence of a transition-metal catalyst. Both the electrophiles and the organometallic nucleophiles are usually

obtained from pre-functionalization of their corresponding hydrocarbons. However, with the development of modern synthetic methodology and the urgent demand for green and economical synthesis, traditional couplings face big challenges on account of their inevitable drawbacks such as low atom economy and considerable generation of harmful by-products. At this point, direct bond formation between two nucleophiles, especially two hydrocarbons, would be an ideal alternative. As for the coupling between two nucleophiles requires an extra oxidant to promote bond formation, this type of reactions are designated as oxidative couplings.

We have recently investigated some novel oxidative annulation reactions for the construction of nitrogen heterocycles such as quinoxalines, quinazolines, bis(indolyl)methanes, and 1,3-benzazoles using amines as reaction partners. Sustainable metal catalysts such as iron or copper salts, and abundant oxidants viz., air or molecular oxygen were used for conducting the oxidative annulation reactions. The results of these studies will be presented in the conference.

### **OIL-08 : Conventional and Microwave Assisted Synthetic Approach of Pyridine Analogous: Their in vitro Antimicrobial, Anti-Mycobacterium and Anti-Protozoal Activity and in-Silico Molecular Docking Studies**

**Navin B. Patel**

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Evaluating potential drug candidate with the desired biological properties is time-consuming and expensive. Microwave-assisted heating under controlled conditions has been shown to be an invaluable technology for medicinal chemistry and drug discovery applications since it often dramatically reduces reaction times, typically from days or hours to minutes or even seconds. The elegance of the reaction, high yield, short time span, simplified work-up procedure and eco-friendly conditions are the main advantages of the method and so that the Microwave assisted organic synthesis have revolutionized organic synthesis. An efficient procedure for the synthesis of pyridine analogous contributing various heterocyclic via microwave irradiation to offer newer analogous of pyridine with improved potency that compared with standard drugs has been carried out. Currently, “Neglected Diseases” such as Chagas, malaria, tuberculosis and leishmaniasis disease are still serious public health problems in developing countries and their prevalence continues to increase, because of the constant

migratory flow in endemic countries new strategies to speed drug development to treat these diseases are required. Moreover, the increasing rate of bacterial resistance to clinical antimicrobial agents is the major problem that facing world today. This provides a great opportunity to synthetic chemists for the synthesis of new compounds possessing lower cytotoxicity and with better antimicrobial potency. Compounds containing pyridine cores have a broad spectrum of different biological activities. The ability of these heterocyclic compounds to undergo various chemical reactions has made them important for molecule planning, such as, 1,2,4-triazole, Manich base, Schiff base, etc., using various amino benzimidazoles, quinoxalines, benzothiazoles etc. with enormous biological potential. All the newly synthesized scaffolds were subjected to in vitro anti-bacterial (*S. aureus*, *S. pyogenes*, *E. coli*, and *P. aeruginosa*), anti-fungal (*C. albicans*, *A. niger*, and *A. Clavatus*), anti-mycobacterial (*M. tuberculosis* H<sub>37</sub>Rv), anti-malarial (*P. falciparum*) anti-trypanosomal (*T. cruzi*) and anti-leishmanial (*L. Mexicana*) activity. We have also carried out in silico molecular docking study of our targeted compounds with different PDBs as biological target to understand binding interaction of targeted compounds.

### **OIL-09 : Total Synthesis Driven Methodologies**

**C. V. Ramana**

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The structural complexity and skeletal diversity of natural products have served as inspirations to organic chemists for the discovery and design of new synthetic methods en route to their chemical synthesis. Our group focuses on the development of new methodologies that are specifically designed in the context a total synthesis of natural products of biological relevance. In this presentation, we wish to provide a comprehensive compilation of various novel transformations that have been developed in our group along with some salient aspects of the accomplished total synthesis.

### **OIL-10 : Palladium and CO Gas Free Carbonylation of Aryl Iodides : An Easy Access to the Synthesis of Various Heterocyclic Compounds**

**Siddaiah Vidavalur**

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Heterocyclic compounds are privileged scaffolds that have been found in a wide variety of natural products and biologically potential

molecules. Particularly, nitrogen heterocyclic compounds such as 1,2,4-triazoles, N-fused 1,2,4-triazoles, 1,2,4-oxadiazoles, benzimidazoles, benzoxazoles and oxygen heterocyclic compounds such as flavonoids have recently received significant attention in the field of chemistry, biological and material sciences. These scaffolds are known to exhibit a wide range of biological properties including antibacterial, anti-inflammatory, antiviral, anti-tumor, anti-asthmatic and anti-oxidant activities. Five membered nitrogen heterocyclic have also been used as bioisosters of esters, amides and as dipeptidomimetics in a number of pharmacologically important molecules. Moreover, these five-membered ring scaffolds act as intermediates in the synthesis of many drugs such as maraviroc, sitagliptin, triazolam, penipranolol and ataluren. Palladium-catalyzed carbonylation with a subsequent intramolecular cyclization reaction has been shown to be an efficient process for the straightforward synthesis of heterocycles. However; this method has some drawbacks such as the requirement of expensive palladium reagents and the use of the toxic and cumbersome to handle CO gas. Recently, group VI metal carbonyl complexes such as  $\text{Cr}(\text{CO})_6$ ,  $\text{W}(\text{CO})_6$ ,  $\text{Co}_2(\text{CO})_8$ ,  $\text{Mo}(\text{CO})_6$  etc., have been used as solid sources of CO. Among them,  $\text{Mo}(\text{CO})_6$  has emerged as an ideal candidate and has been used in several organic transformations. Inspired by these advances and in view of the diverse applications of the above heterocycles, we have developed a simple, efficient, green and CO gas free method for the synthesis of the above mentioned heterocycles from aryl halides. In this method  $\text{Mo}(\text{CO})_6$  acts as a convenient and reliable solid source of carbon monoxide.

## **OIL-11 : Novel Heterocycles and their Pharmacological Assay**

**V. Padmavathi**

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In this conference we would like to discuss the synthesis of a variety of heterocycles linked by different pharmacophoric groups. The methodologies adopted to optimize the yield and pharmacological assay will be addressed.

## **OIL-12 : Synthesis and Bioassay of Bis Heterocyclic Compounds**

**A. Padmaja**

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Oxadiazoles, thiadiazoles, triazoles and pyrimidines have gained

importance due to their applications in pharmaceutical and material science. My talk on bis heterocycles includes the synthesis, characterization and biological studies of bis oxadiazoles, bis thiadiazoles, bis triazoles and pyrimidinyl bis azoles.

### **OO-CYSA-01 : Conventional and Microwave Assisted Synthesis of New Biomolecule-Based Coumarin-Maltol Hybrids as Potent Anti-Cancer Agents, their DNA Cleavage and Docking Studies**

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A series of new coumarin-maltol hybrids (2a-2k) has been synthesized by using conventional as well as microwave irradiation protocols. Microwave irradiation caused a significant increase in the yields of all the derivatives. The synthesized compounds (2a-2k) were evaluated for their in-vitro anticancer activity against two human cancer cell lines viz., A-549 (human lung carcinoma) and HeLa (human cervical cancer). The results revealed that, the compounds (2a) and (2d) exhibited very significant anticancer activity against the A-549 cell line, whereas compound (2a) was active against the HeLa cell line. A DNA cleavage study using plasmid pBR322 DNA by gel electrophoresis method revealed that compounds (2a), (2j) and (2k) were found no traces of DNA. Furthermore, Molecular docking study performed for all the synthesized compounds with Clorobiocin (PDB code: 4TZK) and results were obtained, the compounds (2d), (2g) and (2k) have higher C score values.

### **OO-CYSA-02 : I<sub>2</sub>-Catalyzed Oxidative C-N and N-S Bond Formation: Facile Synthesis of 1,2,4-Thiadiazoles and 1,2,4-Triazoles**

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Heterocyclic compounds are important structures found in natural and synthetic compounds. Development of new synthetic protocols for the synthesis of biologically active N-heterocyclic compounds through various C-N, N-N, N-O and N-S bond formations is still in high demand. As a result, a plethora of methods were developed for carbon-heteroatom and heteroatom-heteroatom bond formation. Amongst

these, metal-catalyzed protocols for C-N, N-N, N-O and N-S bond construction have limitations, such as the metal contamination, drastic reaction conditions, cost-factors, air-sensitivity and scalability issues.<sup>1</sup> Earlier, metal free protocols were developed for C-N, N-N, N-O and N-S bond connection, of all these iodine catalyzed reactions played a major role owing to its environmentally friendly nature, oxidizing ability, inexpensive, easily available in solid form and easy to handle.<sup>3</sup>

Inspired by these advances, we have developed a mild and green protocols for the construction of the C-N and N-S bond by employing molecular iodine as a catalyst for the synthesis of N-fused 1,2,4-thiadiazole and 5-imino-1,2,4-thiadiazoles in acetonitrile<sup>4</sup> and 3- amino-1,2,4-triazoles, and 5- amino-1,2,4-thiadiazoles in water.

### **OO-CYSA-03 : Synthesis and Biological Evaluation of Some Novel Bis-((3-Methyl-5-Phenoxy-1-Phenyl-1H-Pyrazol-4-Yl)Methylene)-1-Phenyl-1H-Pyrazole-3,4-Dicarbohydrazide Via 1,3-Dipolar Cycloaddition of Sydnone**

**Balakrishna Kalluraya\* and Asma**

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Nitrogen-containing heterocyclic compounds have been extensively studied due to their versatile biological properties such as antibacterial, antifungal, antitubercular, analgesic, anticancer activities and other potential applications. Whereas pyrazole derivatives being five-membered nitrogen-containing heterocyclic compound have drawn considerable importance due to the variety of biological activities associated with them such as antibacterial, antiviral, anticancer, anti-inflammatory, antidiabetic, anti-depressant, antioxidant, antitubercular, antihypertensive etc. Hydrazones possessing -NHN=CH- group constitute an important class of precursors as they serve as best binding site for many receptors.

Encouraged by these observations, we have synthesized a series of bis-((3-methyl-5-phenoxy-1-phenyl-1H-pyrazole-4-yl)methylene)-1-phenyl-1H-pyrazole-3,4-dicarbohydrazide by the condensation of 1-aryl pyrazole-3,4-dicarbohydrazides with 5-aryloxy-3-methyl-1-phenyl-1H-pyrazolecarbaldehydes. The structure of these compounds was confirmed by NMR, LCMS, XRD, and elemental analysis. The results of biological studies of the synthesized compounds will be presented.

## **OO-CYSA-04 : Synthetic Transformations of Active Methylene Compounds to Structurally Intriguing Hybrid Molecules**

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Synthetic organic chemistry is one of the most profound, vibrant and fascinating areas of research. The impact of synthetic organic chemistry on science and technology does not stop with biology and medicine but encompasses several other prominent fields like supramolecular chemistry and nanotechnology. Most of the life-saving drugs available today have been realized through synthesis. In addition several compounds that find applications as materials, dyestuffs, fluorescent sensors, polymers, etc. have been obtained via synthesis. The universe of compounds prepared by synthetic transformations is very large and could be almost infinite.

For the past seven years our research group has been focusing on synthesizing several library of novel hybrid molecules using active methylene compounds like 1,3-cyclohexanedione, N-alkyl-4-piperidone, thiophen-3-ones, cyclooctanone, cyclododecanone, thiazolidine-2,4-dione, aroyl acetonitriles, malononitrile and steroids such as estrone, trans-androsterone and dehydroandrosterone) as starting materials. The synthesized hybrid molecules include multi-spiro heterocycles, thiaspirodecadienes, fused bi/tri/tetra-cyclic systems, tri/tetra-cyclic cage like compounds, benzo/hetero-cycle fused cyclooctanoids/cyclododecanes, fused pyrans, etc. These hybrid molecules comprise a maximum of up to seven hetero atoms (N, O or S) in the ring systems. The syntheses of these hybrid molecules have been achieved employing environmentally benign protocols like multi-component domino reactions and atom economic 1,3-dipolar cycloadditions. In total 1323 numbers of novel hybrid molecules have been synthesized in our laboratory. The structure of all these hybrid molecules has been characterized unambiguously using one- and two-dimensional NMR spectroscopy and in 118 cases the structure has been further supported by single crystal X-ray studies. With an intention to explore the biological significances, 194 of these hybrid molecules were evaluated for their AChE inhibitory activity and 131 molecules were screened for their activity against tuberculosis. In addition 21 compounds exhibited good fluorescence properties and were identified as selective sensors of picric acid, Fe<sup>3+</sup> or Hg<sup>2+</sup>. These findings have resulted in 23 publications since 2013 in peer reviewed journals of high impact.

The lecture will bring out some significant features observed during the synthesis and characterization of the above hybrid molecules.

## **OO-CYSA-05 : Desulfurization of Thiopeptides to 1, 5-Disubstituted Tetrazole Peptidomimetics using HgCl<sub>2</sub>**

**N. R. Sagar and Vommina V. Sureshbabu\***

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The bio-isosteres like triazole, tetrazole, etc., are being explored to overcome the inadequacies such as oral bioavailability, rapid metabolism by proteolysis and their interactions at multiple receptors posed by the native peptides. The cis-amide bond plays a significant role in molecular recognition and biological activity of peptides. Peptide analogs with cis-amide bond surrogates are attractive to study the topology of active sites of native peptides. To increase the utility of valuable conformationally constrained peptidomimetic for molecular recognition studies, we have demonstrated the selective insertion of tetrazole in to peptides. 1,5-disubstituted tetrazole peptidomimetics were synthesized by the desulfurization of thiopeptides by using HgCl<sub>2</sub> in presence of NaN<sub>3</sub>/TEA in DMF in good yields. HgCl<sub>2</sub> was found better among various other desulfurizing agents screened. The site selective insertion of tetrazole in to peptide-thiopeptide hybrids in the protocol display advantage over earlier methods. Also, the protocol was found compatible with Fmoc, Boc, Cbz protecting groups. Two tetrazole peptidomimetics Cbz-Ala-ψ[CN<sub>4</sub>]-Phe-OMe and Boc-Pro-ψ[CN<sub>4</sub>]-Val-OMe were obtained as single crystals as confirmed by X-ray crystallography.

## **OO-CYSA-06 : N-Propyldiamine Sulfonic Acid Encapsulated on Fe<sub>3</sub>O<sub>4</sub> Magnetic Silica Nanoparticles: An Efficient and Magnetically Reusable Heterogeneous Catalyst for the One-Pot Synthesis of 1, 8-Dioxo-Decahydroacridine Derivatives in Solvent-Free Conditions**

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The preparation of n-propyldiamine sulfonic acid-functionalized Fe<sub>3</sub>O<sub>4</sub>-magnetic core-shell silica nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-SiO<sub>2</sub>-n-SO<sub>3</sub>H-nH-SO<sub>3</sub>H) as a new recoverable and heterogeneous nanocatalyst is

described. The properties of this nanocatalyst were characterized by FT-IR, EDX, SEM, XRD, XRF and elemental analysis.

This heterogeneous nanocatalyst was explored to present high catalytic performance for the synthesis of 1,8-dioxo-decahydroacridine derivatives in solvent-free conditions. Easy separation of the nanocatalyst by using an external magnet, recyclability, non-toxicity, versatility and high stability of the catalyst combined with low reaction times and excellent yields make the present protocol very useful and attractive for the synthesis of the titled products.

## **OO-01 : Isolation of Active Constituents from Medicinal Plants : An Approach Leading toward Drug Discovery and Development**

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Drugs discovered from natural sources have undoubtedly revolutionized medicine, like antibiotics (e.g. penicillin, tetracycline, erythromycin), antiparasitics (e.g. avermectin), antimalarials (e.g. quinine, artemisinin), lipid control agents (e.g. lovastatin and analogs), immunosuppressants for organ transplants (e.g. cyclosporine, rapamycins), and anticancer drugs (e.g. paclitaxel, irinotecan). New drug discovery is facing serious challenges due to reduction in number of new drug approvals. Recently, there has been a renewed interest in natural product research due to the failure of alternative drug discovery methods to deliver many lead compounds in key therapeutic areas such as immunosuppression, anti-infective and metabolic diseases. Moreover, it is very challenging task to provide effective treatment to the patients suffering from parasitic diseases due to the development of drug resistant parasitic strain has emerged as major challenge to the medicinal chemists to discover new effective therapeutic agents. Our ongoing programme and continuous effort to identify the novel active constituent from medicinal plants as we have isolated and identified the many active constituents form medicinal Keeping in view importance of the aforesaid facts previously, we have observed anti-giardial activity in the ethanolic extract of the *Phlebophyllum kunthianum* and recently isolated a new ursane triterpenoid from this plant. The details isolation procedure, structural elucidation of the isolated ursane triterpenoid will be discussed during presentation.

## **OO-02 : Synthesis of Some New Series Of 1,3,4-Thiadiazolo-2-Thiol-Thiazolidino-5-Arylidines and their 2-Oxo-Azetidines : Biologically Active Molecules**

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Heterocycles and medicines are both inter related. As appeared in the literature that most of the modern reported life saving drugs contains the heterocyclic moiety in their structures. Heterocycles and their derivatives have attracted much attention to the scientists and the chemists because of their broad spectrum biological and pharmacological activities associated with this class of the compounds specially heterocycles having N-C-S linkage which exhibited marked chemotherapeutic activity. 4-oxo-thiazolidines and their 5-arylidines derivatives possess N-C-S linkage in thiadiazoles ring makes them of versatile biological interest and chemotherapeutic agents. The reactivity of azetidinones influences largely on substitution at position-2. I have selected 5-methyl-1,3,4-thiadiazol-2-thiol for the present study. The –SH group present at position 2 in 5-methyl-1,3,4-thiadiazol-2-thiol was used as the target for the chemical modifications. Several new class of 2-arylidenylamino-1,3,4-thiadiazoles ; 4-substituted-aryl-3-chloro-2-oxo-azetidines; 2-substituted aryl-4-oxo-thiadiazolidines and 5-arylidine-2-aryl-1,3-thiazolidin-4-ones were synthesized. The structures of the products were confirmed by spectral and chemical methods. Most of the synthesized products were screened for their antifungal activity against some selected fungi. The ED<sub>50</sub> values of active antifungal products were also calculated on a log probit scale from percent inhibition growth data. The antibacterial activity of the compounds were also determined against some bacteria. Some of the products were found to exhibit acceptable biological activity.

## **OO-03 : Novel Environmentally Benign One-Pot Synthesis of Isothiocyanates and Cyanamides**

**Upasana Bora Sinha**

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With environment protection becoming more and more important, there is an on-going effort to develop newer, environmentally benign alternatives to existing synthetic protocols. In acknowledgment of this, a highly efficient and simple methodology for the synthesis of Isothiocyanates and Cyanamides has recently been developed. This method is a general, economical and environmentally benign strategy

for the preparation of isothiocyanates and cyanamides from their corresponding dithiocarbamic acid salts. The use of non-toxic and eco-friendly reagents and solvents without the formation of any side products makes this methodology potentially useful. High environmental acceptability of the reagents, cost effectiveness and high yields are the important attributes of this methodology.

### **OO-04 : Potassium Fluoride: An Efficient Catalyst for the Synthesis of Aryl-14H-Dibenzo[A.J.] Xanthenes**

**Sayujiata R. Vaidya<sup>1\*</sup>, Kawade D. S.<sup>2\*</sup>, Jaishri J. Chamergore<sup>2\*</sup> and Jaidatt B. Gore<sup>1\*</sup>**

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The Synthesis of Xanthenes, especially benzoxanthene has emerged as a powerful tool in organic synthesis due to their wide range of biological and therapeutic properties such as antibacterial, antiviral, and anti-inflammatory activities, There are several methods for the synthesis of xanthenes.

An efficient and convenient synthesis of Aryl-14H-Dibenzo[a.j.] Xanthenes derivatives have been achieved via one pot cyclocondensation of aromatic aldehydes and  $\alpha$ -naphthol using Potassium fluoride in water under reflux condition. Potassium fluoride act as an efficient catalyst and has advantages over other catalysts such as high yield of products, reusable catalyst, shorter reaction time, easily available and simple workup procedure.

### **OO-05 : Synthesis and Biological Evaluation of Some Novel Hydrazones Carrying Benzimidazole and Pyrene Moiety**

**Desta Gebretekle, Balakrishna Kalluraya<sup>1\*</sup> and Manju N.**

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Benzimidazole is the “key core” in several bioactive compounds, and they exhibit varied pharmacological activities like antimicrobial, antioxidant, anti-inflammatory, anticancer, anti-tuberculosis, anti-hypertensive. Imidazole ring is found in many natural products like purine, histamine, histidine and in the nucleic acids.

Pyrene is a special class of polycyclic aromatic compound (PAH)

consisting of four fused benzene rings. A series of pyrene-containing molecules have been synthesized and used for the fluorescent label of oligonucleotides. Fluorescent labels are efficient tools for structural and functional investigations of nucleic acids of particular interest are fluorophores capable of DNA binding and exerting microenvironment-dependent emission. Pyrene derivatives are convenient in modelling and studying properties of fluorescent conjugates, since pyrene has an elevated lifetime of the excited state. In addition, pyrene derivatives are stable and fully compatible with chemistry of DNA synthesis. Encouraged by the above observations, we synthesized hydrazones bearing benzimidazole and pyrene moiety through one pot nitro reductive cyclization. The structures of the newly synthesized compounds were confirmed by IR, <sup>1</sup>H NMR, and mass spectra. The synthesized compounds were evaluated for their antioxidant activity and also studied for the photo physical properties.

## **OO-06 : Catalytic Performance of Palladium (II) Salen Complexes in Cross Coupling of Organobismuthines with Acid Chlorides: Synthesis of Aromatic Ketones**

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The cross-coupling of aryl organometallic reagents with acyl halides is a useful methodology for the synthesis of various functionalized aromatic ketones that find applications in many natural products, pharmaceuticals and in liquid crystalline materials. The development of atom-efficient organometallic reagents is important as many of these reagents are used in industrial scale synthesis. Since the coordination sphere of palladium determines the activity of the palladium complex for a particular reaction, it was decided to screen Pd(II) complexes having salen ligands and to investigate their activity and efficiency for cross coupling reactions.

Triaryl bismuth(III) derivatives Ar<sub>3</sub>Bi (Ar = Ph, m-Tol, p-Tol, p-anisyl) were synthesized in excellent yields by salt metathesis reaction and were tested as cross coupling partners with acyl halides in presence of synthesized palladium catalyst (2-4 mol%). In this synthetic transformation triaryl bismuth compounds react with corresponding acyl halides affording the aromatic ketones in regioselective manner in good yields. The results showed that the Pd (II) salen complex F catalysed the reaction and gave complete conversions. The optimization of various reaction conditions such as effect of solvent, bases, Pd

precursors, temperature on the reactivity of organobismuth compounds and on selectivity of cross coupling were also studied.

### **OO-07: ZnO Nanostructures: An Efficient Catalyst for the Multicomponent Synthesis of Dihydropyrano[2,3-C]Pyrazole Derivatives**

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Pyranopyrazole derivatives are significant class of biologically active heterocycles. They exhibit various biological activities such as anticancer, antimicrobial, analgesic, anti-inflammatory, molluscicidal and fungicidal activities. The traditional synthetic methodologies offers efficiency; but most of them suffers from certain drawbacks such as low yields of the products, use of harsh reaction condition, toxic solvents and catalysts. In this regards we have developed a simple, efficient, non-toxic nanostructured ZnO as a heterogeneous catalytic system for the multicomponent synthesis of dihydropyrano[2,3-c]pyrazole derivatives via one pot four component reaction in good to excellent yield. The major advantage associated with this methodology includes ease of separation, reusability of catalyst, easy work-up and short reaction time.

### **OO-08 : Chemo-Enzymatic Approaches towards Enantioselective Synthesis of Bioactive Molecules**

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Despite tremendous advances accomplished through developing cheaper and more versatile chemical catalysts and optimizing the reaction media, the global needs for clean manufacturing technologies, management of hazardous chemicals and waste present new research challenges to both chemistry and biotechnology. Recent advances in biocatalysis, fueled by either protein engineering or screening, greatly improved the number of synthetic opportunities from small chiral polyfunctional molecules to highly complex analogs.

Chiral 1,2-amino alcohols, 1,3-diols and carboxylic acids are the vital structural components of a large number of biologically active molecules with potential pharmaceutical relevance and in chiral auxiliaries. In the present work, we seek to highlight the biocatalytic

approach towards the synthesis of these molecules and other useful precursors of bioactive molecules by panel of microorganisms bearing lipases/oxedoreductases belonging to IIIM-Jammu repositories as well as those procured from commercial sources.

### **OO-09 : Reaction of N<sub>1</sub>-Hydroxy Imidazole with Maldrum's Acid Derivative**

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Maldrum acid derivatives are very much attractive for the synthetic organic chemists for their use in the synthesis of various natural products. Thus, this made us to see the reactivity of N<sub>1</sub>-hydroxy imidazoles with the Maldrum's acid derivative. Maldrum's acid derivatives were synthesized by condensation of various aromatic aldehydes with Maldrum's acid. These synthetic derivatives are subjected to reactions with hydroxy imidazoles to get the derivatives. The products were purified and analysed using NMR.

### **OO-10 : 0.1 Molar Calcium Hydroxide is an Efficient Catalyst for Synthesis of 2'-Amino Chalcone**

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0.1M Calcium hydroxide was found to be an efficient catalyst for the condensation reaction between 2-amino acetophenone and substituted aldehyde to afford corresponding 2'-amino chalcone. 0.1M calcium hydroxide solution was prepared by dissolving calcium hydroxide in water. The method is applicable to various substituted aromatic including electron donating as well as electron withdrawing group. The merits of this method include shorter reaction time, inexpensive and easily available catalyst, high yield, and easy workup compared to other reported methods.

### **OP-CYSA-01 : Thionation of Di and Tripeptides Employing Thiourea as a Sulfur Transfer Reagent**

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Peptide bond modification by replacement of an amide bond by a thioamide moiety has attracted considerable attention in recent years

for several reasons. The receptor interactions of sulfur analogues of biologically active peptides may be more selective or more potent than their parent compounds. In addition, the enhanced stability against enzymatic action can be expected towards various proteolytic enzymes. Thiopeptides, popularly known as thiopeptides, used as a precursor for a wide range of peptidomimetics including triazole, tetrazole, thiazole and reduced amide isosteres as well. Initially, peptide was treated with  $\text{PCl}_5$  in the presence of catalytic amount of DMF for 20 min at room temperature followed by the addition of thiourea in acetonitrile. After 15 min of the reaction, the expected thiopeptide was obtained in good yield. The protocol was extended to prepare peptidyl-thio, dithio and aryl thioamides in good yields.

### **OP-CYSA-02: Nano Au/TiO<sub>2</sub> Catalytic Hydrothiolation of Acetylenic Ketone- A Mechanistic View using DFT and their Molecular Docking and Toxicity Studies**

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The hydrothiolation of acetylenic ketones with 5-aryl-1,3,4-oxadiazol-2-thiol leads to the formation of anti-hydrothiolation in various solvents in presence of nano Au/TiO<sub>2</sub>. The mechanism of anti-hydrothiolation was proposed by density functional theory calculations. Gold nanoparticles are alkynophilic in nature and therefore initial interaction was expected between acetylenic ketone and thiol. The relax calculations showed that the acetylenic ketone preferentially get adsorbed on gold catalyst at  $\alpha$  carbon with respect to carbonyl group. This will facilitate the nucleophilic attack of sulfur on  $\beta$  carbon to give Z-isomer. The in-vivo anti-inflammatory activity was well noticed at 2<sup>nd</sup> to 3<sup>rd</sup> hour of inflammation. Further the molecular docking studies of these anti-inflammatory agents showed good ligand-protein interactions and docking scores of -9 to -12.

### **OP-CYSA-03 : Synthesis of Some Novel Imidazole Carrying Thiadiazole Derivatives through One-Pot Nitro Reductive Cyclization**

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Thiadiazole, benzimidazoles, and pyrazoles are novel class of heterocyclic compounds possessing a broad spectrum of biological activities. Fused heterocycles play a prominent role in the investigation of bioactive molecules due to the drastic enhancement in their biological activity. One pot reactions are known for their high yield and efficacy in synthetic organic chemistry.

One pot nitro reductive cyclization catalyzed by sodium dithionate provides a platform for the synthesis of new class of benzimidazole in minimal time with easy work-up process. Traditional method used for the synthesis of benzimidazole requires harsh condition and tedious workup process this one eliminated by the sodium dithionite reagent.

Here we synthesized a thiadiazole fused triazole and benzimidazole carrying pyrazole through one pot nitro reductive cyclization catalyzed by sodium dithionite reagent and all the synthesized compounds were characterized by analytical and spectral analysis. Structure-activity relationship studies also reported for the newly synthesized compounds. Majority of the synthesized compounds exhibited prominent antimicrobial and antioxidant activity.

## **OP-CYSA-04 : Synthesis of Saccharumoside B with Potential of Antiproliferative and Pro-Apoptotic Activities**

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Cancer has become the major cause of death in the world with the changes in the living habitat of people and environment. Breast cancer is the leading cause of cancer deaths in women with an estimated 1,383,500 new cases and 458,400 deaths annually. Hence, chemotherapeutic agents have been developed throughout the world by pharmaceutical industries and academic institutions but their usage is limited due to poor efficacy and adverse effects.<sup>2</sup> Thus, discovery and development of safer and effective molecules is urgently required to reduce the burden of cancer. Phenolic glycoside esters (PG) are some of the most abundant secondary metabolites in plants with novel bioactivities. Several PG have been isolated from the plants of the different families. Previously, Tao et al.<sup>3</sup> isolated four new PG esters including saccharumoside B from the bark of *Acer saccharum* (sugar maple tree) and reported cytotoxic activity of saccharumoside B in cancers remains to be elusive. The present work reports the first time synthesis of anticancer natural product saccharumoside B and

its analogs with with good yields. Further, in vitro anticancer and pro-apoptotic studies of synthesized saccharumoside B and its analogs were performed.

## **OP-01 : Synthesis of Nitrogen and Oxygen Containing Disubstituted Tetrazolo Naphthalenes**

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Naphthalene nucleus is commonly found in compounds of commercial importance. A number of pharmaceutical and agricultural agents have naphthalene framework. Some of the commonly known examples include LY326315 (a selective estrogen receptor modulator) naproxen & nabumetone, naphazoline & pronethalol. Owing to the wide variety of practical application of naphthalene nucleus as building blocks, it is paramount to develop synthetic strategies around this nucleus to gain easy access to variety of naphthalene derivatives. The compound (7-methoxy-naphthalen-1-yl)-acetonitrile reacted with hydroiodic acid in the presence of Red Phosphorous to provide the corresponding (8-Hydroxy-naphthalen-1-yl)-acetonitrile. This compound was treated with  $\text{NaN}_3$  in the presence of  $\text{NH}_4\text{Cl}$  as a catalyst in dimethyl formamide as solvent to provide the corresponding 8-(1H-tetrazol-5-yl) methyl)-naphthalen-2-ol, which on reaction with aryl halides in the presence of  $\text{K}_2\text{CO}_3$  yielded the corresponding N-1H and 2H-substituted tetrazolonaphthalenes. The newly synthesized compounds were established by Infra Red,  $^1\text{H}$ ,  $^{13}\text{C}$  Nuclear Magnetic Resonance, mass spectroscopy data and their elemental analyses.

## **OP-02 : Synthesis and Antimicrobial Activity of Some New Products Derived from 5-Methyl-Benzimidazole Interlinked with Thiazolidinones : Potential Applications in Medicine**

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Heterocyclic ring systems containing N and S exhibit potent chemotherapeutic activity. 4-oxo-thiazolidines are important synthones for various types of biologically active molecules. Benzimidazoles and their derivatives are the important class of heterocycles because of

their wide spectrum of biological activity shown by the molecules. Incorporation of acetylamino-4-oxo-thiazolidines in 5-methyl-benzimidazole have been considered as an important pharmacophore for introduction to design the biologically active molecules. Hence in the present study 5-methyl-benzimidazole containing a -NH group at position-1 was used as the target for chemical modification. 5-methyl-benzimidazole on treatment with  $\text{ClCOCH}_2\text{Cl}$  in the presence of  $\text{Et}_3\text{N}$  followed by  $\text{N}_2\text{H}_4$  and various substituted aldehydes/ketones to afford arylidene hydrazino-acetyl- 5-methyl-benzimidazoles, 1. The compound 1 on reaction with thioglycolic acid yielded substituted aryl-[(acetylamino)-1,3-thiazolidin-4-ones]- 5-methyl-benzimidazoles, 2. The compound 2 on further treatment with various substituted aldehydes / carbonyls gave arylidene-substituted-arylated-(acetylamino)-1,3-thiazolidin-4-ones]-5-methyl-benimidazoles, 3. The structures of all the products were confirmed by spectroscopic data and chemical methods. The products were assayed for their antifungal activity against some selected fungi . The  $\text{ED}_{50}$  values of active antifungal products were also calculated on a  $\log_{10}$  probit scale from percent inhibition growth data. The antibacterial activity of the products were also determined against some selected microorganisms. Some of the products were found to exhibit appreciable activity.

### **OP-03 : Synthesis, Characterizations and Antifungal Activity of Some New Series of Halogenated Multifunctionalised Uracil Derivatives**

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In medicinal chemistry pyrimidine derivatives have been very well known for their therapeutic applications like 5-fluorouracil as anticancer; idoxuridine and trifluoridine as antiviral; zidovudine and stavudine as antiHIV; trimethoprim, sulphamethiazine and sulphadiazine as antibacterial; sulphadoxin as antimalarial and antibacterial; minoxidil and prazosin as antihypertensive; barbiturates eg. phenobarbitone as sedative, hypnotics and anticonvulsant; propylthiouracil as antithyroid; thionzylamine as H1-antihistamine; and toxoflavin and fervennuline as antibiotics. Life threatening infections caused by pathogenic fungi are becoming increasingly common, especially in those individuals with suppressed immune systems such as cancer patients and patients with AIDS. This is in part due to the emergence of strains resistant to currently available antibiotics. Therefore, in order to provide effective treatment to the

patients suffering from parasitic disease the discovery of the new and effective drugs is urgently needed. Pyrimidine nucleus was not widely explored as antifungal agents except few reported in literature. Keeping in view importance of nitrogen heterocycles in antiparasitic area and our continuous effort to search the novel bioactive nitrogen heterocycles, recently, we have synthesized a new series of halogenated multi-functionalised uracil derivatives for their antifungal activity. Synthesized compounds were screened in vitro against some human pathogenic fungi using ketoconazole as a positive control. Some of the synthesized halogenated multifunctionalised uracil derivatives have exhibited promising antifungal activity. In this presentation, the detailed antifungal activity profiles, synthetic procedure, mechanisms of the reactions and characterizations of the synthesized compounds by their spectral data ( $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR, EIMS, UV and IR) analysis will be discussed.

### **OP-04 : Montmorillonite K-10-Supported Palladium Nanoparticles for Copper-Free Acyl Sonogashira Reaction**

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Ynones are the versatile intermediates useful in the synthesis of a variety of heterocycles including pyrazoles, triazoles, furanones and pyrimidines. They also serve as key precursors for the synthesis of many bioactive molecules and natural products. Preparation of palladium nanoparticles supported on montmorillonite K-10 clay is described. The utility of thus prepared catalyst was examined for copper free acyl Sonogashira reaction of acid chlorides with phenyl acetylenes to achieve various ynone scaffolds. Coumarin derived ynones were also synthesized under mild optimized reaction conditions. All the title compounds were obtained in good to excellent yield. The recycling efficiency of the catalyst was extremely good and used successfully for seven cycles without significant drop in the yield. Herein we describe the preparation of palladium nanoparticles supported on montmorillonite K-10 clay which is first of its kind. Further, the utility of thus prepared catalyst was examined for copper free acyl Sonogashira reaction of acid chlorides with phenyl acetylenes to achieve various ynone scaffolds. Also the catalyst worked well to afford coumarin derived ynones under mild optimized reaction conditions. All the title compounds were obtained in good to excellent yield. The recycling efficiency of the catalyst was extremely well and used successfully for seven cycles without significant drop in the yield.

## **OP-05 : Staudinger Aza-Wittig-Type Reaction : A Simple Synthesis of Selenoureidopeptides Employing LiAlHSeH**

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A facile one-pot procedure for the synthesis of selenoureidopeptides employing lithium aluminum hydride hydroselenide (LiAlHSeH) as a selenating agent via a Staudinger aza-wittig type reaction is described. The protocol is simple, mild and involves the condensation of N<sup>β</sup>-urethane-protected aminoalkyl azide and an isothiocyanato ester leads to carbodiimide generation in situ, which further reacts with LiAlHSeH to form selenoureidopeptides in good yields. The obtained compounds were well characterized by <sup>1</sup>H, <sup>13</sup>C and <sup>77</sup>Se NMR studies.

## **OP-06 : PVC-Supported Palladium Nanoparticles as an Efficient Catalyst for Suzuki Cross-Coupling Reactions**

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Palladium-catalysed cross-coupling reactions are imperative tools for the construction of C-C bonds in fine chemicals, pharmaceuticals, advanced functional materials and natural products. Suzuki-Miyaura cross-coupling reactions are extensively employed protocol for the construction of biaryls and hetero biaryls compounds and they have been used on an industrial scale for the synthesis of the Sartan family of hypertensive drugs and the fungicide boscalid. Palladium nanoparticles since overcome the limitations of use of palladium complexes, exhibit a wide range of applications in both chemistry and biology. Polyvinyl chloride (PVC), commercially available polymer supported palladium(0) nanoparticles in ligand-free Suzuki cross-coupling reaction is demonstrated. Unmodified PVC-Polymer was swelled in ethanol, followed by the reduction of PdCl<sub>2</sub> in to Pd(0) using NaBH<sub>4</sub> at elevated temperature for 10 min to obtain PVC-Pd(0) catalyst. Desired biaryls were synthesized by treating PVC-Pd(0) to the solution aryl iodide/chlorides/bromides, arylboronic acid and Na<sub>2</sub>CO<sub>3</sub> in 1:1 EtOH-H<sub>2</sub>O in good yields.

As found in ICP-OES, recovered catalyst could be reused up to four times with negligible metal leaching. The PVC-Pd(0) was found

efficient and recyclable catalyst system for Suzuki reaction under mild conditions.

### **OP-07 : Microwave Assisted Synthesis and Characterization of Carboxymethyl Lignin from Lignin Bio-Polymer Obtained From Biomass of Bagasse Pulping**

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In the present study, a simple and efficient method is described for the synthesis of biodegradable soluble Carboxymethyl lignin (CML) using insoluble Kraft lignin bio-polymer which was isolated from bio mass of bagasse pulping under microwave irradiation. The present work revealed that rapid synthesis of CML and CML's degree of substitution (D.S.) was studied with respect to reaction time, microwave power and concentration of reactants. Further the characterization like FTIR, and PSD studies were carried out to evidence the changes observed in the CML.

### **OP-08 : Asymmetric Catalyst for Stereoselective Michael Addition and Henry (Nitroaldol) Reaction**

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Asymmetric synthesis has occupied central stage in the organic transformations. Among the various methods accessible for asymmetric catalysis, asymmetric catalysis is the most preferred method for the purpose of such synthesis. A series of enantiopure divalent metal complexes such as PdL1 – PdL4 and NiL1 – NiL4 are synthesized from optically pure chiral schiffs base ligands (CSBLs) L1 to L4. These CSBLs are easily obtained by simple condensation of variety of enantiopure  $\beta$ -aminoalcohols with o-hydroxybenzaldehyde in water at room temperature. Metal complexes thus prepared by mixing stoichiometric amounts of metal salts and CSBLs are used as asymmetric catalyst for stereoselective Michael addition and nitroaldol(Henry) reactions and studied for their % ee. Among the eight chiral catalysts of Pd(II) and Ni(II) studied, palladium complexes exhibited high % ee in both Michael addition and nitroaldol (Henry) reactions while nickel complexes showed moderate % ee.

## OP-09 : Ionic Liquid Mediated Synthesis of Novel Substituted Coumarin Containing Benzo[1,3]Oxazine-4-Ones

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Heterocyclic skeletons serve as ideal scaffolds on which pharmacophores can be appended to yield potent and selective drugs. In this respect, the utility of the benzo[b][1,4]oxazine scaffold as a privileged structure for the generation of drug like libraries in drug discovery programs has been amply demonstrated. The benzo[b][1,4]oxazin derivatives have been used as the basic framework for substances of interest in numerous therapeutic areas, such as anti-candida albicans, antifungal, and kinase inhibitors. Our interest concentrated on the construction of benzo[b][1,4]oxazin derivatives containing coumarin structural platform are known to serve as better biological activities in [Bmim]BF<sub>4</sub> as Ionic liquid. We are synthesized 2,3-dihydro-2-methyl-2-(2-oxo-2H-chromen-3-yl)-3-arylbenzo(e)[1,3]oxazine-4-one 4(a-e) from 3-acetyl coumarin I by Green synthesis. The compound 1 treated with substituted aniline in methanol refluxed for 4 h to form corresponding Schiff's base 3(a-e), which were treated with salicylic acid in [Bmim]BF<sub>4</sub> as ionic liquid heated at 80 °C to form corresponding title compounds.

## OP-10 : WEB : A Green Catalytic System for the Synthesis of Biologically Active Benzimidazole Derivatives

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Benzimidazoles and its derivatives represent one of the most biologically active classes of compounds. Its nucleus is structurally similar to purine bases and found in a variety of naturally occurring compound such as vitamin B12 and its derivatives. In this sense, synthetic protocols aiming to achieve this heterocycle core is a permanent interest, and many methods have been reported to accomplish this purpose. However, recent reports have been focused on the reaction of o-phenylenediamine with derivatives of carboxylic acid such as nitriles, amides, o-esters and acyl chlorides. These methods exhibit various advantages, but some of them suffer from one or more drawbacks such as prolonged reaction time, high temperature and

moderate to low yields, use of toxic reagents, tedious workup and stronger acidic conditions. Therefore, the present work is to develop a greener and economical approach for the synthesis of biologically active Benzimidazole derivatives. The approach for the synthesis of Benzimidazole derivatives using *o*-phenylenediamine and substituted benzoyl chlorides catalyzed by a natural feedstock extract of WEB (Water Extract of Banana) assisted by ultrasonication at room temperature.

## **OP-11 : CuBr/Air-Catalyzed C–N Bond Formation Via Cross-Dehydrogenative Coupling of 3-Phenyl Quinazoline-2,4(1H,3H)-Dione(N–H) And Methylarenes(C–H)**

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Quinazoline-2,4(1H,3H)-diones have elicited considerable interest among medicinal chemists because these are privileged in many pharmaceutical agents as well as in synthetic chemistry.<sup>1</sup> In particular, compounds containing N-benzyl-3-phenyl quinazoline-2,4(1H,3H)-dione substructures exhibit a wide range of biological activities<sup>2</sup> such as such as antibacterial, anti-inflammatory, anti-tubercular, anticonvulsant, hypoglycaemic, analgesic, antifungal, antiviral, antidepressant and anti-parkinsonism activities. Despite the potential applications of these molecules, very few methods are available for the direct N-alkylation of 3-phenyl quinazoline-2,4(1H,3H)-dione. Generally, they are synthesized by the reaction of 3-phenyl quinazoline-2,4(1H,3H)-dione with dimethyl carbonate.<sup>3</sup> However, this method has some drawbacks such as the use of harsh reaction conditions and expensive catalysts and reagents in many cases. Therefore, facile convergent approaches for accessing an array of N-benzyl-3-phenyl quinazoline-2,4(1H,3H)-dione derivatives are in high demand. Recently, metal-free Cross-Dehydrogenative-Coupling (CDC) of carbon–hydrogen (C–H) and nitrogen–hydrogen (N–H) bonds under oxidative conditions has emerged as powerful tool for the construction of carbon–nitrogen (C–N) bond. Thus, in continuation of our work on the development of new synthetic methodologies for the synthesis of heterocyclic compounds. Herein, we report a simple and efficient protocol for the direct synthesis N-benzyl-3-phenyl quinazoline-2,4(1H,3H)-dione via an oxidative C–N formation involving sp<sup>3</sup> C–H bond from non prefunctionalized methylarenes with 3-phenyl quinazoline-2,4(1H,3H)-dione by using CuBr/air catalyzed system.

## **OP-12 : Synthesis of Substituted (3-Chlorophenyl)(1-(5-Phenyl-1,3,4-Oxadiazol-2-Yl)Indolizin-3-Yl)Methanone and their Biological Applications.**

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Indolizine derivatives possess valuable biological activities and have been studied for their anti-inflammatory, anti-mycobacterial agent, anticancer agent, anticonvulsant agent etc. Many substituted indolizines are subject of extensive research due to their biological applications.

Substituted indolizine derivatives incorporated with oxadiazole was synthesized from substituted carbohydrazide and were prepared using hydrazide derivatives with corresponding indolizine acid. The acid was prepared from corresponding indolizine ester. Further, the ester was prepared using pyridinium bromide. All the above organic reactions were monitored by TLC. The structures of these compounds were confirmed by elemental analyses, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectral data. The substituted (3-chlorophenyl)(1-(5-phenyl-1,3,4-oxadiazol-2-yl)indolizin-3-yl)methanone biological activity in progress.

## **OP-13 : Copper-Catalyzed Synthesis of $\alpha$ -Acyloxy Ethers From Benzyl Amines Via Oxidative C-O Bond Formation**

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$\alpha$ -Acyloxy ethers are an important class of organic compounds and mainly appear as vital structural units in various biologically active compounds such as the antimalarial drug artemisinin and sanguin H-5. Despite of their applications in various fields, very few methods have been reported for the synthesis of  $\alpha$ -acyloxy ethers. Generally, they synthesized by the reaction of ethers with carboxylic acids and aldehydes. However, these methods have some disadvantages such as using toxic reagents and long reaction times. Therefore, there is a need to develop simple and efficient methods for the synthesis of  $\alpha$ -acyloxy ethers. Recently, the oxidative cross-coupling reaction has emerged as a power full tool for the construction of C-C and C-N bonds, relatively very few studies have involved in the formation of C-O bonds. Based on this, herein, we report an efficient method for

the construction of  $\alpha$ -acyloxy ethers from benzylamines and ethers via oxidative C-O bond formation in the presence of copper acetate and TBHP.

### **OP-14 : Synthesis of Arylcyanamides through Copper-Catalyzed C-N Cross-Coupling Strategy**

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An efficient method was developed for the synthesis of aromatic cyanamides from thiourea using readily available and air stable copper source as catalyst under moderate reaction conditions. The reaction process involves desulphurization followed by C-N cross-coupling techniques. All the substrates were given their corresponding target products in good yields. Various substituted iodobenzenes produced their respective C-N cross-coupled products in good to excellent yields under the optimized reaction conditions.

### **OP-15 : Synthesis and Antimicrobial Activity of Novel N-(5-Methylisoxazol-3-Yl)-2-(5-Phenyl-1,3,4-Oxadiazol-2-Yl)Acetamide Derivatives**

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2,5-Disubstituted 1,3,4-oxadiazoles constitute a unique class of nitrogen and oxygen containing five membered heterocyclic compounds with a wide range of biological activities such as antibacterial, antitubercular, antitumor, antifungal, anti-inflammatory antiviral, antihypertensive, anticonvulsant, and anti-diabetic properties. Isoxazole derivatives exhibit various biological activities such as, anticonvulsant, anticancer, anthelmintics, anti-inflammatory, adenosine antagonist, fungicidal, herbicidal, hypoglycemic, muscle relaxant, antiviral and antimicrobial. As a sequel to our work on screening for new biologically active molecules possessing isoxazole moiety, we report the synthesis and antimicrobial activity of novel N-(5-methylisoxazol-3-yl)-2-(5-phenyl-1,3,4-oxadiazol-2-yl)acetamides.

Ethyl 2-(5-methylisoxazol-3-ylcarbonyl)acetate was prepared and

it was converted into 3-hydrazinyl-N-(5-methylisoxazol-3-yl)-3-oxopropanamide, with hydrazine hydrate in ethanol and converted into hydrazones by reacting with different aromatic aldehydes in methanol. These hydrazones were treated with Chloramine-T underwent oxidative cyclization to afford N-(5-methylisoxazol-3-yl)-2-(5-phenyl-1,3,4-oxadiazol-2-yl)acetamides. The structures of all newly synthesized compounds were confirmed by their IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectral analysis. The newly synthesized title compounds have been screened for antimicrobial activity

### **OP-16 : Selective Synthesis of 3-( $\alpha$ , $\alpha$ -dibromoacetyl)-4-hydroxy-6-methyl-2H-pyran-2-one as an Excellent Precursor for the Synthesis of 2-substituted 4-(4-hydroxy-6-methyl-2-H-2-oxopyran-3-yl)thiazoles as Antimicrobial and Antifungal Agents**

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$\alpha$ -Bromoketones are well known for their use as precursors for synthesizing a myriad of  $\alpha$ -functionalized ketones, carbo- and heterocyclic compounds. These bifunctional compounds are readily accessible from bromination of the corresponding ketones. In spite of their multifaceted utility in organic synthesis, there is always need of exploring their alternatives because of the lachrymatory properties associated with them. In view of these facts and based on the recent developments on the use of  $\alpha$ ,  $\alpha$ -dibromketones as a safer and superior alternative to  $\alpha$ -bromoketones, we became interested in the synthesis of some new 2-substituted 4-(4-hydroxy-6-methyl-2-H-2-oxopyran-3-yl)thiazoles.

A selective synthesis of 3-( $\alpha$ ,  $\alpha$ -dibromoacetyl)-4-hydroxy-6-methyl-2H-pyran-2-one (3) has been achieved by bromination of DHA using CuBr<sub>2</sub>. The reaction of 3 with different thioureas and thiomides offers a convenient and efficient method for the syntheses of 2-substituted 4-(4-hydroxy-6-methyl-2-H-2-oxopyran-3-yl)thiazoles. These thiazoles were evaluated for their antimicrobial and antifungal activity.

This study further establishes that  $\alpha$ ,  $\alpha$ -bromoketones are superior and safer alternatives to  $\alpha$ -bromoketones, particularly when nucleophile is sulfur. The details of methods of synthesis, characterization data of the synthesized compounds, and mechanistic aspects of these reactions will be presented.

## **OP-17 : Synthesis, Characterization and in vitro SIRT1 Inhibition Studies of Some Indole Derivatives**

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SIRT1, a NAD<sup>+</sup>-dependent deacetylase enzyme, belongs to the family of class III histone deacetylase and is involved in diverse cellular processes. Since SIRT1 is involved in various physiological functions both in normal and diseased conditions, a strategy of designing small molecules to act on SIRT1 has been emerging out as a promising approach in medicinal chemistry research. Based on our ongoing effort to identify indole based potent SIRT1 inhibitors and also considering the promising sirtuin inhibition of isoxazolone derivatives, we synthesized a new set of 3-methyl-4-[(1-methyl-1H-indol-3-yl)methylene]isoxazol-5-one derivatives (I<sub>1-18</sub>) which contain substituted amide (I<sub>1-9</sub>), substituted 1,2,3-triazole (I<sub>10-15</sub>) or substituted benzylic ether (I<sub>16-18</sub>) at position-2 of the indole nucleus. The molecules were screened against three human cancer cell lines to evaluate their in vitro cytotoxic property. Most of the trifluoromethyl substituted derivatives exhibited better growth inhibition activity than their methyl substituted analogues. The SIRT1 inhibition activity of two potent molecules (I<sub>17</sub> and I<sub>18</sub>) was investigated and the SIRT1 IC<sub>50</sub> values are 35.25 and 37.36 μM respectively for I<sub>17</sub> and I<sub>18</sub>. The molecular docking studies with SIRT1 enzyme revealed favourable interactions of the molecule I<sub>17</sub> with the amino acids constituting the receptor enzyme.

## **OP-18 : Synthesis and Antibacterial Activity of (E)-N-(2-(3-Chlorophenyl)-1-(Pyridin-3-Yl)Ethyldene) Methanamine**

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Heterocycles are abundant in nature and are of great significance to life; hence they have attracted considerable attention towards the design of biologically active molecules and advanced organic materials. Among wide variety of heterocycles that have been explored for developing pharmacologically important molecules. Pyridine unit, constitutes an important group due to wide variety of biological activity such as antitumor, antioxidant, anti-inflammatory, analgesic, anti-diabetic and chemotherapeutic agents. Schiff's bases and their amine analogues derived from various aromatic aldehydes and ketones

were reported to possess fungicidal, bactericidal, antiviral, antioxidant and antimicrobial activity. In continuation of our interest in designing the synthesis of biologically active heterocycles herein we report the synthesis and antibacterial activity of (E)-N-(2-(3-chlorophenyl)-1-(pyridin-3-yl)ethylidene)methanamine

2-(3-Chlorophenyl)-1-(pyridin-3-yl)ethanone was treated with different primary amines, in methanol in presence of catalytic amount of glacial acetic acid to get the (E)-N-(2-(3-chlorophenyl)-1-(pyridin-3-yl)ethylidene)methanamines. The structure of the synthesized compounds has been elucidated by means of IR, <sup>1</sup>HNMR and Mass spectral data. All the synthesized compounds are evaluated for antibacterial activity.

### **OP-19 : Synthesis, Characterization and Antimicrobial Studies of Some New Dithiodihydrazones**

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A facile synthesis of different dithiodipropionic dihydrazones have been achieved condensation of dithiodipropionic dihydrazide with m-anisaldehyde, thiophene-2- aldehyde and 4-acetyl pyridine resulted in the formation of different dihydrazones viz . m-anisaldehyde dithiodipropionic dihydrazone, thiophene-2-aldehyde dithiodipropionic dihydrazone and 4-acetyl pyridine dithiodipropionic dihydrazone respectively. All the synthesized compounds were characterized by their repeated M.P. determination, TLC for single spot, element analysis, IR and NMR spectral data. They were screened for their antimicrobial activities against two bacteria *Staphylococcus aureus* and *Escherichia coli* and two fungi *Aspergillus niger* and *Aspergillus flavus*. All the synthesized compounds showed appreciable antimicrobial activities in comparison to the constituting fragments.

### **OP-20 : Evaluation of their Antibacterial, Antifungal Activity and Synthesis and Characterization of 6-benzyl-3-(5-methyl-1-(naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)-7H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazine.**

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Synthesis of quiazoline derivatives and also have been evaluated

their biological activity. In this synthesis methodology follows very identical and evaluated their anti microbial activity most of the compounds have been exhibits more or all most equal activity of standered activity. Synthesis of 6-benzyl-3-(5-methyl-1-(naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)-7H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazine from reaction in between 4-amino-5-(5-methyl-1-(naphthalen-1-yl)-1H-1,2,3-triazol-4-yl)-4H-1,2,4-triazole-3-thiol and various phenacyl iodides and these compounds has been charecterization by PMR,CMR,IR and Mass spectral methods.

In this method sucessfully synthesised novel substituted quiazoline derivatives with good yeild and also evaluated their Antibacterial activity towards Gram possitive and Gram negative bacterias and also evaluated their Antifungal activity. In this componds large number of compounds shows more potent antimicrobial activity.

### **OP-21 : Synthesis and in-vitro Studies of Some New Quinoline 1, 3, 4- Thiadiazolo Pyrimidin Derivatives**

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A series of eight new quinoline associated 1,3,4-thiadiazolo pyrimidin derivatives have been developed by using 8-fluoro-4-methylsulfanylthiocarbonylamino-quinoline-3-carboxylic acid ethyl ester, 8-fluoro-4-hydrazine thiocarbonylamino-quinoline-3-carboxylic acid ethyl ester and 3-amino-7-fluoro-2-mercapto-3H-pyrimido-[5,4-c]quinolin-4-one as main intermediates which have been made from the typical 4-amino-8-fluoro-quinoline-3-carboxylic acid ethyl ester. Structure elucidation of the titled compounds has been done by IR, <sup>1</sup>HNMR and Mass spectral data. Microbial activity of the target compounds has been verified against various microorganisms.

Further studies needed for the development of anti microbial activity and other biological activities.

### **OP-22 : Natural Products from Marine Environment**

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The marine environment is a rich source of both biological and chemical diversity. This diversity is immense and therefore is an extraordinary resource for the discovery and development of various novel drug leads. Because of the different physical and chemical conditions found in the marine environment, almost every class of

marine organism affords a variety of molecules with unique structural features. Research into the biological as well as pharmacological properties of marine natural products has led to the discovery of many potentially active agents considered worthy of clinical application.

### **OP-23 : Comparative Study of Metal Concentrations in different Parts of *Coldenia procumbens* Linn. by ICP-AES**

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*Coldenia procumbens* Linn. is the most widely used medicinal plant in Sidha and Ayurveda for the treatment of different diseases. The objective of this paper is to compare metal concentrations in different parts of the plant i.e. leaves and leaf twigs. The leaves extract showed major concentrations of Ca, Na and minor concentrations of B, Cu, K, Mg, Mn, Ni, Zn. The leaf twigs extract showed higher concentrations of Ca, K and least concentrations of Cu, Mn, B, Ni & Zn. The heavy metals like As, Pb, Hg and Cd are not detected in these extracts. All these concentrations were within the permissible limits. Hence the *Coldenia procumbens* Linn. is safe enough to be consumed as a drug for treating various diseases like arthritis, cancer and diabetes.

### **OP-24 : GC-MS Analysis of Stem Bark of *Syzygium Samarangense***

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*Syzygium samarangense* (Blume) Merr. & L.M. Perry is a famous deciduous tree belongs to Myrtaceae family, which is being cultivated in India mainly for their edible fruits. It is also well known as java apple and water apple. Hexane extract of *Syzygium samarangense* stem bark was subjected to Preparative Thin Layer Chromatography which was separated into two bands. For further purification, these bands were again subjected to Preparative Thin layer Chromatography in a different solvent system and these bands were analysed by using GC-MS analysis. In band one, hydrocarbons are the major components followed by fatty acids and steroids. In band two, Steroids are the major components followed by hydrocarbons and fatty acids. The present study gives detailed information about the GC-MS analysis of Hexane extract of *Syzygium samarangense* stem bark.

## **OP-25 : An Efficient Synthesis and Biological Applications of Chalcogen Derived Pyridine, Pyrimidine based Coumarins**

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An efficient synthesis of novel series of coumarin-pyrimidine hybrids derived from coumarin chalcones and Isonicotinamide hydrochloride are reported here. Structures of the synthesized compounds were characterised by IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, and Mass spectroscopic techniques. Investigation of all the compounds revealed its potency towards anti-microbial activity. The synthesized compounds were also explored for their in vitro anticancer activity and IC<sub>50</sub> reveals significant cytotoxicity against two human cancer cell lines A-549 (human lung carcinoma) and HeLa (human cervical cancer) with IC<sub>50</sub><100 μM. DNA cleavage exhibited that most of the synthesized compound inhibited the growth of pathogenic organism by genome cleavage as no traces of DNA were found. The present investigation points out that the synthesized coumarin-pyrimidine analogs are promising in targeted drug delivery systems, may be designed for cancer therapy.

## **OP-26 : An Efficient Synthesis of New Polycyclic Aromatic Hydrocarbons through C-H Bond Activation**

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Synthesis of new pyrazolo[1,5-f]pyrazolo [1',5':1,2] quinolino [4,3-j] phenanthridine and its derivatives via C-H bond activation and conventional direct arylation techniques have been reported. The photocatalytic activity of the Pd-complexes depends on the bandgap energy, surface area, and photostability. Therefore, we studied the photocatalytic activity of the new catalysts are compared with existing Pd(II) catalysts. Overall photostability of the new photocatalysts is high in the aquatic solutions than known Pd(II) catalysts. The activity of the Pd(DPTTP)Cl<sub>2</sub> and Pd(TPTTP)Cl<sub>2</sub> performed better than existing Pd(O) complexes due to higher surface area and lower bandgap energy.

## PHARMACEUTICAL CHEMISTRY SECTION

### Sectional President's Address

#### **Kinetic and Mechanistic Patterns in the Oxidation of L-cysteine and L-cystine – A Comparative Study**

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Oxidation of organic compounds and in particular amino acids is an important transformation in synthetic organic chemistry. L-Cysteine and L-Cystine are the two non essential sulfur containing optically active amino acids that take part in protein and enzyme synthesis. The deficiency of these two amino acids results in anemia and necrosis of liver and kidneys. A considerable effort was made to explore the mechanism of oxidation of these two sulfur containing amino acids basing on the kinetic results obtained with different oxidants like chromium(VI), cerium(IV), hexachloroiridate(IV), pyridinium chlorochromate(PCC), pyridium bromochromate (PBC), manganese (III) and thallium(III) in acid medium and hexacyanoferrate(III) uncatalysed and catalysed (Osmium(VIII) or Ruthenium(III)) and periodate in alkaline medium. The kinetic trends, mechanisms of oxidation and oxidation products of the monomer (cysteine) and dimer (cystine) were compared. It was noticed that the oxidation of L-Cysteine with pyridinium chlorochromate(PCC) proceeds complexation between the substrate and oxidant while that of PBC proceeds with the formation of an intermediate (no kinetic evidence for complexation), though the final oxidation product is cysteic acid( $\text{RSO}_3\text{H}$ ) in both the reactions. While in the oxidation of L-Cysteine by periodate in alkaline medium, the end product is cysteine sulfinic acid( $\text{RSO}_2\text{H}$ ). Further in the uncatalysed and Osmium(VIII) catalysed oxidation reactions of L-Cystine with HCF(III) cysteic acid is the end product but Ruthenium(III) catalysed oxidation of HCF(III) resulted in the formation of 2-oxo-ethylsulfonyl acetaldehyde. So it is evident from these observations that sulfur atom is the primary site of attack in the oxidation of these two sulfur containing amino acids with all these oxidants.

## **PCIL-01 : Practical Approach for the Quantification and Risk Assessment of Elemental Impurities in Pharmaceutical Products**

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Elemental impurities in pharmaceutical products can be introduced from a number of sources, including catalysts, raw materials, production processes, and packaging materials. New methods and guidelines are coming from United States Pharmacopeia (USP) Chapters USP <232>, <233> and <2232> and counterpart guidelines from International Conference on Harmonization (ICH), referred as ICH Q3D which are adopted by the European Medicines Agency (EMA).

The implementation of the new USP chapters <232> and <233> on elemental impurities, in January 2018, will redefine how the pharmaceutical industry shall perform tests for elemental impurities in drug products. This abstract provides a practical guidance for determining Elemental Impurities in Pharmaceutical Products (both in Active Ingredients and in Dosage forms) by employing a generic method developed on the instrumental technique (ICP-MS).

Elemental impurities included in the ICH Q3D have been categorized in to three classes i.e. Class 1 elements (As, Cd, Hg & Pb) are human toxicants that have limited or no use in the manufacturing process, Class 2A (Co, Ni & V) and Class 2B (Ag, Au, Ir, Os, Pd, Pt, Rh, Ru, Se & Tl) elements are generally considered as route dependent human toxins and Class 3 (Ba, Cr, Cu, Li, Mo, Sb & Sn) elements have relatively low toxicities by oral route of administration but may require risk assessment for inhalation and parenteral routes.

The generic method was developed using ICP-MS (Agilent 7800 ICP-MS system with auto sampler IAS and Mass hunter 4.3 workstation used as data acquisition software) by optimizing conditions like cell gas flow rate, plasma Rf power, dilution gas to achieve all 24 elements in a single acquisition scan. However, the sample preparation technique with Microwave digestion system (CEM, Mars 6 model used) was adapted with necessary optimization of preparation method in order to achieve the complete sample digestion, reduce matrix interference and recovery of elemental impurities in the range of LOQ to 150% of specification level.

To check the suitability of method and for risk assessment at predefined specification levels, a generic method is adapted for feasibility studies of drug substance or drug product. To achieve the

better accuracy, method optimization of sample preparation includes but not limited to changing the acid composition, altering the sample concentration, usage of complex formation agents like Thio Urea in mild acidic condition.

Few challenges were faced during the method optimization primarily due to the complexity of sample matrix interferences, detectability of elements present at trace levels, contamination at trace levels, on the type of sample preparation and its route of administration. After the method optimization Method validation was performed as per USP <233>. In order to assess the risk of class 1, 2A, 2B and 3 elemental contaminants in commercial products under distribution, a maximum daily dosage of 10 grams/day considered as worst case scenario for setting specification limits for oral, inhalation and parental route of administration.

## **PCIL-02 : Nanotechnology – A Strategic Tool for Drug Delivery in Pharmaceutical Industry**

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The classical research model in the development of new drugs are capital and time exhaustive. Nevertheless, several drugs fail in their clinical study phase causing a huge loss to an organization making pharmaceutical companies explore new means of meeting market demands. The technological advances in the field of human health care had made the generic firms evolve from conventional dosage form to Novel Drug Delivery System (NDDS) changing from classical model towards creating value-added products. These methods enable pharma companies to reformulate existing drugs in the market which extends product life, enhance drug performance, increase patient safety and reduce healthcare costs. Nanotechnology in drug delivery has a profound impact on disease prevention, diagnosis and treatment of chronic diseases such as cancer, HIV and diabetes. Normally, drugs work through the entire body before they reach the disease affected area. Using Nano formulations, the drug can be targeted to a precise location which would make the drug more effective and reduce the chances of possible side-effects. Nano based delivery systems can also protect drugs from degradation, improves drug bioavailability, reduces the number of doses required and hence quicker and cheaper treatments can be developed. For the generic industry, the field of drug delivery extends to all therapeutic class and represents a strategic tool for expanding drug markets because new delivery systems have reduced development time, hastened approval from regulatory, making the drug cost effective.

## **PCIL-03 : Recent Pharmaceutical Approach Leading to the Discovery of Drugs from Medicinal Plants**

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The high mortality rate associated with parasitic diseases is mainly due to the development of parasitic multi-drugs resistant strain and hence drugs currently in the markets are not effective due to their limited pharmacological efficacy. Therefore, in recent scenario, the discovery of new drugs in parasitic area has become a challenging task for pharmaceuticals/medicinal chemists. In 21<sup>st</sup> century the pharmacological effects of traditional medicinal plants have been considered as a promising source of future drug for the treatment of various challenging diseases and recently, there has been a resurgence of interest to rediscover medicinal plants as a source of potential drug candidate/ lead molecule. The plants derived lead molecules have played an important role in pharmaceutical industries to optimize the activity of lead candidate in order to develop new effective drugs in treating the various diseases. In our continuous effort and work for the development of new therapeutic agents from medicinal plants for parasitic diseases, recently, we have isolated and identified the many new lead bioactive constituents from terrestrial medicinal plants i.e. novel anthraquinones, spirostan saponins and ursane triterpenoids along with many other inactive constituents. In this presentation, recent pharmacological trends toward the discovery of new therapeutic agents from plants and our finding on the isolations, characterisations and bioactivity profiles of the bioactive lead molecules isolated in our Laboratory will be discussed in detail.

## **PCIL-04 : Design, Synthesis and Biological Evaluation of Pyrimidine Analogous**

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Pyrimidine found to be pharmaceutically and synthetically resourceful substrates, where they can be used for the synthesis of a large variety of heterocyclic compounds and as organic matter for drug synthesis. In medicinal chemistry pyrimidine derivatives have been very well known for their therapeutic applications. The presence of a pyrimidine base in thymine, cytosine and uracil, which are the essential binding blocks of nucleic acids, DNA and RNA is one possible

reason for their activity. Another important pharmacophore group is an isoniazid incorporated in a wide variety of therapeutically important drugs. Isonicotinic acid hydrazide (Isoniazid, INH) has very high in vivo inhibitory activity towards *M. tuberculosis H<sub>37</sub>Rv*. Finding numerous biological significance, we have utilized pyrimidine as building block by incorporating with different biologically active nitrogen and/or sulphur containing heterocyclic moieties like isoniazid, triazole, thiazolidinone and studied their biological activities. Our efforts are focused on the introduction of chemical diversity in the molecular frame work in order to synthesize pharmacologically interesting compounds. Astonishing pharmacological activities of pyrimidine nucleus and resistance against microorganism prompted us to study biological activity of newly synthesized pyrimidine clubbed analogs towards different biological evaluation viz., antimicrobial, antimalarial and antitubercular. We have also carried out *in silico* molecular docking study of our targeted compounds with different PDBs as biological target to understand binding interaction of targeted compounds.

## **PCIL-05 : N-Arylhydroxamic Acids as Anti-Breast Cancer Agents**

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Hormonal imbalance is generally responsible for Breast Cancer which is one the most frequent cancer and second leading cause of cancer deaths in women. To design a biologically active compound, lots of money is required for the synthesis of huge number of molecules and to perform their biological characterization, followed by separation of active compound, its testing and modification. Therefore, knowledge of QSAR parameters of a series of compounds is helpful in saving time and money as there is some quantitative relationship between molecular structure and biological activity.

In the present investigation, hydrophobic, electronic and steric parameters of a series of N-arylhydroxamic acids have been measured and that of quantum mechanical indices are computed. Cytotoxicity of these molecules have been determined in-vitro towards breast cancer cell line, MCF-7 by MTT assay. All molecules show anti-tumour activity. The best molecule CBHA, with IC<sub>50</sub> value 89.96  $\mu$ M was chosen for in-vivo studies. The results showed that it killed 90% of cancer cells per kg wt. of mice within 16 days.

QSAR parameters were then correlated with biological activity following the multiple regression analysis (MRA). This generates five

equations for hydrxamic acid's functionality and resulted that the parameters,  $M_R$ ,  $\log K_w$ ,  $E_{LUMO}$  and HBD strength are responsible for the biological activity of these molecules. This is also inferred that introduction of more bulky substituents are favourable to make the molecules more potent against breast cancer.

## **PCIL-06 : Polymorphic Transformations in Pharmaceutical Drug Substances - A Case Study with Lenalidomide**

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Comprehensive studies on the isolation/characterization of pharmaceutical solids such as polymorphs, salts, hydrates, solvates, co crystals, etc. are integral parts of the pharmaceutical industry. Further, the selected solid form should meet the basic requirements of optimal stability, reproducibility, and scalability, which will eventually lead to devising a robust and reliable process for its manufacture. The existence of more than one crystal structure for a chemical substance is referred as polymorphism. Polymorphs of active pharmaceutical ingredients (APIs) have always drawn attention in view of their physical and intellectual property. Polymorphs can exhibit different physical and chemical properties, including melting point, density, stability, manufacturability, solubility, bioavailability, etc. The importance of polymorph screening can be visualized by a fact of sudden appearance or disappearance of a polymorphic form during manufacturing and storage. The goal of any specific solid form screening/development is to identify such triggering factors deciding the polymorphic phase stability. Hence, it is essential and important that the API solid form is monitored closely to understand the dehydration/desolvation pathways. The main objective of the current work was to discover novel

Polymorphs of Lenalidomide and to investigate the reasons behind it.

## **PCIL-07 : Newer Diversity Oriented Methodologies for the Molecules of Biological Importance**

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Newer methodologies to develop molecules of biological importance is the attractive area of research, thereby creating library of known

and unknown molecules having potential biological applications. Synthetic methods that allow rapid access to large number of diverse structural arrays is growing constantly, which served as a new driving force for the new innovations. In order to synthesize large number of molecules with high level of diversity and complexity, In addition to developing new synthetic techniques and reagents, organic chemists are exploring new methods to design and to evolve new molecules, strategies for new molecules leading to new source of diversity and improving the quality of compound libraries. This diverse new methodologies that will create structurally diverse compounds efficiently in high yields and with excellent purity and with wide range of functional groups as handles to expand them further. One of the richest source of diversity in drug discovery are small molecule heterocycles, which in addition to exhibiting biological activity, also serve as rapid scaffolds for further display of broad range of functionalities. For several years M.V.Basaveswara Rao have been engaged in design and development of new efficient methodologies for a wide variety of heterocycles, displaying a range of skeletal and functional group diversity. The biological properties of heterocycles in general make them one of the prime interests of the pharmaceutical industry, storage device platforms for opto-electronic industry. We have synthesized various heterocyclic skeletons initially and utilized them for making other heterocycles. All the synthetic methodologies reported by us are simple efficient and does not involve hitherto costlier chemicals, circuitous reaction pathways, drastic reaction conditions and corrosive molecules. We have exploited [4+2]cycloaddition reactions, [3+3]Cycloaddition reactions, indolo[2,3]quinodimethanes and dienolates, anion assisted aromatic annulations, heteroaromatic annulations and doubly handled reactions. Our aromatic and heteroaromatic annulation strategies are highly efficient, simple and results in variety of molecules with quantitative yields.

## **CYSA-PCO-01 : DNA Binding Parameters and Cytotoxicity of Hydroxamic Acid-Metal Complexes**

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DNA is the potential target of numerous drugs utilized widely in clinical cancer therapy. The present study embodies the detail of interaction of N-p-tolylbenzohydroxamic acid-Cobalt(II) complex [N-p-TBHA-Co(II)], N-p-chlorophenylbenzohydroxamic acid-Vanadium(V) complex [N-p-ClPBHA-V(V)] and (N-phenylbenzohydroxamic acid-Tungsten(VI) complex [N-PBHA-W(VI)] with ct-DNA and its

consequences by UV-Visible and fluorescence spectroscopy, viscosity measurements and molecular docking. The intrinsic binding constant,  $K_b$  of complexes were determined which follows the order as N-p-TBHA-Co(II) > N-p-CIPBHA-V(V) > N-p-PBHA-W(VI) along with hyperchromism and bathochromic shift for the complexes. Fluorescence quenching method also reveals an interaction of N-p-TBHA-Co(II), N-p-CIPBHA-V(V) and N-p-PBHA-W(VI) with ct-DNA suggesting the decrease in fluorescence intensity of the complexes. Mode of binding was also disclosed by ethidium bromide displacement method. The increase in the relative viscosity of ct-DNA with increasing the concentration of the N-p-TBHA-Co(II), N-p-CIPBHA-V(V) and N-p-PBHA-W(VI) complex is also revealed. The docked posture of ct-DNA with N-p-TBHA-Co(II), N-p-CIPBHA-V(V) and N-p-PBHA-W(VI) uncover the strong binding interactions as it has smaller value of binding energy. Finally, the *in-vitro* cytotoxicity studies indicate that the complexes have excellent anticancer activity against the breast cancer cell line, MCF-7. The observed results would be a great tool in the design and development of hydroxamic acid-metal complexes as potent anti-cancer agent.

### **CYSA-PCO-02 : Synthesis, Characterization and In-vitro Antioxidant Properties of 4-(((4-((5-((Substitutedphenoxy)Methyl)-1,3,4-oxadiazol-2-yl)sulfanylmethyl)-1H-1,2,3-triazol-1-yl)methyl)-6-methyl)-2H-Chromene-2-one and 1-(((4-((5-((Substitutedphenoxy)Methyl)-1,3,4-oxadiazol-2-yl)sulfanylmethyl)-1H-1,2,3-triazol-1-yl)-Methyl)-3H-Benzo[f]Chromene-3-one**

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Development of new synthetic strategies for the construction of heterocycles is attracting the attention of organic chemists since last few decades. This is because of the fact that, fine tuning of biologically important motifs lead to various derivatives of heterocycles. One of those derivatization involve alkylation and arylation of the side chain of the heterocycle which is an important method since this technique is used to link one heterocycle to the other. One such method is S-alkylation of 2-mercapto-1,3,4-oxadiazole. Several methods are reported for the S-alkylation of 5-substituted-2-mercapto-1,3,4-oxadiazole. Herein we report a green chemistry process for the S-alkylation of 2-mercapto-

1,3,4-oxadiazole derivatives with propargyl bromide by using sodium bicarbonate in aqueous medium. The resulting alkynes containing substituted oxadiazoles underwent 1,3-dipolar cycloaddition reaction with 4-azidomethyl coumarins/chromenes under "Click Chemistry" condition to yield the title compounds. All the newly synthesized compounds are screened for their *in-vitro* anti-oxidant properties by DPPH radical scavenging assay method. Structures of the newly synthesized compounds were confirmed from analytical and spectral data.

### **PCO-01 : Microwave Assisted Synthesis and Characterization of Carboxymethyl Lignin from Lignin Bio-polymer Obtained from Biomass of Bagasse Pulping**

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In the present study, a simple and efficient method is described for the synthesis of biodegradable soluble Carboxymethyl lignin (CML) using insoluble Kraft lignin bio-polymer which was isolated from bio mass of bagasse pulping under microwave irradiation. The present work revealed that rapid synthesis of CML and CML's degree of substitution (D.S.) was studied with respect to reaction time, microwave power and concentration of reactants. Further the characterization like FTIR, and PSD studies were carried out to evidence the changes observed in the CML.

### **PCO-02 : Influence of Electron Donating and Electron Withdrawing Substituents on *in-vitro* Antioxidant Activity of Different-1, 4 - Dihydropyridine Dicarboxylates**

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A series of different 1, 4 - dihydropyridine dicarboxylates were synthesized and subjected to their antioxidant activity. The antioxidant activity of these compounds were determined by using 1,1-Diphenyl-2-picrylhydrazyl (DPPH) radical scavenging activities, 2,2-azino-bis-(3-ethylbenzothiazoline-6-sulphonic acid) (ABTS) radical cation scavenging

activities and measuring its ability to reduce  $\text{Fe}^{3+}$  to  $\text{Fe}^{2+}$  by Ferric Reducing Ability of Plasma (FRAP) test. Butylated hydroxytoluene (BHT) was used as standard antioxidant. Activity data reveals that this class of compounds has significant radical scavenging ability. Especially, electron donating substituents at C4 position enhances antioxidant activity while electron withdrawing substituents reduces the antioxidant activity of different-1, 4 - dihydropyridine dicarboxylates.

### **PCO-03 : Encompassment of Benzyl Isothiocyanate in Cyclodextrins : Distinct Focus on Stability and Biological Applications**

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The use of methodical and innovative sonication method has been explored for the fabrication of inclusion complex of Benzyl Isothiocyanate, a potential anticancer and -antimicrobial agent. The advancement involved investigation of inclusion behaviour, characterisation and an in-depth study of thermal and UV stability of Benzyl Isothiocyanate with cyclodextrins;  $\beta$ -CD and hp- $\beta$ -CD. The sonication driven encompassment in cyclodextrins helped to overcome the hindrance of low solubility and high volatility. Investigations of physical and thermodynamic parameters using UV-visible spectroscopy, FTIR, XRD, TGA etc confirmed stability of inclusion complexes. Both  $\beta$ -CD and hp- $\beta$ -CD based inclusion complexes retained the antimicrobial property of the free Benzyl Isothiocyanate, indicating their potential utility as antimicrobial agents. Haematological safety and cellular uptake data gives direction to in-depth analysis for its exploitation of anti-tumour activity.

### **PCO-04 : Metallopharmaceuticals**

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Synthesis, structural and biological properties of metal complexes has been one of the research areas of the principal investigator. The present work is written with an interest in the broad exploration of pseudohalogens containing metal complexes in terms of synthesis, structural and anti-cancer biological evaluation. Mixed-ligand metal complexes containing pseudohalogens as primary ligand and an organic molecule of N-hetroaromatic ligand's family such as imidazole, bipyridine, 1,10-phenanthroline, 2,4,6-Tris(2-pyridyl) 1,3,5-triazine and

essential amino acid: tyrosine and arginine as secondary ligand. It is well known that these hetroaromatic and amino acid ligands and their derivatives, as well as many of their complexes, are exhibiting anti-bacterial, anti-microbial, anti-fungal, anti-viral and antitumor. The paper will focus on synthesis of a broad spectrum of pseudohologen based metal complexes using different synthetic methods and studies on structural properties of these metals. Electronic properties like energies, structures, vibrational frequencies of metal complexes and reactive systems will be predicted by utilizing ab initio, density functional theory, semi-empirical, etc. with the help of in silico programs like Gaussian etc. and the results will be correlated with experimental values. Furthermore, the synthesized complexes will be evaluated for anticancer, antioxidant and antimicrobial for the use as metallopharmaceuticals.

### **PCO-05 : Phytochemical Screening and GC-MS Analysis of Tridax Procumbens Leaves**

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Tridax procumbens Linn.is a weed found throughout India. The plant is known as “vetukkayathalai”, in English activity, hypotensive effect, immuno modulating property, bronchial, dysentery, diarrhoea. The present investigation was carried out to determine the qualitative analysis of phytochemical screening and possible chemical components Tridax procumbens. The further phytochemical compounds are identified using GC-MS analysis popularly called ‘coat buttons’ and is dispensed for “Bhringraj” by some of the practitioner of Ayurveda. Tridax procumbens is a widely occurring medicinal herbs used by ethnomedicinal practitioner. It has known for its number of pharmacological activities like hepatoprotective activity, anti inflammatory, wound healing, antidiabetic.

### **PCO-06 : Molecular Modeling Studies of some Synthesized Pyrazolines as Antitubercular Agents**

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A series of pyrazoline analogs, have been synthesized in good yields in the present research and structures of these compounds were established by IR, <sup>1</sup>H NMR and mass spectral analysis. And evaluated for their antitubercular activities. Some of the tested

compounds displayed promising anti-tubercular activity. The docking of inhibitors into MtSK using Sybyl-X 2.0 software revealed the vital interactions and binding conformation of the inhibitors. Physicochemical properties and Lipinski's 'Rule of Five' analysis predicted higher intrinsic quality of the synthesized compounds and revealed that these compounds have good bioavailability and druglikeness properties.

### **PCO-07 : Effect of Inorganic Cations on the Complexation of Pluronic F-127 and Rhodamine-B Dye**

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In this paper complexation of pluronic F-127 and cationic dye Rhodamine-B in presence of chlorides of  $\text{Sr}^{2+}$ ,  $\text{Cr}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Cu}^{2+}$  and  $\text{Co}^{2+}$  as quenchers is studied. The characterization studies employed were UV visible spectroscopy, fluorescence spectroscopy, lifetime studies, scanning electron microscopy (SEM), Dynamic light scattering (DLS) studies. There was increase in size of the F-127 after incorporation of Rh-B dye in the first step and further increase in size after addition of quenching salts in the second step. Out of all the salts  $\text{Cu}^{2+}$  was to be the best quencher in the group.

### **PCO-08 : Isoxazoles as Potent Pharmacophores Against Strong Pathogenic Isolates**

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Isoxazoles are nitrogenous five member heterocyclic moieties play a vital role as non selective COX inhibitors, widely used in the treatment of several ailments for a long time. Possessing anti inflammatory, analgesic and antipyretic properties, this class of agents are chiefly used to treat chronic inflammation states. 3-(substituted phenyl)-1-(2,2,8,8-tetramethyl-3,4,9,10-tetrahydro-2H, 8H-pyrano[2,3-f]-chromen-6-yl) isoxazoles exhibited potential activity. The synthetic protocol includes preparation of chalcones via chromans. The formed chalcones are treated with Hydroxylamine hydrogen chlorides in presence of potassium hydroxide / ethanol and refluxed for about 6-8 hours. The novel isoxazoles isolated (4a-4g) are screened against human pathogenic Isolates *Salmonella typhi*, *Vibrio cholerae*, *Shigella dysenteriae*.

## **PCO-09 : Microwave Induced Synthesis, Biological Evaluation, Molecular Docking and Molecular Dynamic Simulation of Newer Pyridine Clubbed Benzimidazole**

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The present work highlights the synthesis of a newer biologically active Mannich bases contributing benzo[d]thiazole and aminopyridine via N-Mannich reaction by conventional method as well as microwave heating approach as a part of an environmental benign synthetic protocol. All the synthesized compounds were characterized by spectral analysis and were screened for in vitro antimicrobial, antitubercular and antiprotozoal activity. One of the synthesized compound was found to be most active against *E. coli* (50  $\mu$ M), *S. aureus* (12.5  $\mu$ M), *C. albicans* (100  $\mu$ M) and *M. tuberculosis* (50  $\mu$ M) MIC value in the primary screening. Whereas one of the N-Mannich derivative showed potency against *L. mexicana* and *T. cruzi* with MIC value 1.01 and 3.33  $\mu$ M better than reference drug Miltefosina and Nifurtimox. To provide understandable evidence to predict binding mode and approximate binding energy of a compound to a target in the terms of ligand-protein interaction, all synthesized compounds were docked against different biological target (PDBs). Moreover, molecular dynamics (MD) simulations are performed for up to 20 ns simulation time investigating the stability of a ligand-protein complex. The computational studies revealed that Mannich derivatives have a high affinity toward the active site of enzyme which provides a strong platform for new structure-based design efforts. The Lipinski's parameters showed good drug-like properties and can be developed as oral drug candidate.

## **PCO-10 : Kinetics and Mechanism of Oxidation of L-threonine by Periodate in Alkaline Medium**

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The oxidation of L-threonine by periodate was studied spectrophotometrically at 280 nm in alkaline medium at 30°C. The reaction was found to be first order with respect to [periodate] and fractional order with respect to [L-threonine]. The oxidation product is identified to be 2-hydroxy propanaldehyde by infra red spectral studies. Increase in ionic strength increases the rate of the reaction.

A plausible mechanism is proposed and the activation parameters for the slow step, energy of activation,  $E_a$  and entropy of activation,  $\Delta S^\ddagger$  are computed by linear least squares method and are found to be  $91.34 \pm 2.05 \text{ kJ mol}^{-1}$  and  $2.23 \pm 8.12 \text{ JK}^{-1}\text{mol}^{-1}$  respectively.

### **PCO-11 : Formation of Binary Complexes of Co(II), Ni(II) and Cu(II) with L-Dopa in DMF-Water Mixtures**

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Complexation of essential metal ions with (S)-2-amino-3-(3,4-dihydroxyphenyl) propanoic acid (dopa) in (0-60% v/v) DMF-water mixtures has been studied pH-metrically at a temperature of 303 K and an ionic strength of 0.16 M. The existence of different binary species was established from modeling studies using the computer program MINQUAD75. The best-fit chemical models were selected based on statistical parameters like crystallographic R factor and sum of the squares of residuals in mass-balance equations. The models for binary complex systems contain the chemical species ML,  $ML_2$ , MLH,  $ML_2H$  and  $ML_2H_2$  for Co(II), Ni(II) and Cu(II) in DMF-water mixtures. The trend in the variation of stability constants with change in the mole fraction of the medium was explained based on electrostatic and non-electrostatic forces

### **PCO-12 : Speciation Studies of L-Cysteine Complexes of Pb<sup>II</sup>, Cd<sup>II</sup> and Hg<sup>II</sup> in Dioxan-Water Mixtures**

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L-Cysteine complexes of Toxic metal (Pb<sup>II</sup>, Cd<sup>II</sup> and Hg<sup>II</sup>) ions were studied pH-metrically in various concentrations (0.0- 60.0% v/v) 1, 4- Dioxane-water mixture maintaining an ionic strength of 0.16 mol L<sup>-1</sup> at ambient conditions. Exhaustive modeling was performed to identify the species present in the present systems. The models contain ML, MLH and  $ML_2$  for Pb<sup>II</sup> and Cd<sup>II</sup> and ML and  $ML_2$  for Hg<sup>II</sup>. The appropriate experimental conditions were verified by introducing errors intentionally in the concentrations of ingredients. The trend in the variation of stability constants with the dielectric constants of dioxan is explained on the basis of electrostatic and non-electrostatic forces. The bioavailability of metals and their transportation are explained based on the distribution diagrams.

## **PCO-13 : An Efficient Protocol for the Synthesis of 4-Arylidene-2-Phenyl-5(4H)-Oxazolones and their Antimicrobial Evaluation Against Selected Human and Phytopathogens**

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A simple and convenient method has been developed for the synthesis of a series of 2-(4-substituted phenyl)-4-(substituted arylidene)-1,3-oxazol-5-ones (5a-j) via reactions of hippuric acid with differently substituted aromatic aldehydes (4a-j) in different metal acetates viz., sodium acetate, potassium acetate, calcium acetate and ammonium acetate, which were tested for their efficiency as catalysts in both conventional and microwave assisted synthetic methods in presence of 4°A zeolites. The title compounds were evaluated for their antimicrobial properties against selected human pathogens (bacterial and fungal) and phytopathogens (fungal) and compared with standard drugs. All the 5(4H)-oxazolones synthesized exhibited moderate to high activity. The results of the study will be presented.

## **PCP-01 : N-Arylhydroxamic Acid as Antisickling Agents**

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Sickle cell disease (SCD) is a genetic blood disorder that affects the shape and transportation of red blood cells (RBCs) in blood vessels, leading to various clinical complications. The N-arylhydroxamic acid (RC(O)NHOH, HA) exhibit diverse biological activity, including hypotensive and antisickling properties associated with formation of nitroxyl (HNO) or nitric oxide (NO). N-p-Tolyl-p-chlorobenzohydroxamic acid (N-p-T-p-CBHA) and N-p-chlorophenyl-o-chlorobenzohydroxamic acid (N-p-C-o-CBHA) that contain an N-hydroxy group react with oxyhemoglobin to form methemoglobin and variable amounts of nitrite/nitrate. Antisickling activity and the minimum concentration of extract required to normalize sickled cells was determined by gel electrophoresis test. The potential of Hydroxamic Acids in sickle cell disease management was investigated in vitro using freshly prepared 2% sodium metabisulfite for sickling induction. Treatment of sickling cells with extracts at different concentrations showed that a decrease of the percentage of sickling cells formation was found in both induced

and non induced sickling cells. The results indicated that the percentage of sickled cells, which was reduced to 29.3%, 32.8%, in the presence of N-p-T-p-CBHA and N-p-C-o-CBHA, respectively, where the rate of polymerization inhibition was 5.9 and 6.6 ( $\times 10^{-2}$ ) accordingly. These results suggest that the N-p-T-p-CBHA and N-p-C-o-CBHA demonstrated the most significant antisickling effect with a potential for use in the clinical management of SCD.

### **PCP-02 : Kinetics and Mechanism of Oxidation of L-tyrosine by Iron(III)-1,10-phenanthroline Complex in Perchloric Acid Medium**

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L-tyrosine is an aromatic non-essential amino acid and it is formed from L-phenylalanine which is a nutritionally essential amino acid. It is a precursor of levodopa, melanine, thyroxine and triiodo thyroxine. We have investigated the oxidation of L-tyrosine by various oxidants like hexachloroiridate(IV), thallium(III) and tetrachloroaurate(III) in perchloric acid medium. In continuation of our studies on the oxidation of L-tyrosine, the kinetics of oxidation of L-tyrosine by Fe(III)-1,10-phenanthroline complex was studied spectrophotometrically at 510 nm in perchloric acid medium at  $30 \pm 0.1$  °C . The reaction was found to be first order with respect to Fe(III) and zero order with respect to tyrosine. The rate of the reaction was found to be decreased with increase in acid concentration and second order with respect to phenanthroline concentration. Basing on these results, a plausible mechanism is proposed and rate law is derived.

## PHYSICAL CHEMISTRY SECTION

### Sectional President's Address

#### Role of Physical Chemistry in Emerging Areas of Applied Sciences

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The term "Physical Chemistry" was coined by Mikhail Lomonosov in 1752 at Petersburg University, Russia. Physical Chemistry has always filled a knowledge gap in material science, as long as we take physics and chemistry in a narrow sense. The current status of Physical Chemistry in Indian Universities and the difficulties associated with research in Physical Chemistry will be discussed in brief. Physical Chemistry finds its application in almost all branches of basic as well as applied sciences. The application of physical chemistry in daily life usually focused in the fields of Biology and Medicine i.e., in the determination of three dimensional arrangement of atoms in biological assemblies, Protein folding and unfolding, Rational drug design and Biological energy conversions. The importance of Physical Chemistry is highlighted by variety of outstanding drug withdrawals in recent years through the exploitation of the tools of Physical Chemistry. Another important application of Physical Chemistry involves in the study of both physical and chemical interactions in foods as well as the applications of physical/chemical techniques and instrumentation for the study of foods. Finally, how the simple principles of Physical Chemistry are useful in enrichment of an energetic material, RDX from a crude RDX-HMX mixture by solubility modification through the results obtained by our group will be discussed.

## **PIL-01 : Conducting Polymer Based Electrochemical Biosensor for Polyphenol Antioxidants**

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Antioxidants are considered as important bioactive compounds because of their health benefits and their role in delaying oxidative rancidity of numerous foods. Polyphenols are the most abundant antioxidants in the diet. Current evidence strongly supports a contribution of polyphenols to the prevention of cardiovascular diseases, cancers, and osteoporosis and suggests a role in the prevention of neurodegenerative diseases and diabetes mellitus. Consequently, the requirement of a standard assay is very important in order to compare the different results and validation. Reliable, sensitive and rapid determination of antioxidants procedures are in demand throughout the world and the electroanalytical techniques represent the most effective answer to this because of greater reliability and rapid determination of the widest variety of analytes in complex matrices. Electrochemical biosensors are based on biochemical reaction that produces a change in the electrical potential at the surface and a transducer responds to the signal and translates amount of the signal into a measure of the amount of the analyte. The researchers in this area are quite vast and continue to grow and broaden the scope for the analysis. Highly sensitive and selective determinations of biologically important compounds such as antioxidants are the major achievements of electrochemical biosensors. The principal developments in the area of developing biosensors which focus on reducing the detection limit to trace level of antioxidant, down to nM are in need. The modifiers are based on organic semi-conductors such as polyaniline, polypyrrole, polythiophene and their derivatives, prepared on solid electrodes [4,5]. Composites of conducting polymers and other nano materials have also been used to enhance the sensitivity. In this study, electrochemical nano biosensors were developed for catechol, a model polyphenol antioxidant by employing four conducting polymer/copolymer/composites [polyaniline-polyphenol oxidase, poly 3-methylthiophen- Lacasse, polyethylene dioxy thiophene-reduced graphene-ferric oxide-polyphenol oxidase and Poly(aniline-co-ethyl 4-aminobenzoate)-lacasse]. Of the four modifiers, the biosensor developed by the polymerisation of aniline and ethyl 4-aminobenzoate and simultaneous incorporation of LAC enzyme in presence of ionic liquid shows maximum efficiency for catechol. The determination of catechol using the proposed biosensor was simple and rapid with high

accuracy. The lifetime was about two months and it was suitable for real sample analysis. In short, this work would be a significant contribution towards the fabrication of a biosensor for polyphenol.

## **PIL-02 : Role of Adsorption in Chemical Defence**

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The ubiquitous and utilitarian adsorption technique plays an important role in the event of a Chemical agent threat that can come from a wartime attack, terrorist attack or from an industrial accident. The primary focus is on the first responders, for the early recognition of the threat and informing the command and control centres, so that appropriate counter measures can be initiated. The three pronged approach of detection, protection and decontamination (containment) plays a crucial role in mitigating the ill effects of these toxic chemicals in a chemical disaster either deliberate or accidental. As global terrorism escalates, the demand for the rapid, reliable life saving systems from these potentially hazardous materials including toxic industrial chemicals (TICs), explosives, Chemical Warfare Agents (CWA) and narcotics is becoming increasingly critical to military and civilian first responders. Availability of a reliable and rapid sensing chemical detection system immensely helps in identifying the causative chemical agent, so that individual and collective protection measures like donning the appropriate individual protection equipment (IPE), administration of suitable medicines inclusive of antidotes (that may also have toxic side effects if unnecessarily administered) and finally containing the area with suitable decontamination measures. Defence Research and Development Establishment, a premier laboratory of Defence R & D Organisation (DRDO) situated at Gwalior, Madhya Pradesh is working in the area of defences against chemical and Biological warfare (CBW) agents for the last three and half decades. With the experience and expertise gained in the related areas DRDE continues to play its role as the key institution in the CBW Research and Development, and also involved in designing and developing state of the art systems and technologies for chemical and biological defences. A series of adsorbents are used in designing and developing various gadgets used to mitigate the ill effects of these toxic chemical agents. Specially treated silica gels and thermally stable polymeric adsorbents are studied and utilised in design and development of on-site chemical detection systems for various strategic purposes. Activated charcoal and many other adsorbents play an important role in the filtration systems developed for protection against these CWAs. In house

developed Activated Carbon Sphere (ACS) based chemical protective clothing is the nascent development. During the presentation an attempt will be made to discuss the R & D aspects in the development of various Chemical defence equipments having equal potential utility for the protection of both soldiers and society in the event of a chemical threat scenario.

### **PIL-03 : Ammonium Ionic Liquids as Biocompatible Co-solvents for the Structure and Stability of Biomolecule**

**Pannuru Venkatesu**

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We have investigated the biomolecular interactions and related associated structural changes of  $\alpha$ -chymotrypsin (CT) with new ILs by using several biophysical techniques including circular dichroism (CD) and fluorescence. The ILs studied in the present study includes diethylammonium dihydrogen phosphate  $[(\text{CH}_3\text{CH}_2)_2\text{NH}][\text{H}_2\text{PO}_4]$  (DEAP), diethylammonium hydrogen sulfate  $[(\text{CH}_3\text{CH}_2)_2\text{NH}][\text{HSO}_4]$  (DEAS), triethylammonium dihydrogen phosphate  $[(\text{CH}_3\text{CH}_2)_3\text{NH}][\text{H}_2\text{PO}_4]$  (TEAP) and triethylammonium hydrogen sulfate  $[(\text{CH}_3\text{CH}_2)_3\text{NH}][\text{HSO}_4]$  (TEAS). We observed that all ILs have dominant contribution to the stabilization of the native structure of the CT. Furthermore, the results reveal that phosphate anions of ILs are strong stabilizers and acted as effective refolding enhancers for thermally denatured enzyme structure, whereas the enzyme was not refolded in the sulfate anions of ILs. These findings suggest a new generation of enzyme stabilizers that can be applied to other protein folding studies and biological systems.

### **PIL-04 : Molecular Tools for Controlling Nanoparticle Size/Morphologies**

**Bhagavatula L. V. Prasad**

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Organic molecules/ligand have been demonstrated to play a key role in nanoparticle formation in many aspects viz. controlling their size, morphology and their dispersional stability in a given medium. Different features of ligands, such as bulkiness, binding strength and concentration have been found to influence the size of metal nanoparticles especially spherical nanoparticles. Ligands can also be used to exercise control over the shape of metal nanoparticles by

their specific binding to different crystallographic facets leading to the growth of anisotropic nanoparticles. The exposed group (present at the end opposite to that attached to the nanoparticle surface) of the ligands attached to nanoparticle surface can direct the dispersion of nanoparticles in different solvent media. A dual functioning agent (DFA) is another class of ligands that act as reducing as well as capping agent and are being used extensively these days. In this talk we will briefly review the role of molecules/ligands as tools for controlling nanoparticle size, morphology and dispersion stability in different media.

## **PIL-05 : Solvation Behaviour of Bioactive Molecules in the Presence of Additives**

**Harsh Kumar Manchanda**

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The stabilization or destabilization of the proteins is transmitted by the addition of specific molecules to protein solutions. Because of solvent effects or their direct binding, the protein conformation is sometimes influenced by these added co-solutes. The most happening interactions like hydrogen bonding and electrostatic interactions are non covalent in nature. A significant perception about the conformational stability and folding/unfolding behavior of globular proteins is delivered by the study of these interactions. The conformation and properties of proteins like solubility, denaturation and dissociation into subunits, the activity of enzymes etc. are remarkably effected by salt solutions. Due to complexity of proteins and non feasibility of direct thermodynamic studies, various fundamental structural units of proteins such as amino acids and peptides have been reviewed to achieve a better knowledge of interactions that may arise in the solutions. Since amino acids are, among other compounds, the basic structural building units of biomolecules, so the behavior and properties of amino acids in solutions have been always a stuff of attention. Amino acids occur as dipolar ions in aqueous medium that explicit a unique hydration behavior linked to the vital biological phenomenon. This linkage leads to the important study of amino acids in unfolding the character of dipolar ions in the biological system. The elucidation of several interactions that exist in the solutions have been manifested by interpreting the effect of concentration of various additives and temperature on the thermodynamical properties of aqueous amino acids. In aqueous and mixed aqueous solvents, thermodynamic properties of these building blocks (amino acids and peptides) provide information regarding solute-

solvent and solute-solute interactions which further helps in understanding the effect of various additives on biomolecules. Here, the main focus is on interactions of amino acids and peptides with citrate, phosphate salts and drug molecules with reference to volumetric, acoustic and spectroscopic studies.

### **PIL-06 : Selective Probes with Sensing Property for Multiple Analytes in Mixed Aqueous Media Based on Imine Linkage**

**S. K. Mehta and Kamaljit Kaur**

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A simple salicylaldehyde derived Schiff base has been synthesized which demonstrates simultaneous dual channel chromogenic and fluorogenic signaling towards  $\text{HSO}_3^-$  and  $\text{Zn}^{2+}$  respectively in mixed aqueous media. The probe exhibits high selectivity over other competitive ions with high detection limit. Solvatochromism has been employed systematically for anion detection using UV-vis spectroscopy. DFT calculations and  $^1\text{H}$  NMR spectroscopy further support the results based on shifting of equilibrium. Moreover, the sensor has shown large fluorescence enhancement and blue shift of 48 nm upon  $\text{Zn}^{2+}$  addition. Importantly, this is one of the rare reports in which schiff base has been utilized for the fabrication of chromogenic or fluorogenic sensor using solvent effect for multianalyte detection.

### **PIL-07 : Micellar Kinetics**

**K. Ramakrishna**

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The information from kinetic parameters in micellar media opened a new window in synthesis of conventional/novel/unique/smart materials in aqueous media adhering to principles of green chemistry. This method avoids use of toxic organic solvents, yet resulting in prospective improvement in reaction rates. The focus of our laboratory over last two decades is kinetics of a variety of chemical reactions in micellar media. The intrinsic hydrophobic/hydrophilic interactions in cationic /anionic and neutral micellar solutions was the base of choice of systems viz. reaction, micelle etc. The decrease in effective dielectric constant in bulk medium has prospective kinetic consequences, for instance in this region the reactants are more easily dissolved promoting formation of transition state and increasing reaction rate. In this talk, illustrative case studies and mathematical treatment of micellar kinetics will be presented.

## **PO-CYSA-01 : Cholinium Based Ionic Liquids: Exploring their Suitability for Beta-Lactoglobulin**

**Anamika Sindhu, Kavya Bhakuni and Pannuru Venkatesu**

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Milk proteins find vast application as drug carriers for several therapeutic and medical purposes. In recent years, the use of beta-lactoglobulin (BLG) has attracted researchers as nanodrug carrier for several hydrophobic poorly absorbed nutraceuticals. On the other hand, ionic liquids (ILs) have emerged as the novel solvents for solubilizing hydrophobic drug molecule. Hence, it is an interesting aspect to use BLG as a drug carrier agent for the hydrophobic drugs in the presence of the ILs. However, in the primary approach, it is essentially required to explore the stability of BLG in the presence of selected ILs. We have selected cholinium-based ILs, such as, choline chloride [ChCl], choline hydroxide [ChOH], choline bitartrate [ChBit], choline acetate [ChAc], choline oxalate [ChOx]. The stability of the BLG was observed in different concentration of the ILs. Enhanced thermal stability by 10 °C was observed in the presence of [ChCl] and [ChAc], indicating, as most biocompatible among the ILs. Further, to examine the structural changes in BLG due to the ILs, circular dichroism, fluorescence, dynamic light scattering (DLS) and UV techniques.

## **PO-CYSA-02 : Controlled Synthesis and Enhanced Structural, Optical and Electrical Properties of Metal Telluride Nanoparticles**

**Deepika Jamwal and Surinder Kumar Mehta**

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Metal tellurides represent a class of compounds that received attention due to size and shape dependent properties and potential applications in electronic, optical, thermo-electrical, magnetic and biological fields. Owing to these properties and applications, the present study is focused on a systematic and extensive work to synthesize and characterize lead telluride nanoparticles by using a special type of size and shape controlling agents i.e. Gemini surfactants. These surfactants represent a new class of surfactants and characterized by much lower critical micelle concentration (CMC) values and stronger surface tension reduction efficiency than the corresponding conventional surfactants.

In the present work, Dimethylenebis(dodecyl-dimethyl ammonium bromide)-stabilized cubical PbTe nanoparticles were synthesized by a

simple hydrothermal method. We proposed a possible reaction mechanism to explain the influence of different precursors. The structural, optical and electrical properties of the prepared PbTe nanoparticles were investigated. The average particle size of the nanoparticles was 20 nm. The optical band gap of prepared nanoparticles determined from the UV-Vis spectroscopy was 0.5 eV indicating quantum confinement shift. The electrical conductivity of lead telluride nanoparticles was 0.02-0.06 S cm<sup>-1</sup>.

### **PO-CYSA-03 : Development of Electrochemical Method for the Determination of Chlorzoxazone Drug and its Analytical Applications to Pharmaceutical Dosage Form and Human Biological Fluids**

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The electrochemical behavior of chlorzoxazone drug at glassy carbon electrode has been investigated for the first time using cyclic and square wave voltammetric techniques. The dependence of the current on pH, concentration and scan rate were investigated to optimize the experimental conditions for determination of chlorzoxazone. The anodic peak was characterized and process was diffusion-controlled. The number of electrons transferred in the oxidation process was calculated and a plausible oxidation mechanism was proposed. In the range of  $8.0 \times 10^{-7}$  to  $1.0 \times 10^{-5}$  M, the current measured by square wave voltammetry presents a good linear property as a function of the concentration of chlorzoxazone with a detection limit of  $4.41 \times 10^{-8}$  M with good selectivity and sensitivity. The proposed method was successfully applied to chlorzoxazone determination under physiological condition in pharmaceutical samples and for the detection of chlorzoxazone in human biological fluids. This method can be employed in clinical analysis, quality control and routine determination of drugs in pharmaceutical formulations.

### **PO-CYSA-04 : Crowded Milieu Tuning the Stability and Activity of Stem Bromelain**

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Proteins are under an extremely crowded environment when

considered in vivo. The presence of large biological macromolecules (known as crowders) offers limited volume available to protein mainly affects its functioning and structure in a cell. During in vitro studies for protein stability, these macromolecular crowding is sometimes ignored. However, if large concentrations of crowders are used to examine protein stability in vitro, their effects on protein inside the cell, as stated, can be understood. Keeping this in context, we have investigated the effects of macromolecular crowding on stem bromelain (BM) with the help of different crowding agents of varying molecular weights such as dextran (40 kDa and 6 kDa) and ficoll (70 kDa). Activity and stability of BM were examined using UV-Vis, fluorescence and circular dichroism spectroscopy. Further, docking methods were used to complement the results to quantify the crowding effects on the stability and activity of BM. The results reveal that the presence of high concentration of crowding agents where the excluded volume effects are quite prominent, it was observed that the overall effect of crowding on BM was destabilizing and deactivating. These observations were in contrast to available reports on the classical stabilizing nature of macromolecular crowding on protein structure. Our detailed investigation on the effect of crowders on BM reveals that the structural stability and activity is concentration dependent. We observed that the decrease in stability and activity can be related to the soft interactions between the crowding agents and BM.

### **PO-CYSA-05 : Chemical Speciation Studies on the Complexation of Ditopic Ligands: Interaction of Terephthalic Acid Dihydrazide and L-Proline with Mn(II), Cu(II) and Zn(II) in Aqueous Medium**

**Nirmala Devi Danabala, Satyanarayana Atreyapurapu and Shyamala Pulipaka**

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Chemical modeling study on the solution equilibria of ternary complexes of Terephthalic acid dihydrazide (L) and L-Proline (XH) with the metal ions  $Mn^{2+}$ ,  $Cu^{2+}$  and  $Zn^{2+}$  was carried out potentiometrically in aqueous medium using Calvin-Wilson titration technique and the data were analyzed using the Miniquad-75 program. Terephthalic acid dihydrazide is capable of binding two metal ions on either side through carbonyl and terminal amino groups of the hydrazide moieties. Further interaction of these metal ions with proline may lead to the formation of a variety of mixed ligand species. The best-fit models obtained were found to contain both monometallic and

bimetallic ternary species of the type  $M_mLX_xH_h$  ( $M= Mn^{2+}/ Cu^{2+}/ Zn^{2+}$ ,  $m= 1$  or  $2$ ,  $x=1$  or  $2$ ) indicating the ambidentate and ditopic nature of the dihydrazide. The values of  $h$  were found to vary from  $+3$  to  $-1$  in different species depending on the degree of protonation of the ligands. Negative values of  $h$  indicate deprotonated or hydroxylated species. The ternary complexes were found to be more stable than the corresponding binary species.

## **PO-CYSA-06 : Development of Nanoprobes for Selective Imaging of Biologically Important Molecules : A Review**

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Reactive nitrogen species (RNS), such as nitric oxide (NO) and its higher oxides, are a class of chemically reactive species that act as cell signaling molecules in human biology. NO homeostasis is crucial to its proper functions in physiological events that take place in the cardiovascular, nervous and immune systems, and any type of misregulation/disturbance of NO production is concerned to the large number of pathological processes including cancer, neurodegenerative injury and inflammation. Other RNS species, such as peroxynitrite (ONOO<sup>-</sup>), nitrate (NO<sub>3</sub><sup>-</sup>) and nitrogen-dioxide radical (NO<sub>2</sub><sup>·</sup>) are also involved in physiological and pathological processes. These essentially inspired a wide range of research to identify the precise roles of RNS in biology. Since RNS diffuses through most of the cells and tissues, it is very difficult to follow immediately after their production. Hence, a selective probe to detect the formation and migration of RNS in living cells is highly desirable. In this aspect, a review on current fluorescence-based detection techniques for RNS will be presented.

## **PO-CYSA-07 : Synthesis and Delineation of Choline-Tryptophan Based Gold Nanoparticles to Enhance Their Water Solubility and Biological Properties**

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Ionic liquids (ILs) being expeditious compounds in chemistry that have been used in many interdisciplinary research, either as a novel solvent for biological macromolecules or solvents for the eradication of toxic organic compounds. A major novel properties of ILs which have been recently observed in the literature, is the formation and

stability of metal based NPs. In this context, gold nanoparticles (AuNPs) have been considered extremely beneficial to biological systems due to their anticancer activity. Hence, it is advantageous to use benevolent nature of both ILs and AuNPs. In the present research we used amino acids based ILs for the synthesis of functionalised AuNPs. More specifically, we used choline-tryptophan and tetraethyl ammonium-tryptophan based ILs for the synthesis of AuNPs, further the obtain results were compared with previously prepared AuNPs in the presence of  $\text{NaBH}_4$ . The synthesised AuNPs were characterized by UV-Vis spectroscopy, dynamic light scattering, scanning electron microscopy and transmission electron microscopy and their functionalities and charge were confirmed by Fourier-transform infrared spectroscopy and zeta potential techniques. A comparison with the literature reveals that choline-trp and tetraethyl ammonium based AuNPs systems are more stable and hydrophilic than these AuNPs with  $\text{NaBH}_4$ . Biocompatibility of choline -trp AuNPs in cell media has been confirmed in the presence of E-coli cell culture by calculating the growth of bacterial cell.

### **PO-CYSA-08 : An Unexplored Remarkable PNIPAM-Osmolyte Interaction Study : An Integrated Experimental and Simulation Approach**

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We investigate the aggregation and collapse of water soluble amphiphilic polymer, poly(N-isopropylacrylamide) (PNIPAM), in aqueous solution containing variable amount of trehalose, sucrose and sorbitol. The effect of osmolytes on the coil to globular transition of the PNIPAM is studied by the use of comprehensive biophysical techniques like UV-Visible spectroscopy, fluorescence spectroscopy, dynamic light scattering and Fourier transform infrared spectroscopy (FTIR). The polarization induced by these additives makes the collapse of PNIPAM polymer much faster as compared to the pure PNIPAM in aqueous solution. The decrease in the LCST of polymer with increase in the concentration of osmolyte is due to the significant changes in the interactions among polymer, osmolyte and water. The high affinity of these additives toward water destabilises the hydrated macromolecular structure via preferential interactions. To investigate the molecular mechanism behind the decrease in the LCST of the polymer in presence of the osmolytes, a molecular dynamics (MD) study was performed. The MD simulation has clearly shown the reduction in hydration shell of the polymer after interacting with the osmolytes.

## **PO-01 : Study of Magnetic Properties of Mn<sub>3</sub>O<sub>4</sub> Nanoparticles Prepared by a Novel Combustion Synthesis Route at Two Different Temperatures**

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Hausmannite Mn<sub>3</sub>O<sub>4</sub> nano particles were prepared at two different temperatures of 300°C and 500°C using combustion synthesis route with Mn(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O precursor and Allium Cepa. The morphology, functional and magnetic properties were characterized by XRD, FT-IR, EDX, SEM and VSM respectively. A detailed field dependent magnetization study of the synthesized sample is depicted in this work. The XRD peaks of Mn<sub>3</sub>O<sub>4</sub> exhibited good agreement with JCPDS (#024-0734) but 59.82360 appeared in XRD spectrum of Mn<sub>3</sub>O<sub>4</sub> prepared at high temperature of 500°C. It is observed that the crystallinity of nano powder increased when temperature increases from 300°C to 500°C. The irregular particle size of nano compound from XRD and SEM is 10-25nm at 300°C and increases to 30-50nm at 500nm. The EDX result also confirms the formation of Hausmannite Mn<sub>3</sub>O<sub>4</sub>. FT-IR analysis exhibits stretching vibrations of metal ions in tetrahedral and octahedral co-ordination confirming crystal structure. Magnetic studies of the as synthesized samples revealed paramagnetic behaviour at room temperature for both samples at 300 and 500°C. The saturation magnetization and hysteresis was not reached in the region of measured field strength showing maximum magnetization ( $M_{max}$ ) of 2.12 and 1.13emu/g at 10K respectively. With decrease in temperature, ferromagnetic behavior increases. The maximum magnetization was smaller than the saturation magnetization for bulk Mn<sub>3</sub>O<sub>4</sub> which is 38emu/g. The smaller value of magnetization is due to the core-shell structure with aligned moments in the core and canted surface moments which reduces the magnetization. The obtained remnant magnetization for both samples is 5.4emu/g and coercivity is 10500 and 7250 Oe respectively.

## **PO-02 : A DFT Study on Electronic Structure and Linear Optical Properties of Visible Absorbing Squaraine and Thiosquaraine Dyes**

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Squarains are with planar structure and zwitterionic in nature.

These are generally considered as donor-acceptor-donor (D-A-D) type of molecules and are having strong interaction with light, exhibit intense absorption and emission in visible to near infrared region. Due to the advantage of intensive absorption with tunable wavelength, squaraine dyes are very good candidates for diverse applications (optoelectronic properties), such as colorimetric sensors, imaging, nonlinear optical devices, photodynamic therapy and organic solar cells. By varying donor substituents on central four membered acceptor ring and increasing the  $\pi$ -conjugated systems, the absorption wavelength can cover the long wavelength visible to near-IR region. Replacement of carbonyl oxygen of central four membered acceptor ring with sulphur results thiosquaraines and these are showing longer wavelength absorption than squaraines. The nature of lowest electronic excitations and charge transfer characteristics of visible absorbing squaraines and thiosquaraines are studied by DFT and TDDFT method.

### **PO-03 : Molecular Interactions in Ternary Liquid Mixture Involving Quinoline**

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The ultrasonic velocity( $u$ ), density( $\rho$ ), and viscosity( $\eta$ ) have been measured for ternary mixtures of quinoline, methanol and phenol at different temperatures (303.15, 308.15, 313.15, 318.15 K) over the entire composition range. These experimental data have been used to estimate the parameters such as adiabatic compressibility ( $\beta$ ), intermolecular free length ( $L_p$ ), internal pressure ( $p_i$ ), free volume ( $V_f$ ), acoustic impedance ( $Z$ ), surface tension ( $S$ ) and their excess values. The results are used to estimate the molecular interaction between the components of the mixture.

### **PO-04 : Nano-Crystallites**

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Nano-crystallites of Lithium Titanium Oxide (LTO) and Lithium

Nickel Phosphate (LNP) type materials are prepared by means of ball milling methodology. High energy milling changes structural properties and morphological patterns. LTO and LNP have been investigated as prominent lithium-ion battery materials due to their excellent structural stability and safety. In this paper LTO and LNP nano particulates are characterized structurally and morphologically. Lithium-ion batteries, which are considered as promising power sources, have been extensively applied on electronic devices due to advantages such as high energy density, long cyclic life and no memory effect.

### **PO-05 : Study of Mixed Surfactant on Photoelectric Parameters in Solar Cell**

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Effect of mixed surfactant on photoelectric parameters in solar cell was studied. Solar cells are those cell in which sunlight is converted into electrical energy via formation of energy rich species that exhibit the photo-solar effect. Photo-solar effect was studied in solar cell containing photosensitizer with mixed surfactant in aqueous solution of reductant. The observed cell performance was discussed in terms of electrical parameters such as maximum value of photo potential, photocurrent, power, work efficiency and cell performance.

### **PO-06 : Chemical Speciation Studies on the Interaction of Adipic Acid Dihydrazide and Glycine with Some Essential Divalent Metal Ions in Aqueous Medium**

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Chemical speciation studies on the ternary systems of essential metal ions  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  with adipic acid dihydrazide as primary ligand and glycine as a secondary ligand were carried out potentiometrically in aqueous medium. The data acquisition was made using Calvin-Wilson potentiometric titration technique in aqueous medium at an ionic strength of 0.1M and temperature 303K. The data were analyzed using the SOPHD and Miniquad-75 computer programs and species distribution diagrams were generated using the HYSS program. The best-fit models obtained by chemometric analysis were

found to contain both monometallic and bimetallic species with different degrees of protonation, supporting the ambidentate and ditopic nature of the dihydrazide. The stabilities of ternary species relative to those of corresponding binary species were discussed on the basis of  $\Delta\log K$  parameter.

### **PO-07 : Synthesis and Characterization of Modified SBA-15 Mesoporous Silica and its Application in the Removal of Cu(II) and Ni (II) from Water**

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A new hybrid sorbent, Trans 1,2-Diaminocyclohexane-Functionalized SBA-15 mesoporous silica was prepared, characterized and used in the removal of heavy metal ions, Cu(II) and Ni(II) from water. The organic-inorganic hybrid material was prepared by successive grafting of SBA-15 silica with 3-aminopropyl-trimethoxy silane and Trans 1,2-Diaminocyclohexane as shown in the scheme. The material was characterized by elemental analysis, XRD, TEM, SEM, FT-IR,  $^{13}\text{C}$  and  $^{29}\text{Si}$  NMR spectroscopy, Nitrogen adsorption-desorption isotherms, and thermo gravimetric analysis. The application of hybrid material as sorbent in the removal of Cu and Ni was studied by optimizing the experimental parameters, pH contact time, initial concentration, and adsorbent dose. Experimental data was analyzed by kinetic parameters and found that sorption of metal ions followed pseudo-second-order. Langmuir isotherm model fitted well to data as represented by high values of correlation coefficient (i.e.  $R^2 \approx 1$ ). Maximum removal (for Cu(II) 98.1%, for Ni(II) 96.8%) for both the metal ions was observed at pH 6.0 with an initial metal ion concentration of 50 mg/L. The regeneration of spent sorbent for recovery of metal ions and reuse of the sorbent was studied using HCl solution.

### **PO-08 : Ultrasonic Speed Measurements in Binary Mixtures Containing Xylenes at Temperatures from 303.15 to 313.15K**

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Density and ultrasonic speed have been measured in pure and binary mixtures containing Diethyl carbonate with o-xylene, m-xylene

and p-xylene over the whole composition range at 303.15, 308.15, and 313.15K. From these values, isentropic compressibility and intermolecular free lengths as well as excess quantities for sound speed, isentropic compressibility and intermolecular free length have been calculated. The results have been fitted to Redlich-Kister polynomial equation. The results have been explained on the basis of intermolecular interactions.

### **PO-09 : Photocatalytic Bleaching of Textile Wastewater of Bhilwara (Rajasthan) by Photo Fenton Reagent**

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Textile industries produce large volume of coloured dye effluent which are toxic and non-biodegradable during the last decade. Bhilwara textile industry is one of the most water and chemical intensive industries. About 200-400 litres of water is needed to produce 1 kg of textile fabric in textile factories and discharge polluted wastewater. Photocatalytic- degradation of Textile wastewater by fenton reagent has been investigated by using U.V. light in Photochemical Reactor at 254nm. The progress of reaction was observed spectrophotometrically. The effects of various parameters like concentration of catalyst, pH on the rate of degradation and decolourisation were also studied.

### **PO-10 : Interactional Behaviour of Ionic Liquids in the Presence of Different Additives**

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Ionic liquids (ILs) are novel class of molten salts which are in liquid state around room temperature. The molten salts or fused salts having low melting points can be considered as ILs. Ionic liquids thereby have low melting point, this is mainly due to 'Packing frustration' which are caused as a result of asymmetric cations and anions which fails to gain crystallinity. ILs are different from organic molecular solvents, and grabbing the special attention of scientific community due to their impressive properties as minimal or no vapour pressure, non-flammability, high mechanical stability, high conductivity and excellent ability to solubilize various substances. Scientific community is extensively engaged in the exploration of the properties

of ionic liquids alone and in the presence of various additives which range from amino acids/peptides, drug molecules, proteins, surfactants etc. The aqueous solutions of surfactants having micelles are of interest in present scenario. The effective use of surfactants which have ability to form spontaneous self-assembled structures, makes them persuasive as these have vast applications in colloidal formulation.. Further, these mixtures have wide applications which includes a micro emulsion used the enhanced recovery of oil, Synthesis of nano-particles in micro emulsion drug delivery system and disperant application. Here in this abstract we have focused on study of interactional behaviour of ionic liquids with two different additives like organic salts and surfactant molecules. Micellization behaviour of mixtures along with apparent molar properties have been analyzed from the experimental measurements. The interactional behaviour has been studied using spectroscopic, conductometric, volumetric and acoustic measurements. The results have been discussed in terms of different interactions prevailing in these mixtures depending upon the cation and anions present in the ionic liquid and additives.

### **PO-11 : Synthesis, Characterization and Kinetic Studies of Sodium Alginate Grafted IPN Hydrogels for Controlled Release of Anticancer Drug**

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The aim of present study is designing of dual responsive interpenetrating polymer network (IPN) hydrogels for the controlled release of an anticancer drug, imatinib mesylate. In the course of preparation of these hydrogels, first N-Acryloyl-L-phenylalanine grafted sodium alginate copolymer (NaAla-g-PAPA) was synthesized through free radical polymerization. The grafting parameters were calculated comparatively. The optimum grafting conditions were obtained by alteration of the reaction conditions such as the reaction time, temperature, monomer and initiator concentrations. Then novel dual responsive smart hydrogels were prepared through free radical polymerization reaction. The hydrogels were characterized by FTIR, SEM, DSC and XRD studies. Various network parameters of hydrogels such as volume fraction in the swollen state ( $\phi$ ), the average molecular weight of the polymer chain between two neighboring crosslinks ( $M_c$ ), Flory-Huggins interaction parameter ( $\chi$ ), crosslink density ( $V_c$ ) and

mesh size ( $\xi$ ) were calculated. The dynamic and equilibrium swelling studies were performed in different pH conditions. The in vitro drug release experiments were conducted in pH 1.2 and pH 7.4 buffer solution at 25°C and 37° ± 5 °C. The drug release data were fitted into different empirical kinetic models such as zero order, First order, Higuchi Square root, Hixson-Crowell cube root and Koresmeyer-Peppas equations.

### **PO-12 : Adsorption Studies of (Cr (VI), Cd (II), and Cu (II)) Metal Ions from Aqueous Solutions by Synthesized Fe<sup>3+</sup> and Ag<sup>+</sup> co-doped TiO<sub>2</sub> Nanoparticles.**

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The present communication has been addressed to the removal of Cr (VI), Cd (II) and Cu (II) from aqueous solutions by Fe<sup>3+</sup>-Ag<sup>+</sup>/TiO<sub>2</sub> nano metal oxide synthesized by Sol-Gel technique and characterization was done by XRD, SEM, TEM, EDS, and FTIR. Batch equilibrium experiments were performed for various concentrations of 0.1 mg/L to 1 mg/L and the effect of contact time, pH and adsorbate dosage was investigated. The adsorption kinetics was well fitted to pseudo-second order kinetic model, Weber-Morris & Reichenberg Kinetic equations. Langmuir and Temkin isotherms were found well fitted with the data.

### **PP-CYSA-01 : Fabrication of Functionalized Gadolinium Oxide and Their Biological Study**

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Gadolinium oxide nanoparticles synthesis has gained attention due to their diverse bio- applications. However, their functionalization with amino acids has not been reported yet to the best of our knowledge. The present report describes the synthesis of 2 nm size gadolinium oxide nanoparticles using co-precipitation method via sonication. The interactions of serum protein (BSA) with synthesized nanoparticles have been demonstrated using UV-visible spectroscopy, Fluorescence spectroscopy and Circular Dichroism (CD). The conjugation with nanoparticles was confirmed by FT-IR and Differential Scanning Calorimetric analysis. The synthesized nanoparticles demonstrated potential for anti-microbial, which has been tested

against two bacterial strains *Escherichia coli* and *Staphylococcus aureus*. The cell viability, MTT assay on HaCaT cell lines revealed the non-toxicity of synthesized nanoparticles

### **PP-CYSA-02 : Palladium (II) Catalysed Oxidation of Atropine Sulfate Monohydrate in Alkaline Copper (III) Periodate Complex : A Kinetic Study**

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Atropine sulfate monohydrate (ASM) is an anticholinergic drug, having a wide spectrum of activity. Hence, the kinetics of oxidation of ASM by diperiodatocuprate (DPC) in the presence of micro amounts of Pd(II) catalyst has been investigated spectrophotometrically in aqueous alkaline medium at  $I = 0.50 \text{ mol dm}^{-3}$ . The reaction between DPC and ASM exhibits 1:2 stoichiometry (ASM:DPC) i.e., one mole of ASM require two moles of DPC to give products. The main oxidation products were confirmed by spectral studies. The reaction is first order with respect to [DPC] and [Pd(II)], while the order with respect to [ASM] and [OH<sup>-</sup>] was less than unity. The rates decreased with increase in periodate concentration. The catalytic constant ( $k_c$ ) was also determined at different temperatures. A plausible mechanism was proposed. The activation parameters with respect to slow step of the mechanism were calculated and the thermodynamic quantities were also determined. Kinetic experiments suggest that the active species of Cu(III) and Pd(II) are  $[\text{Cu}(\text{H}_2\text{IO}_6)(\text{H}_2\text{O})_2]$  and  $[\text{Pd}(\text{OH})_2\text{Cl}_2]^2$ .

### **PP-CYSA-03 : Fully Aromatic High Performance Thermoset via Sydnone Maleimide 1,3-Dipolar Cycloaddition**

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Growth in the aerospace and microelectronic industries increasingly requires the development of lightweight materials with excellent chemical, thermal, and mechanical robustness. Thermoset polymers, having densely cross-linked networks of organic repeat units, offer a modular and flexible synthetic approach to such materials with desired

properties to be tuned via the macromolecular structure. Specifically, rigid networks with high contents of aromatic units lead to increased heat resistance and improved thermo mechanical properties such as high performance thermosets (HPTs) offering significant promise. However, the synthesis of fully aromatic structures is a major challenge since it requires the efficient formation of aromatic connecting points between aryl monomers without using metal catalysts. To address the criteria of efficient and noncatalytic chemistry, cycloaddition reactions were selected for thermoset formation and we have developed an efficient synthetic platform for the preparation of a new class of high performance thermosets based on the 1,3-dipolar cycloaddition of a functionalised sydnone with bis-maleimides. These processable materials possess outstanding thermal stability and a weight loss of <0.1% per day. Key to this performance is the stability of the starting functional groups that allows for reactive  $\beta$ -staging via simple thermal activation to give fully aromatic and highly cross-linked polyimide -based thermosets.

### **PP-CYSA-04 : Energetics of Reduction and Protonation Pathways of p-Benzoquinone for Quinone to Quinol Interconversion: A DFT Study**

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Quinones, a versatile class of organic compounds, perform various functions in biological, electrochemical and medicinal applications due to their redox and protonation abilities. These are also extensively studied as an electrode material in energy storage devices. The quinone-hydroquinone redox couple is well recognized as an organic redox electrode for pH measurements. Proton and electron transfer processes in photosynthesis and respiration are also the consequences of quinone to quinol interchange in which they exhibit nine possible oxidation- and protonation-states. In the present work, the energetics of all these possible oxidation and protonation pathways is studied using density functional theory (DFT). The adiabatic electron and proton affinities are analysed with frontier molecular orbitals of each oxidation and protonation state of p-benzoquinone (BQ), a prototypical example of the class of quinones. The study traces a good correlation of electron and proton affinities of the states with their respective highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO).

## **PP-CYSA-05 : Effect of AOT on Hydrolysis of Di-2,3-Dichloroaniline Phosphate**

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The effect of anionic surfactant, di-octyl sodium sulphosuccinate (AOT) on the hydrolysis of di-2,3-dichloroaniline phosphate has been studied spectrophotometrically at 303 K. AOT strongly catalyzes the hydrolytic reaction. With a progressive increase in [AOT], the reaction rate increased and after achieving a peak  $k_p$  decreased at higher concentrations of AOT. The Effect of temperature, added salts and dielectric constant of the medium has also been studied. The various thermodynamic activation parameters have been evaluated. The role of anionic micelle has been explained by the Menger-Portnoy, Piszkiwicz and Berezin models and the binding constant, rate constant in the micellar phase, cooperativity index ( $n$ ) have been calculated.

## **PP-CYSA-06 : Influence of Various Globular Proteins on the Phase Behavior of Thermosensitive Polymer**

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Poly (N-isopropylamide) (PNIPAM) has been recognized as a model system to understand the influence of various environmental effects on the stability of biological macromolecules. Protein is one of essential biopolymers employed in living systems to maintain biological homeostasis. PNIPAM contain both hydrophilic group (amide group) and hydrophobic group (isopropyl group), able to exhibit both well-solvated coil conformation at lower temperatures and precipitated globular conformation at higher temperatures. Comprehensive insight into the interaction between PNIPAM and proteins is crucial to understand the behavior of PNIPAM, which is widely used in biological, pharmaceutical and medicinal applications. Hence, in this work we have investigated the effect of various globular proteins such as Cytochrome C, Bromelian, Beta-lactoglobulin and myoglobin on the phase transition temperature of PNIPAM in aqueous solution with the aid of U.V. absorbance spectroscopy, steady-state fluorescence spectroscopy, thermal fluorescence spectroscopy, dynamic light scattering, Fourier transform infrared spectroscopy and field emission scanning electron microscopy measurements. Interestingly, we

observed that the phase transition in PNIPAM significantly varied with the type of protein.

### **PP-CYSA-07 : Structural and Thermo-responsive Behavior of Aqueous PNIPAM in the Presence of CNTs**

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The world of nanoscience is gaining popularity due to their vast applications in the field of biotechnology. In this context, nanomaterials such as carbon-nanotubes (CNTs) are highly popular because of their use as molecular transporters. It is very interesting that, CNTs overcome the challenges of drug delivery, such as targeted delivery of cancer drugs in the blood stream, overcoming the cell penetration issues and low toxicity levels. In spite of the wide application of CNTs, it is highly essential to examine the effects of CNTs on the physical properties of macromolecular systems. Hence, we have examined the effects of CNTs on the thermo-responsive behavior of aqueous poly (N-isopropylacrylamide) (PNIPAM). PNIPAM is very well known, in drug delivery system and a representative of protein structures due to the presence of amide-linkage within its structure. The experiment is divided in two sections: (a) increasing the solubility and dispersion of CNTs by functionalization with –COOH group, (b) examining the effect of functionalized CNTs on the phase transition of PNIPAM. The results, as observed using DLS, fluorescence and UV analysis, represent that CNTs have influence the thermo-responsive behavior of PNIPAM, indirectly correlating with the biocompatible nature of –COOH functionalize.

### **PP-CYSA-08 : Synthesis and Characterization of Europium Oxide Nanoparticles**

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Lanthanide oxide based nanoparticles are receiving great attention due to their excellent luminescent and magnetic properties and can be used in biomedical applications. Among various lanthanide nanoparticles, europium oxide nanoparticles are widely used in high performance luminescence devices, catalysts and other functional materials because of the electronic, optical and chemical characteristics originating from their 4f electrons. The Europium oxide nanoparticles

were prepared via sonication method of aqueous solution of europium nitrate in the presence of ammonia. The properties of these nanoparticles were characterized by X-ray diffraction, thermogravimetric analysis, differential scanning calorimeters, fluorescence and transmission electron microscopy.

### **PP-01 : Study of Molecular Interactions in Binary Liquid Mixtures Containing Glycols**

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Data on sound velocity offer a convenient method for determining certain thermodynamic properties of liquids and liquid mixture, which are not obtained by other methods. Extensive work has been carried out by many workers to investigate liquid state through analysis of ultrasonic propagation parameters and to correlate ultrasonic velocity with other physical and thermodynamic parameters. The experimental data of binary mixtures of Cyclohexane in 2-Methoxyethanol have been used to compute some acoustic and thermodynamic parameters such as intermolecular free length ( $L_p$ ), free volume ( $V_p$ ), relaxation time ( $\theta$ ) and acoustic impedance ( $Z$ ) at different temperatures over the entire composition range. The non-linear variations of these derived acoustical parameters with different concentration of the solute have been explained on the basis of structural changes occurring in a solution. The variation in ultrasonic velocity and other parameters play an important role in understanding solute solvent interaction between the constituent molecules are presented with some possible reasons.

### **PP-02 : Refractive Properties of Binary Mixtures of 1,4-Butanediol with Cresols**

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Refractive indices,  $n_D$ , and densities,  $\rho$ , have been measured for binary mixtures of 1,4-butanediol (1,4-BD) +o-cresol/ m-cresol/ p-cresol over the entire composition range at different temperatures (303.15,

308.15, 313.15 and 318.15 K). Some empirical and theoretical relationships like, Arago-Biot (A-B), Eykman (E), Eyring and John (E-J), Gladstone-Dale (G-D), Heller (H), Lorentz-Lorenz (L-L), Newton (N), Oster (Os) and Weiner (W) have been applied to study the dependence of the measured and derived quantities on temperature and composition. Furthermore, refractive index deviation,  $n_D$ , molar refraction, R, and molar refraction deviation,  $R$  have been calculated. Results have been fitted to Redlich-Kister polynomial equation to obtain the adjustable parameters and standard deviations between the measured and fitted values, respectively.

### **PP-03 : Kinetic and Mechanistic Study of Oxidant of Lower Oxyacids of Phosphorus by TSSD**

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Kinetic and mechanistic study of oxidant of lower oxyacids of phosphorus by TSSD in DMSO lead to the formation of corresponding oxyacids with phosphorus. The reaction is first order in TSSD. Michaelies-Menten type of kinetics is observed with respect to the oxyacids. The reaction is catalysed by hydrogen ions. The oxidation of deuteriated phosphinic and phenylphosphinic acids exhibited a substantial primary kinetic isotope effect. The oxidation was studied in nineteen different organic solvents. The solvent effect has been analysed by using Kamlet's and Swain's multiparametric questions. A mechanism involving transfer of a hydride ion in the rate determining steps has been proposed.

### **PP-04 : Role of Electrolyte on The Micellization and Clouding Phenomenon of Amphiphilic Antidepressant Drug Imipramine Hydrochloride: Conductometric, Dye Solubilisation, Tensiometric and Fluorometric Studies**

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In the present study, we report the micellization and clouding behavior of an amphiphilic antidepressant drug viz., amitriptyline hydrochloride (AMT) at different fixed temperatures and KCl concentrations in aqueous solutions. The critical micelle concentration

(CMC) of AMT, as measured by conductivity method, increases with increasing temperature and decreasing with KCl concentration. The thermodynamic parameters viz., standard Gibbs energy ( $\Delta G_m^0$ ), standard enthalpy ( $\Delta H_m^0$ ), and standard entropy ( $\Delta S_m^0$ ) of micellization of AMT are evaluated. The values clearly indicate more stability of the AMT solution in presence of KCl. Like surfactant, AMT also shows phase separation behaviour. The cloud point (CP) of AMT in water decreases with increase in pH of the medium because of the deprotonation of the drug molecule. The CP values increase with increasing KCl concentration and AMT concentrations, clearly indicating the micellar growth at higher concentration. Furthermore, for better understanding of the behaviour of drug molecule in water, we evaluated various thermodynamic parameters of the above drug molecule at CP.

### **PP-05 : The Influence of Adenosine on The Micellization of Cationic Gemini Surfactant, Hexanediyl-1,6-Bis(Dimethylcetylammmonium Bromide Solutions : Conductometric, Dye Solubilisation, Tensiometric Fluorometric and <sup>1</sup>NMR Studies**

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Herein we report the influence of adenosine and temperature on the micellization of cationic gemini surfactant, hexanediyl-1,6-bis(dimethylcetylammmonium bromide) (16-6-16) aqueous solutions. In absence and presence of adenosine (additive), the critical micelle concentrations (CMC) of 16-6-16 were measured by the conductivity, surface tension measurements, dye solubilisation, fluorescence methods. An increasing trend of the CMC values was found with addition of additive. We also studied the temperature effect on the micellization by conductometric method and found the CMC values increases with increasing the temperature. The energetics (viz., standard Gibbs energy ( $\Delta G_m^0$ ), standard enthalpy ( $\Delta H_m^0$ ), and standard entropy ( $\Delta S_m^0$ )) of micellization of 16-6-16 were evaluated. The evaluated energetics indicates less stability of the 16-6-16 solution in presence of additives. The aggregation number ( $N_{agg}$ ) of 16-6-16 (in absence and presence of adenosine) also determined by using fluorescence experiment.

## **PP-06 : Ultrasonic Velocity and Other Allied Parameters of Barium Carboxylates in Non-Aqueous Medium**

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The ultrasonic velocity of solutions of Barium Carboxylates (caprate, laurate and myristate) were measured in a mixture of chloroform-propylene glycol (70%-30% v/v) at a constant temperature. The data obtained were used to evaluate the critical micelle concentration (CMC) and to study the soap-soap and soap-solvent interactions. Various acoustic parameters, viz., adiabatic compressibility, intermolecular free length, apparent molar compressibility, specific impedance, and salvation number have been evaluated. The results show that the values of CMC are in agreement with the values obtained from other micellization properties.

## **PP-07 : Study of Thermo Excess Acoustical Parameters in Binary Liquid Mixtures of Butyl Acetate and o-Anisidine at Four Different Temperatures**

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Ultrasonic speeds( $u$ ), densities( $\rho$ ), and viscosities( $\eta$ ) have been measured in liquid mixtures containing butyl acetate and o-anisidine at different temperatures  $T=(303.15, 308.15, 313.15$  and  $318.15)K$  over the entire mole fraction range. From the experimentally measured data, excess thermo-acoustical parameters such as excess internal pressure, excess enthalpy, excess molar volume, excess acoustic impedance have been calculated. The results are fitted to the Redlich-Kister polynomial equation and they have been explained on the basis of molecular interactions between the components of liquid mixtures.

## **PP-08 : Density, Viscosity and Excess Thermodynamic Properties of Binary Liquid Mixtures of Aniline with 1-Propanol and 2-Propanol at 293.15 and 303.15K**

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The excess thermodynamic properties viz., excess molar volume

( $V^E$ ), excess Gibbs free energy of activation of viscous flow ( $\Delta G^{\#E}$ ) and viscosity deviation ( $\Delta\eta$ ) of the binary liquid mixtures of aniline with 1-Propanol and 2-Propanol have been calculated from experimentally determined at 293.15 and 303.15K temperatures. These derived excess functions have been fitted to Redlich-Kister equation and viscosities have been correlated with several viscosity models. The results have been interpreted in terms of molecular interactions.

### **PP-09 : Physico-Chemical Studies on Micellar Properties of Dysprosium Soaps in a Liquid Mixture**

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Various physical measurements like density, viscosity and conductivity of Dysprosium soaps (Myristate, palmitate and stearate) have been made to study the micellar properties in a mixture of Benzene-methanol (50%-50%) v/v. The results show that the CMC of these soaps decreases with increasing the chain length of fatty acid constituent. The density and viscosity results confirm that the molecules of the soap do not aggregate appreciably below the CMC and a sudden change in the aggregation takes place at the CMC. The results are explained in terms of well-known equations proposed by Einstein, Moulik, Vand and Jones-Dole.

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<b>S</b>			PO-CYSA-01, 05, 07, 08
Sandhya G.	PO-12		PP-CYSA-06, 07
Sangeeta	PP-06	<b>W</b>	
Satyaveni S.	PP-01	Ware A. P.	PP-CYSA-05
Seshaiah K.	PO-07	<b>Y</b>	
Shweta S.	PO-CYSA-06	Yadav R.	PO-CYSA-08
Siddiq A. M.	PP-05		PP-CYSA-07
Sindhu A.	PO-CYSA-01		



