INDIAN COUNCIL OF CHEMISTS

(www.chemicc.com)

XXXV Annual Conference

2016

ABSTRACTS BOOK

Haribhai V. Desai College, Pune

in association with

College of Engineering, Pune

on

22nd - 24th December, 2016

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 XXXV Annual Conference of ICC from 22nd - 24th December, 2016 at Haribhai V. Desai College, Pune in association with College of Engineering, Pune.

The leading researchers and key opinion leaders in Chemistry have been invited to facilitate sessions and deliver lectures at XXXV 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 Pune. You can enjoy there too.

Thank you for your participation.

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

PROVISIONAL PROGRAMME

Thursday, 22nd December, 2016

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

Friday, 23rd December, 2016

09:00 to 01:00 PM	Symposium ICC 2016 on "Role of Indian Women Researchers in Chemical Sciences"
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

Saturday, 24th December, 2016

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

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IN ASSOCIATION WITH
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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.

- You should be printing and bringing your poster to the conference.
- The dimensions of poster **should NOT exceed 90 cm wide × 120 cm high.**
- 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.
- Allocate the top of the poster for the title and authors as stated on the submitted abstract.
- The text, illustrations, etc. should be bold enough to be read from a distance of two meters.
- Double sided tape and technical equipment will be available for the mounting of posters. Staff will also be available to assist you.
- 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.
- 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 35th Annual Conference at Pune on 22nd - 24th December, 2016 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 35 years of its existence.

The Council is grateful to Dr. G. R. Pathade, Principal, H.V. Desai College, Pune, Dr. B.B. Ahuja, Director, College of Engineering, Pune and Dr. G. S. Gugale, Head, Department of Chemistry, H.V. Desai College, Pune 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

CONTENTS

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
RWS	- Symposium

Life Time Achievement Awardee Lecture Abstract

Development of Electroanalytical Techniques for the determination of the Drugs at Pre-Treated Graphite Pencil Electrode and Their Applications

Sharanappa T. Nandibewoor

P. G. Department of Studies in Chemistry, Karnatak University, Dharwad-580003

Analytical Chemistry plays an important role in the development of a compound from its synthesis to its marketing stage as a part of drug formulation and analysis. In 1959, Prof Heyrovsky was awarded Nobel Prize in Chemistry for his discovery of the polarographic methods of analysis. Since then voltammetric methods have become a popular and indispensable tool for the study of electrochemical reactions, in coordination chemistry, in solar energy conversion, in environmental monitoring, in industrial quality control, for the study of redox mechanisms and in the determination of trace concentrations of biological and clinically important compounds. Cyclic voltammetric (CV) methods have found to have extensive applications for evaluation of thermodynamics and mass transport phenomena of a number of redox reactions and associated chemical reactions. CV studies in rat brain, invivo studies in animals, bacteria and even plants are picking up. With the introduction of newer electrode materials of small size, these methods of chemical analysis in living systems might grow even faster. It is important to develop a simple, low cost, rapid, reliable and reproducible method for detecting ingredients in drugs since it is essential in quality control laboratories. Many electrodes were developed in our laboratory for the determination of important drugs and the proposed methods were applied in pharmaceutical formulations and real samples. As an example, a simple and rapid electrochemical determination of ketoconazole (KTZ)

drug, an antifungal drug, in physiological pH, 7.4 at pre-treated graphite pencil electrode (PGPE) was developed. After the pretreatment, graphite pencil electrode (GPE) exhibited excellent electrocatalytic activity with good reproducibility and more stability. The voltammetric behaviour of KTZ for physiological buffer at pH 7.4 was observed to be sharper and better oxidation peak was obtained. From the scan rates (v) of both linear sweep and cyclic voltammeric techniques, KTZ was found to be irreversible and diffusion controlled electrode process, and there was transfer of unequal number of protons and electrons. Differential pulse voltammetry exhibited a good linear range of 5.0×10^{-8} M to 5.5×10^{-7} M with a detection limit of 3.98×10^{-9}M and square wave voltammetry in concentration range from 1.0×10^{-8} M to 5.0×10^{-6} M with a detection limit of 0.96×10^{-9} M for KTZ. Effect of several possible interfering substances on the determination of KTZ was investigated. The proposed method was applied to the determination of ketoconazole in real and pharmaceuticals samples.

To be presented in
Physical Chemistry Section

Prof. W. U. Malik Memorial Awardee Lecture Abstract

Green Solvents in Thin-Layer Chromatography of Surfactants

Ali Mohammad

Department of Applied Chemistry, Faculty of Engineering & Technology, Aligarh Muslim University, Aligarh-202002
Email: alimohammad08@gmail.com

Analysis of surfactants is important because of their effects on aquatic plants and organism. Surfactants are organic compounds and by virtue of their easy solubility in water these are capable to enter into water systems through wastewater discharge from domestic as well as industrial sources. Therefore, it becomes necessary to develop simple and selective methods for their identification in water bodies using eco-friendly solvent systems (e.g. Green solvents). Because of environmental concern, the trend of using volatile organic solvents in chemical analysis by chromatography is being currently discouraged. To reduce the harmful impact of toxic organic and mixed organic solvents used in thin layer chromatography, green solvents have recently introduced in the analysis of surfactants. In this direction, efforts are being made in our laboratory and certain highly effective water based mixed organic solvents have been identified as green solvents for efficient separation of surfactants from their multi-component mixtures by thin layer chromatography. Thin layer chromatographic procedures involving the use of lower alcohols (C1-C4), aqueous sodium thiocyanate solution, acetone, ethyl acetate, ethyl methyl ketone, water, ethylene glycol etc. have been successfully applied for on-plate identification of surfactants with preliminary separation on different static phases of sorbents. Different chromatographic parameters and limits of detection of the separated surfactants have been determined in order to check the efficiency of green solvents.

To be presented in Environmental & Analytical Chemistry Section

Prof. S.P. Hiremath Awardee Lecture Abstract

Molecular Hybrids Based Drug Design : A Myth or Reality

Diwan S. Rawat

Department of Chemistry, University of Delhi, Delhi-110007
E-mail : dsrawat@chemistry.du.ac.in

The design of new molecules with improved ADME properties along with effective pharmacological potency; lack of toxicity and devoid of resistance for the treatment of infectious diseases has remained a big challenge for the scientific community. In order to address these issues concept of hybrid molecules was put forward which deals with the covalent hybridization of two or more distinct pharmacophores into a single molecule that may lead to a hybrid molecule with improved efficacy. This approach may solve the problem of drug resistance and reduce the undesired side effects. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. Towards these goals we have synthesized various molecular hybrids and tested these for antimalarial, anti-Parkinson and anti-cancer activities and efforts will be made to present our recent work.

To be presented in
Pharmaceutical Chemistry Section

Prof. Kaza Somashekhar Rao Awardee Lecture Abstract

A Review on Plasmonic Metal–TiO_2 Composite for Generation, Trapping, Storing and Dynamic Vectorial Transfer of Photogenerated Electrons Across the Schottky Junction in a Photocatalytic System

L. Gomathi Devi

Department of Post Graduate Studies in Chemistry, Central College City Campus, Dr. Ambedkar Street, Bangalore University, Bangalore-560001
E-mail : gomatidevi_naik@yahoo.co.in

The titania based nanomaterials are an attractive candidates for energy and environmental applications. TiO_2 is one of the most important photocatalyst for its special multiple characteristics like high reactivity, low toxicity, low cost, high flexibility, long term stability especially in aqueous medium, shows relatively high energy conversion efficiency, easy to prepare several modifications with various morphologies, with good recycle ability, favorable band edge positions and superior physicochemical and optoelectronic properties. However, large band gap of titania and massive charge carrier recombination impairs its wide photocatalytic applications. As an alternative to various strategies reported extensively in the literature, noble metal deposition on the titania surface seems to be effective and reliable method for increasing the life time of excitonic pairs and to extend the band gap absorption to visible range of the solar spectrum. In this presentation, the fundamental and critical issues in the photocatalytic activity of metal deposited titania by taking into consideration the influence of various parameters like preparation methods, metal dispersion on titania, formation of heterojunctions and optimum metal loadings on the interfacial charge carrier dynamics will be discussed.

The metal deposition on titania of varied hierarchical morphology, crystal structure, defective surface along with extended modification like simultaneous doping and heterostructure coupling with other semiconductors is also highlighted. It was revealed that deposited metal is involved in multiple crucial roles like; (i) it serves as passive electron sink with high capacity to store electrons to suppress photogenerated charge carrier recombination; (ii) it facilitates rapid dioxygen reduction to generate reactive free radicals; (iii) visible light response of titania can be achieved through surface plasmon resonance effect; (iv) direct excitation of metal nanoparticles especially under visible light and vectorial electron transfer to the TiO_2 CB. This presentation attempts to provide a comprehensive update of design and fabrication of metallization on the surface of TiO_2 semiconductor particles highlighting some of the advancements made in the energy and environment applications.

To be presented in the
Physical Chemistry Section

Dr. Arvind Kumar Memorial Awardee Lecture Abstract

Design and Applications of Ionic Liquids as Green Solvents for the Extraction, Absorption and Dissolution Processes

Ramesh L. Gardas

Department of Chemistry, Indian Institute of Technology Madras, Chennai-600 036

E-mail : gardas@iitm.ac.in

Solvents are major contributors and high on the list of environmental damage chemicals, mainly because of their large usage and high volatility. The widespread use of volatile organic compounds (VOCs) in many industrial chemical processes is an issue of great environmental concern. It is an extremely important task to search of potentially green and environment friendly alternatives for VOCs. At least a partial solution to this problem may offer by a novel class of molten salts referred to as ionic liquids (having melting point, generally, below boiling point of water), as they possess unique combination of particular properties, unlike molecular liquids, namely negligible vapour pressure (~ 10^{-11} to 10^{-10} bar at room temperature), wide thermal window (~ -50°C to +250°C), wide electrochemical window (~ ±3 Volt vs. NHE), non-flammability, high ionic conductivity and a highly solvating capacity for organic, inorganic and organometallic compounds. This unique combination of particular properties leads them to be exploited as “green solvents” and giving them increasing attention in academic and industrial research. The research areas on ionic liquids are growing very rapidly and the potential application are numerous, mainly due to the fact that simple changes in the cation and anion combinations or the nature of the moieties attached to each ion allow the physical properties of ionic liquids such as hydrophobicity, viscosity, density, coordinating ability,

ion selectivity, and chemical and electrochemical stability to be tailored for specific applications. Proposed talk will include the introduction of green solvents, ionic liquids, general applications of ionic liquids and understanding unique thermophysical properties of novel ionic liquids for metal ion extraction, solar refrigeration system, dissolution of tank bottom sludge and dissolution and stability of biomolecules. Further, the effects of thermophysical properties of ionic liquids on these applications will be discussed.

To be presented in
Physical Chemistry Section

Symposium on "Role of Indian Women Researchers in Chemical Sciences"

Chairman Remarks

Role of Women in Science

N. S. Rajurkar

Ex-Head, Department of Chemistry, S.P. Pune University, Pune
E-mail : rnilima@rediffmail.com

Women have made significant contributions to science from the ancient times. However, the role of women in India has been subject to many great changes over the past few millennia. From equal status with men in ancient times to lower status during medieval time and as of equal rights today.History of women's role in science starts from Gargi and Maitreyee in ancient India. In the beginning of nineteenth century Nobel Laureates Marie (1903,1911) and Irene (1935) Curie played a significant role in chemical sciences which resulted in the betterment of mankind. In 1964 Dorothi Hodgkin received the Nobel prize for developing protein crystallography and after 45 years another women scientist Ada Yonath received the Nobel prize for structure and function of ribosome. Even though women are under-represented in the sciences as compared to their numbers in the overall working population, in the present decade many women scientists are playing very important role in various fields in India. The present lecture gives an overview of the role played by women scientists, especially in chemical sciences.

RWS-IL-01 : Women Chemists from MadamCurie to Charusita Chakravarty

C. P. Bhasin

Department of Chemistry, Hem. North Gujarat University, PATAN- 384 265 (Gujarat)
E-mail : cpbhasin@yahoo.com

Madam Curie the first lady Nobel Laureate in Physics and Chemistry was felicitated in 2011 world wide for her centenary celebration of her second Nobel prize in the field of Chemistry after getting first in Physics in 1903. She was not Indian but is a unique example till date for her outstanding contribution of two generations in the field of chemistry. In India starting fromAsima Chatterjee (1917 – 2006)to Charusita Chakravarty tremendous contribution in chemical sciences has been made by female scientists.It would be worth mentioning that Dr. Kamala Sohonie (1912–1998)of course was the first Indian woman to get a Ph.D. in a scientific discipline was from Botany (tissue culture). She applied to the I.I.Sc. for a research fellowship and met with rejection merely because she was a woman! Prof. CV Raman, then I.I.Sc. Director was dead against having women students. She then became the first of his female students, and performed so well that Prof. Raman gave her permission to pursue further research.While at Cambridge, she found that every cell of a plant tissue contained the enzyme 'cytochrome C' which was involved in the oxidation of all plant cells. In fact, her 40 page PhD thesis was based on this. The subjects of her research were often on food items consumed by the poorest people. She started her pioneering work on the nutritional value of Neera.Charusita Chakravarty wasa professor of Chemistry at the Indian Institute of Technology, Delhi since 1999 till last. Born in the USA, she relinquished her U.S. citizenship and now works in India. She had won several awards for her work, most notably, the Shanti Swarup Bhatnagar Prize. She was an Associate Member of the Centre for Computational Material Science, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.She was outstanding &brilliant Chemist worked in the field of chemical physics, theoretical and computational chemistry.In 2009 she was conferred Shanti Swarup Bhatnagar Prize for Science and Technology in the field of Chemical Science. In 1999, she received B.M. Birla Science Award.

RWS-IL-02 : Role of Indian Women Researchers in Chemical Sciences

Vidya Gupta

National Chemical Laboratory, Pune
E-mail : vs.gupta@ncl.res.in

It is a general assumption that studies in the science faculty are highly rigorous and need wholehearted dedication to complete them successfully. Among the various subjects within science faculty Physics, Chemistry and Mathematics are generally considered to be male dominating as compared to Biology even today. Especially at the higher levels of education such as at postgraduate and Ph. D. level it is more obvious. This is the phenomenon observed not only in India but also globally. Within India various social, economical and cultural issues are responsible for such unequal gender proportion in higher education in general and science education in particular. In such a scenario entering into science research career is no doubt an adventurous and bold step. However, there are some women who selected research in science as their career and few of them have acquired feathers in their caps. Many of them have also balanced their life and work profiles very carefully.There are some globally important names of women scientists in chemical sciences, such as Madam Marie Curie, Dr. Irene Joliot-Curie and Dr. Dorothy Hodgkin stand out who have received the Nobel Prizes in Chemistry in early years of twentieth century. In India, Dr. JanakiAmmal, Dr. Kamala Sohonie, Dr. AsimaChatterjee, Dr. DarshanRangnathanand some more can be considered as pioneering women scientists in the area of biochemical and chemical sciences. Contributions of these women scientists and some of the present era scientists would be discussed.

RWS-IL-03 : Women in Science and Intellectual Property Rights-a Discussion

N. V. Khalap

Technology Transfer & Collaboration Division, BARC, Trombay, Mumbai-400085
E-mail : nutanla@barc.gov.in, nkhalap@yahoo.com

Ancient Indian teachers always believed that knowledge is “wealth” and it increases by giving it free to as many seekers as possible. In today’s context of International treaties and world commerce, knowledge needs to be protected and exploited by those who have created it. Different types of creations of human mind such as scientific inventions, books, films, music, software, traditional knowledge, product designs and business trademarks, etc are protected by different country specific laws formulated as per International guidelines. A review of different Intellectual property instruments will be presented.Patenting is the most common form of protection used for scientific inventions and licensing of patents is the most common form of commercialization of patents.

Despite their contribution to all fields of creativity and intellectual endeavors, women remain underrepresented in many areas.Although there are more female than male undergraduate and graduate students in many countries, there are relatively few female full professors, and gender inequalities in hiring, earnings, funding, satisfaction and patenting persist. In the field of science and technology, women representation is on the rise, but patenting by women remains lower than, for example, their authorship of scientific papers. A study in the United States suggests 7.5% of patents are granted to women while only 5.5% of patents commercialized, are commercialized by women.

The contributing factors to this observed disparity and remedial policy suggestions shall be briefly discussed.

RWS-IL-04 : Emerging New Techniques in Forensic Science:Role of Women

S. V. Ghumatkar[1*], P. A. Ghosarvadkar[2], K.V. Kulkarni[2] and B. B. Daundkar[3]

[1]Regional Forensic Science Laboratories, Kolhapur
[2]Regional Forensic Science Laboratories, Pune
[3]Directorate of Forensic Science Laboratories, Mumbai, Vidyanagari, Kalina, Mumbai-4000098
E-mail : svghumatkar@gmail.com

Forensic science involves the application of science to the investigation of legal matters.Forensic Science Laboratory is a Government institution to help the Investigating Officers in the detection of crime in scientific way to help the criminal justice system.There are various divisions in forensic as:General analytical and Instrumentation division, Biology division, DNA division, Prohibition and excise, toxicology, ballastic, cyber division, TASI division, forensic psychology.

In crime investigation, application of chemistry has become inevitable in Comparison of Soil, Paint, Glass, Glass Bangle, Cloth under IPC 302,376, in Analysis of Gold / Metals, in Analysis of Pharmaceutical Drugs and Analysis of Chemicals in Copy Right Act Cases, Restoration of Chassis & ENGINE Number Cases under IPC 420,in Analysis of Brown Sugar(Heroin), Morphine, Cocaine, Ganja, Charas,Bhang in narcotic drug cases. The analytical techniques used are Colour/Chemical tests, TLC/HPTLC, UV/ IR, GC/GCMS, HPLC/ MS.etc. in cases involving biological specimens such as 302-Murder, 307-Attempt of Murder, 376-Rape andWild life poaching cases. Detection of body fluid stains(i.e. blood, semen, vaginal fluid etc.) on clothes of accused, deceased, injured persons, weapons etc.,species origin of the detected body fluid stains to find whether the stain is of human origin or otherwise, individualization of the body fluid stains by blood grouping, hair examination to prove the involvement of the accused in the crime is done to establish corroborative evidence in court.

Women have made significant contributions to science from the earliesttimes. Women in this field have been working right from the beginningstage as reporting officers. They have been attending crime scenes like 26/11 blast, German bakery bomb blast, serial blasts of Pune, Fharaskhana bomb blast, rape and murder cases and have been heading various sections.They have attended court summons, presented papersin international conferences and received awards too. Showcasing strong role models for women, it'simportant to mention the dynamic lady Director of Forensic, Dr

Rukmani Krishnamurthy, who in her tenture started the new techniques like cyber, psychology,TASI in the state of Maharashtra.Thus, women have played a key role in Forensic upbringing.

RWS-OP-01 : Women Chemists in Developing Countries

Nilakshi V. Sadavarte

Polymer Science and Engineering Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune- 411 008.
E-mail : nv.sadavarte@ncl.res.in

Organization for the Prohibition of Chemical Weapons (OPCW), the Hague, the Netherlands organized one day Symposium on Women in Chemistry on 17 May 2016. I had an opportunity to attend this symposium on behalf of India. The Symposium was attended by over 60 participants from 40 countries, including officials from OPCW States Parties, the scientific community, chemical industry, academia and civil society. To further advance the participation of women as key stakeholders in the scientific community, chemical industry, and other fields of chemistry, the Symposium focused on promoting diversity, equal opportunity and cooperation. The day was organized around thematic presentations and discussions featuring prominent role models who addressed various areas of concern for women working in chemistry-related fields. The group discussions engaging the participants sought to identify opportunities and solutions for promoting education, building capacity, and career advancement for women chemists. In addition, the women chemists shared their professional experiences with other participants.

Thus, OPCW provided an interactive forum; I had an opportunity to interact with women chemists from various countries. The symposium illustrated the strength and depth of the contributions of women in chemistry. The group discussions raised awareness of capacity development for women in chemistry and promoted international solidarity and cooperation in this regard.

RWS-OP-01 : Role of Women Chemists in Public Health

Rashmi S. Kumar[1], Neeta Zatakia and N. S. Rajurkar*

Department of Chemistry, Savitribai Phule Pune University, Pune 41007
[1]Department of Environmental Sciences, Savitribai Phule Pune University, Pune 411007
E-mail : rnilima@rediffmail.com

Women have a special role in healthy nutrition of the population. Public health depends upon women's understanding of healthy nutrition issues. Women, therefore, play a key role in implementing a healthy nutrition policy, both in the family and in society as a whole. Women's health status as well as their social status have a great impact on the health of their children and therefore of the future generation.

There are numerous policies designed to reduce the incidences of nutrient deficiencies.Research on impact of these policieson women's general health and nutrition is neglected at the grass root level. Pregnant women are especially prone to nutrient deficiencies owing to increased nutrition demands. Therefore, we decided to take up the issue of iron deficiency anemia and iodine deficiency disorders among pregnant women belonging to lower socio economic strata from peripheral areas of Pune. 367 pregnant women voluntarily participated in the study. Iron and hemoglobin concentration studies in blood samples revealed that 92% women were anemic.Thyroid profile of 163 pregnant women showed that 67.48% women were prone to hypothyroidism. These results were communicated to the participants.They were made aware of the importance of iron and iodine during pregnancy through informal discussions.

RWS-OP-03 : Role of Women in Water Supply, Water Quality and Sanitation Programme

Ranjana Badve
ranjanakw@gmail.com

Water is an important source of life. Without water there is no life and no development. Water has been featuring prominently both on national and international agenda. Stress on water resources is from multiple sources such as urbanisation, increased industrial activities, heavy use of fertilisers and pesticides in agricultural activities, discharge of untreated sewage and industrial effluents into environment. All these activities ultimately leads to both surface and groundwater pollution. A result of this is that the drinking water supply sources both in urban and rural areas are becoming polluted, which results in increase in cost of water treatment. In order to protect the sources from pollution, the importance of community participation in water quantity and quality management, sanitation and health has been raised.

Women constitute half the world's population. They are the caretakers of children , the guardians of family health and wellbeing, managers of household resources. So their participation, involvement and empowerment in all water management programmes at all levels is essential including decision making and implementation. Education of women is essential and she will work as trainer in future. This will help in sustainable development of water resources.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

Sectional President's Address

Analytical Techniques a Boon for Materials Characterization

Satish K. Pardeshi

Department of Chemistry, Savitribai Phule Pune University
(formerly Pune University), Ganeshkhind, Pune-411007
E-mail : skpar@chem.unipune.ac.in

The conference is one of the activities to bring together academicians, research scholars' and students to interact and discuss on various issues. It also exposes participants to new developments through invited talks by academicians, researcher, eminent scientist and technologist. Developing interest of students for undertaking research and studies in the emerging field of Chemistry is also equally important. Current research is focused on synthesizing material of vast variety. Analytical techniques and instruments play a crucial role in characterization of such materials. Various techniques such as TG-DTA-DTG analysis, FT-IR spectroscopy, Raman spectroscopy, UV-Visible Spectrophotometer, X-ray powder diffraction, X-ray Photoemission Spectrophotometer (XPS), Photoluminescence (PL), Scanning Electron Microscopy (SEM), EDX, Transmission Electron Microscopy (TEM), BET measurement for surface area, etc. are routinely used in characterization of inorganic materials. In addition to these techniques, spin properties are studied using ESR/EPR, magnetic studies using VSM, electrochemical studies by CV are done e.g. in tuned graphene, spin properties are monitored using ESR and VSM. Similarly Second Harmonic Generation (SHG) by Kurtz-Perry powder technique and dielectric measurements by LCR meter for non linear optical material are carried. While, ^{1}H NMR, ^{13}C

NMR spectroscopy and various chromatographic techniques are extremely useful for purification and characterization of organic materials. X-ray single crystal structure analysis gives unambiguous high end characterization of organic and organometallic complex compounds especially for configurational confirmations. In the present address discussion with respect to synthesis of pure / modified/ substituted material done by different methods and their characterization by various methods is summarized. On applying such techniques one can get valuable information of materials synthesized for various applications.

AIL-01 : Biorefinery : A Solution for Sustainable Chemical Processes

C. V. Rode

CEPD Division, CSIR-National Chemical Laboratory, Pune-411008
E-mail : cv.rode@ncl.res.in

'Biorefinery' is an integrated facility for the biomass conversion to fuels, power, and chemicals. The biorefinery concept is analogous to the conventional petroleum refineries, which produce multiple fuels and products from non-renewable fossil-derived petroleum in the same complex. The high-value products enhance profitability, the high-volume fuel helps meet national energy needs, and the power production reduces costs and avoids greenhouse-gas emissions. Biorefining is still largely unexplored territory and presents many research and business opportunities for the production of bio-based products from agricultural and forest residues. Among various bio-feedstock options, abundantly available lignocellulosic material at lower cost can be easily converted to a variety of starting materials. In the first decade of 21st century, much research has been aimed at developing new catalytic routes for the conversion of several bio-based platform molecules into fuels and multiple commodity products leading to realization of 'Bio-Refinery' concept.

Oxygen present in the bioderived molecules poses an interesting challenge of selective hydro-deoxygenation reactions by designing appropriate catalyst systems and at the same time should require less number of processing steps as compared to the fossil derived hydrocarbons. Among various bio-feedstock options, co-generated glycerol in biodiesel production and abundantly available lignocellulosic material at lower cost can be easily converted to a variety of starting materials. For example, hydrogenolysis of glycerol gives 1,2-propanediol. While, γ- valerolactone (GVL) can be obtained by the catalytic hydrogenation of LA. Similarly, furfural is also a versatile carbohydrate derived starting material for either direct hydrogenation to give a variety of useful products such as furfuryl alcohol (FAL), tetrahydrofurfuryl alcohol (THFAL), 2-methylfuran (2-MF) and 2-methyl tetrahydrofuran (2-MTHF) or via catalytic alcoholysis (esters of LA) / hydrogenation sequence to give GVL. In this talk, the application of non-noble metal Cu catalysts will be demonstrated for the conversion of two bio-derived platform molecules viz. (i) selective hydrogenolysis of glycerol to 1,2-propanediol (1,2-PDO) and (ii) selective hydrogenation of levulinic acid to γ-valerolactone (GVL). Both these hydrogenations involve more than one type of reactions however, the catalyst responsible

for several reactions is the same and these steps are carried out in a single-reactor system. Moreover, due to safety concerns and handling constraints, both these hydrogenations could be successfully carried out without using external hydrogen under pressure. Autogeneous glycerol hydrogenation was possible due to aqueous phase reforming reaction while, for levulinic acid hydrogenation, formic acid was used as a H-donor.

AIL-02 : Evaluating the Potential of Sustainable Adsorbents for Chromium Detoxification-An Overview

N. Rajesh

Department of Chemistry, Birla Institute of Technology and Science (BITS), Pilani-Hyderabad Campus, Jawahar Nagar, Shameerpet Mandal, Hyderabad-500 078
E-mail: nrajesh@hyderabad.bits-pilani.ac.in

Solid phase extraction has proven to be a vital separation technique in analytical chemistry. Diverse materials such as polymeric resins, biopolymers, clays and carbon (various forms) are known to sequester heavy metals from varying matrices. Among the toxic metals, chromium in the hexavalent form is considered as potentially carcinogenic and therefore it is imperative to look for eco friendly adsorbents to remove chromium from waste water. The talk would highlight the rising importance of customized biopolymers and carbonaceous adsorbents such as graphene oxide for the speciation of chromium. Appealing mechanisms foster the interaction of these adsorbents with chromium in the hexavalent and trivalent state. The functional groups play a significant role in the effective coordination with chromium in its two stable oxidation states. Regeneration of the adsorbent for repetitive cycles is an important aspect. Adequate selectivity, high adsorption capacity and rapid adsorption-desorption kinetics are attainable with the above mentioned adsorbent materials. The sustainable adsorbents are a viable alternative for solvent extraction towards the removal of chromium from industrial effluents.

AIL-03 : Raman Spectroscopy of Carbon Compounds

P. S. Alegaonkar

Department of Applied Physics, Defence Institute of Advanced Technology, Girinagar, Pune-411021
E-mail: prashant.alegaonkar@gmail.com

Raman spectroscopy is facile, non-destructive, and yet simple tool to investigate materials, especially, carbon compounds. In this, the physics of inelastic light scatting process to the technical details of Raman spectroscopy would be discussed. As a case study,

analysis of various carbon compounds, such as graphene, would be presented, briefly.

AIL-04 : Fluorescent Colorants in Environmental Analysis

N. Sekar

Dyestuff Technology Department,Institute of Chemical Technology (formerly UDCT) Matunga, Mumbai-400019
E-mail : n.sekar@ictmumbai.edu.in, nethi.sekar@gmail.com

Fluorescence is a phenomenon which is highly sensitive to microenvironment like polarity, pH, and similar things. Therefore any change perceived in the fluorescence of a molecule gives qualitative and quantitative aspects of microenvironment in question. Fluorescent colorants therefore act as molecular probes and several analytical techniques employ fluorescence probes. In this requirement high performance fluorescent molecules used in the environmental analysis will be discussed. Typical florigenic molecules with large Stokes shift, dual emission, and NIR emission will be discussed with typical examples used in analytical chemistry. Absorption and emission solvatochromism as polarity indicators, and their utility in environmental monitoring – gas sensing – will be explained. Fluorophore-Antibody conjugates are widely used in bio-sensing. The requirement of fluorescent probe molecules for these applications in terms structure, photo-physics, and other photo-physical properties will be discussed.

AIL-05 : Carbon Based Nanomaterials-Cement Composites and their Physicochemical Properties

N. C. Kothiyal

Nanosurface and Environmental Chemistry Laboratory, Department of Chemistry, Dr B. R. Ambedkar National Institute of Technology. Jalandhar – 144011 (Punjab)

Cement mortar is the most commonly used construction materials worldwide. The material suffers from several drawbacks such as limited strength, high porosity, poor flexural behavior, poor crack resistance, loose microstructure and high brittleness. These factors consequently lead to the degradation of the cementitious matrix with time under different environmental conditions. Previous researches have emphasized on the inclusion of different fibers as reinforcing materials (e.g. steel fibers, carbon fibers, glass fibers, polypropylene fibers, etc.) in order to overcome some of these drawbacks. These reinforcing materials exhibit their reinforcement only at macro-level or micro-level, but the drawbacks originating at nanoscale still persist within the matrix.The various drawbacks

of cementitious matrix can be effectively overcome using the carbon based nanomaterials having exceptional mechanical properties. Use of functionalized 1-D carbon nanotubes (FCNTs) and 2-D graphene oxide (GO) provide new dimension to interact with cement matrix due to their better dispersibility in water, high aspect ratio, high surface area and excellent mechanical properties.The focus of the current research was to investigate the use of GO and functionalized multi-walled carbon nanotubes (FMWCNTs) as the reinforcements in the Portland cement mortar samples. The effects of incorporating GO and FMWCNTs in certain dosages on the hydration, microstructure and mechanical properties of cement-based composites have been discussed. Graphite Powder of particle size 100 micron was subjected to high energy ball milling to produce ball milled graphite powder with reduced particle/sheet size. GO was synthesized using Hummers method and FMWCNTs were obtained by oxidation of pure CNT, which were characterized using Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and X-Ray Diffraction (XRD).Further, inclusion of GO and FMWCNT as dispersed phase in cement mortar matrix were investigated for their effects on compressive strength, tensile strength and conductivity behavior at various dosages as a function of curing time (i.e. 7 days, 14 days and 28 days). The results obtained have shown that compressive strength increases for the cement mortar composites remarkably using small concentrations of GO and FMWCNT with respect to the control sample. The compressive strength of cement mortar sample was found to increase by 58.2% with respect to control sample by using 0.50% FMWCNT (% by wt. of cement used) after 28 days of curing. The highest improvement of 77.3% in the compressive strength was observed using 1.00% GO (% by wt. of cement used) with respect to control sample after 28 days of curing. Whereas, tensile strength was found to increase up to a particular concentration of GO and FMWCNT, thereafter decreases. An increase in tensile strength has been observed by 37.5% using 0.25% GO (% by wt. of cement used) as composite, whereas an improvement of 40% in tensile strength was achieved using 0.25% FMWCNT (% by wt. of cement used) as composite with respect to control sample after 28 days of curing. Increase in the compressive and tensile strength was attributed to an increase in the number of active sites for nucleation of hydration products on GO nano sheets and FMWCNT walls due to presence of functional groups. Additionally the microstructures of hydrated cement mortar matrix were found to be regulated with the inclusion of GO and

FMWCNT. The research provides a new pathway to significantly improving both the compressive and tensile strength of cement mortar by using GO as an economical and potential substitute to costly FMWCNTs.

AIL-06 : Green Solvents in Thin-Layer Chromatography of Surfactants

Ali Mohammad

Department of Applied Chemistry, Faculty of Engineering & Technology, Aligarh Muslim University, Aligarh-202002
E-mail : alimohammad08@gmail.com

Analysis of surfactants is important because of their effects on aquatic plants and organism. Surfactants are organic compounds and by virtue of their easy solubility in water these are capable to enter into water systems through wastewater discharge from domestic as well as industrial sources. Therefore, it becomes necessary to develop simple and selective methods for their identification in water bodies using eco-friendly solvent systems (e.g. Green solvents). Because of environmental concern, the trend of using volatile organic solvents in chemical analysis by chromatography is being currently discouraged. To reduce the harmful impact of toxic organic and mixed organic solvents used in thin layer chromatography, green solvents have recently introduced in the analysis of surfactants. In this direction, efforts are being made in our laboratory and certain highly effective water based mixed organic solvents have been identified as green solvents for efficient separation of surfactants from their multi-component mixtures by thin layer chromatography. Thin layer chromatographic procedures involving the use of lower alcohols (C1-C4), aqueous sodium thiocyanate solution, acetone, ethyl acetate, ethyl methyl ketone, water, ethylene glycol etc. have been successfully applied for on-plate identification of surfactants with preliminary separation on different static phases of sorbents. Different chromatographic parameters and limits of detection of the separated surfactants have been determined in order to check the efficiency of green solvents.

AIL-07 : Smart Sensors for Smart Cities

Parag V. Adhyapak

Centre for Materials for Electronics Technology (C-MET), Panchawati off Pashan Road, Pune-411 008
E-mail : adhyapakp@yahoo.com, adhyapak@cmet.gov.in

Smart cities are cities which will work intelligently with self sufficient ways of operating and monitoring all the processes.

Smart sensors play a crucial role in the foundation of smart city. Different sensors like energy sensors, humidity sensors, LPG/CNG sensors (for piping gases), weather prediction sensors, light/ street Light sensors, gas sensors for environmental monitoring, temperature sensors etc will be a integral part of the smart city. For the development of these smart sensors, the use of nanonmaterials is inevitable in view of expected miniaturization, fast response, high sensitivity, long durability, cost effectiveness etc. Semiconductor metal oxide gas sensors have been explored by many researchers all over the world and tremendous amount of research work is being already done on this subject. Semiconductor metal oxides provides several advantageous features such as simple device structure, ease of fabrication, robustness, adaptability to a wide variety of reductive or oxidative gases, high sensitivity and selectivity etc. In general, the semiconductor metal oxides change their electrical properties, e.g. resistance, to notify the gas concentration. The mechanism of sensing depends on the change in the oxygen concentration at the oxide surface which is due to adsorption and heterogeneous catalytic reaction of oxidizing and reducing gaseous species. The electrical conductivity changes with the gas atmosphere and the temperature of the sensing material exposed to the test gas. Along with semiconductor metal oxide nanomaterials, recently, variety of other materials such as ceramics, carbon nanotubes, organic/conducting polymers and polymer/ inorganic hybrid systems have been extensively investigated and used as a sensing material. The present talk covers the development of various sensors at CMET. The major emphasis is on the synthesis and characterization of nanostructured oxides as well as polymer based metal nanocomposites for humidity and gas sensing applications.

AIL-08 : Nanotechnology for Emerging Applications

V. S. Shrivastava

Nanochemistry Research Laboratory, G.T. Patil College, Nandurbar-425412, (M.S.)
E-mail : drvinod_shrivastava@yahoo.com

Nanoparticle and nanomaterials are the worldwide applications in every field of nanotechnology. The nanoparticles have large surface area, their unique size-dependent properties make these materials superior and indispensable in many areas of human activity. Today Researcher focuses on the testing different applications of these nanoparticles and materials for the human welfare and its development. Applications of nanoscience and nanotechnology can be expected to have a significant impact on sustainable development, influencing virtually all industrial sectors

including healthcare, agrifood, transport, energy, materials, and information and communications technologies (ICT). Our present reliance on fossil fuels for energy and transport, and the by-products and waste from manufacturing industries have a major impact on the environment, leaving areas of land and bodies of water unsuitable for other use, and in the worst cases destroying whole ecosystems. The most recent developments in the field of applied nanomaterials and nanoparticles , in particular their application in biology and medicine, and their pollution control applications such as removal of heavy metals, dyes, phenols, pesticides etc. from the wastewater.

AO-CYSA-01 : Seasonal Variability of Chemical Constituents in Particulate Matter and their Effects on Light Extinction

Atar Singh Pipal[1], Rohi Jan[2] and P. Gursumeeran Satsangi[2*]

[1]Space and Atmospheric Sciences Division, Physical Research Laboratory, Ahmedabad, 380009
[2]Department of Chemistry, S. P. Pune University, Pune-411007
E-mail : aspippal@gmail.com

Atmospheric particulate matter is a diverse mixture of many various chemical constituents originating from an assortment of natural and anthropogenic sources. The present study has been conducted to characterize atmospheric aerosol particles in terms of carbonaceous species and ionic constituents for a yearlong period at Pune, India. This study provides the evidence for the ionic chemistry, secondary aerosols formation, temporal variability and its climatic effect in the atmosphere. The average concentrations of $PM_{2.5}$ and PM_{10} were 110 ± 23.2 and 167 ± 4 μg m^{-3}, respectively, by far exceeding National Ambient Air Quality (NAAQ) and World Health Organization (WHO) standards. Seasonal analyses indicated that $PM_{2.5}$ and PM_{10} mass concentrations were higher in the post-monsoon followed by the winter season and lower during the monsoon period. The average concentrations of organic carbon (OC) and elemental carbon (EC) were 32 ± 7.4 and 4.2 ± 2.4 μg m^{-3} for $PM_{2.5,}$ while, 34 ± 6.2 and 5.0 ± 2.3 μg m^{-3} for PM_{10}, respectively. OC and EC data splits into seasons and their mass loadings were in the order of post-monsoon > monsoon > winter > summer for OC and for EC, it was as winter > post-monsoon summer > monsoon. The overall chemical analysis revealed that particulate matter (PM) consist higher concentrations of OC followed by cations and the lowest one is EC. The ionic composition analysis indicated that cations were the abundant parts of PM in comparison to anions and Na^+ and SO_4^{2-} were at a higher concentration amongst

all the ionic species. The estimated light extinction coefficient (b_{ext}) of the aerosol particle signified that the OC is the higher (45%) contributor for light extinction coefficient followed by EC (18%), $(NH_4)_2SO_4$ (17%), coarse (12%) and lower was NH_4NO_3 (8%). Trajectory analysis indicated that the air masses appear as a result of long-range transportation during summer and monsoon period while during the winter and post-monsoon seasons local manmade activities showed dominant influence.

AO-CYSA-02 : NOx Sensing Response of Pristine WO_3 and WO_3@ Graphene at Room Temperature

Amruta Rathi, Parag V. Adhyapak* and I. S. Mulla

Dept. of Nanoscience and Nanotechnology, Centre for Materials for Electronics Technology (C-MET), Panchwati, Off Pashan Road, Pune-411008 (Maharashtra)
E-mail : adhyapakp@yahoo.com, adhyapak@cmet.gov.in

WO_3 has emerged as an outstanding nanomaterial for gas sensing applications. Herein, we report synthesis of WO_3 using two different capping agents such as oxalic acid and citric acid. The effect of capping agent on the morphology of WO_3 material was investigated. The WO_3 materials were characterized by using XRD, FETEM, FESEM, particle size distribution analysis and UV-Visible spectroscopy etc. The WO_3 obtained from both the capping agents were used to study their gas sensing response particularly for NOx gas. The sensing response towards interfering gases such as; ammonia, acetone, ethanol, methanol and triethylamine was also monitored. Further, the composites of WO_3 were prepared with graphene by physically mixing.The composites were tested for sensing at room temperature as well as at 50Ú and 100ÚC. It was concluded that the citric acid assisted WO_3 material exhibits better response towards NOx sensing. The sensitivity of the pure WO_3 material was better than the composite towards NOx gas. All the products showed quick response (in secs) towards NOx gas; however the recovery time was in few minutes.

AO-CYSA-03 : Silver Doped TiO_2 Nanoparticles based Sensor for Clozapine Detection

Nagaraj P. Shetti[1*], Deepti S. Nayak[1], Shweta J. Malode[1] and Raviraj M. Kulkarni[2]

[1]Department of Chemistry, KLE Society's K. L. E. Institute of Technology, Hubballi-580030, Affiliated to Visvesvaraya Technological University, Belagavi, Karnataka
[2]Department of Chemistry, K. L. S. Gogte Institute of Technology (Autonomous), Affiliated to Visvesvaraya Technological University Belagavi-590008, Karnataka

In the current work, silver stood a conspicuous dopant for TiO_2

nanoparticles, to enhance its catalytic activity. Silver doped TiO_2 nanoparticles were synthesized by liquid impregnation method. The characterization of synthesized nanoparticles was accomplished by utilizing XRD, SEM, EDX and TEM analysis. Further, we established the electrochemical behavior and detection of an atypical antipsychotic drug, clozapine (CLZ) by utilizing silver doped TiO_2nanoparticles modified carbon paste electrode (Ag-TiO_2/CPE) at pH 4.2 by employing different voltammetric techniques. Modification enhances the electro-oxidation of clozapine with increased current intensity.The influence of parameters like scan rate, pH, accumulation time, amount of the modifier and concentration on the peak current of the drug were studied.The effect of CLZ concentration variation was studied using square wave voltammetric (SWV) technique and got lowest detection limit compared to reported techniques. The fabricated sensor was employed for the determination of clozapine in pharmaceutical and biological samples.

AO-CYSA-04 : Role of Chemical Constituents of Aerosols in Radiative Forcing Over the Indo-Gangetic Basin

Pratima Gupta[1], Ashok Jangid[2] and Ranjit Kumar[1*]

[1]Department of Chemistry and Computer Science, Faculty of Science Dayalbagh Educational Institute (Deemed University) Dayalbagh, Agra-5
[2]Department of Physics and Computer Science, Faculty of Science Dayalbagh Educational Institute (Deemed University) Dayalbagh, Agra-5
E-mail : rkschem@rediffmail.com

Aerosols are ubiquitous in nature and known for their effects on radiative forcing, climate change, visibility impairment and human health. The effect of aerosols depends upon physical, optical and chemical properties of aerosols. Chemical constituents of aerosols play very important role as even shape and size of aerosol particle depend upon chemical constituents and chemical processes. The nature of organic and inorganic components alters the scattering and absorption of radiation by aerosol. The mass concentrations of PM_{10}, $PM_{2.5}$, $PM_{1.0}$, BC (black carbon) and AOD have been measured at a sub-urban site in Agra over the Indo-Gangetic basin. The concentration of PM_{10} and $PM_{2.5}$ are much higher than the standard set by WHO, USEPA and NAAQS. The level of $PM_{1.0}$ is also very high. The chemical analysis of RSPM reveals the alkaline nature of aerosols over the Indo-Gangetic basin, which probably may be due to soil contribution.The black carbon concentration is in the range of 5-15 μg m^{-3} which is high amongst cities over the Indo-Gangetic basin. The AOD value is also greatly high. The concentration of sulphate and black carbon

encounters the aerosol radiative forcing as black carbon causes positive forcing while sulphate causes a negative radiative forcing. Aerosols chemistry and meteorology play an important role in effects of aerosols.

AO-CYSA-05 : Enhancement of Degradation of Ponceau S Using Ultrasonic, Sonocatalytic, Photocatalytic and Sonophotocatalytic Degradation in Presence of ZnO and Fe Doped ZnO Nano Catalyst

Vilas K. Mahajan and Gunvant H. Sonawane*

Department of Chemistry, Kisan Arts, Commerce and Science College, Parola, Dist.- Jalgaon- 425111 (M.S)
E-mail : mahajanvilas10@gmail.com.

Fe-doped ZnO nano catalyst was synthesized by co-precipitation method. The intrinsic characteristics of a prepared nano Fe-doped ZnO catalyst were studied using a variety of techniques including powder X-Ray diffraction (XRD), scanning electron microscope (SEM) Electron dispersive X-ray spectroscopy (EDS). In this study, degradation of Ponceau S as a dye pollutant was investigated in the presence of ZnO and Fe-doped ZnO nano catalyst using sonolysis, photocatalysis, sonocatalysis and sonophotocatalysis. The UV light and ultrasonic probsonicator at 20 kHz and 150 W powers were used as an irradiation source. The effect of H_2O_2 on sonocatalytic, photocatalytic and sonophotocatalytic degradation was investigated. At optimum conditions the dye degradation efficiency was influenced by addition of H_2O_2, the highest dye degradation was obtained as 98% by US+UV+Fe-doped ZnO+H_2O_2. The experimental kinetic data followed the pseudo-first order model in doped and undoped sonocatalytic, photocatalytic and sonophotocatalytic processes but the rate constant of sonophotocatalysis is higher than sonocatalysis and photocatalysis process. The sonophotocatalysis was always faster than the respective individual processes due to the more formation of reactive radicals as well as the increase of the active surface area of nano catalyst.

AO-01 : Removal of Fluoride from Aqueous Solution by Low-Cost Activated Carbon Prepared from Jackfruit

K. A. Emmanuel[1*] and T.V.Nagalakshmi[2]

[1]Department of Chemistry, Sir C. R. Reddy Autonomous College, Eluru-534 007, A.P.
[2]Department of Chemistry, LakiReddy BaliReddy College of Engineering, Mylavaram -521230, A.P.
E-mail : kaekola@gmail.com

Fluoride is a persistent and non-biodegradable pollutant that

accumulates in soil, plants, wildlife and human beings. Therefore, knowledge of its removal, using the best technique with optimum efficiency, is needed. In this present study removal of fluoride by low cost Activated carbon prepared from Jackfruit (JFC). Batch sorption studies were executed and the results showed that the ability to adsorb the fluoride. The adsorption of fluoride from aqueous solutions was evaluated with respect to various experimental parameters including pH, adsorbent dose, contact time, agitation time, initial fluoride concentration and temperature were investigated. Sorption interaction of fluoride onto JFC obeyed the first order rate equation. Experimental results showed good fit with the Langmuir's adsorption isotherm model. The removal of fluoride was found to be dependent on the pH of the aqueous solution and the adsorption of fluoride was observed to be greater at pH 7. Maximum fluoride sorption was observed at operating 30^0C operating temperature. Considerable changes in the FT-IR spectra was observed after fluoride sorption which is investigative of the involvement of surface functional groups associated with hydrogen atoms in the carboxylic groups in sorption interaction.

AO-02 : Household Waste Water and Associated Problems in Balajipuram Area of Mathura City

Nisha Rathor

Department of Chemistry, K. R. College, Mathura
E-mail : nisharathorkr@gmail.com

In modern civilization, a large number of new cities and towns have come up and the existing towns have grown, as a result of which household wastewater treatment plants have become necessary. An efficient wastewater disposal is important to the health of any community. Effective collection and treatment of wastewater is a critical problem especially in developing countries like India. Nitrogen in wastewater is present either as ammoniacal nitrogen and originally bound nitrogen derived from proteinaceous matters. The ammoniacal nitrogen constitutes about 50-70% of the total nitrogen. The domestic wastewater contains large amount of urine, which consists of about 2.5 % urea, 1 % NaCl and other complex organic substances. The wastewater also includes many inorganic substances such as nitrates and phosphates of detergents and Na^+, K^+, Ca^{++}, Cl^-, HCO_3^- ions, etc. Present day wastewater contains appreciable amounts of synthetic detergents. In addition to surface active agents, they also contribute phosphates of sodium and other builders. The wastewater also includes biodegradable faeces, animal wastes and certain household waste in the form of

organic compounds such as fats, carbohydrates, proteins, etc. As seen previously some of these matters are carried in suspension, others are taken into true solution, still others become so finally divided that they possess the property of colloidal i.e. dispersed, ultramicroscopic particles. There are two important types of bacteria which are present in the sewage in very high quantity. These bacteria are saprophytic &pathogenic in nature. Saprophytic bacteria are harmless and feed upon dead organic matter. A pathogenic bacterium causes disease in man and animals. A large portion of the wastewater of houses is organic in nature and because of its high energy value it is subject to attack by saprophytic bacteria or micro-organism. Household wastewater is therefore unstable, decomposable and may give rise to offensive odours, notably those of H_2S and other objectionable conditions associated with decomposition. Pathogenic bacteria such as Vibrio choleri (causes cholera), Salmonella typhi (causes typhoid) and Shigelladysenteriae (causes bacillary dysentery) are either discharged by persons harbouring intestinal parasites or suffering from infectious diseases (such as typhoid, paratyphoid dysentery and other gastrointestinal infections). Due to water logging the most frequently reported diseases in the study area are malaria, dengue, dysentery, jaundice and typhoid. Balajipuram area of Mathura city has taken as a study area. The aim of present paper is to examine the release of household wastewater and its associated problems. The paper also shows some of the important findings and suggestions.

AO-03 : Solar Photocatalytic Degradation of Rhodamine 6G over Cd-doped Zinc Oxide

Ashokrao B. Patil[1,2] and Satish K. Pardeshi[1*]

[1]Department of Chemistry, Savitribai Phule, Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
[2]Department of Chemistry, K. M. C. College, Khopoli (Affiliated to Mumbai University) Pin-410203
E-mail : skpar@chem.unipune.ac.in

$Cd_xZn_{1-x}O$ (x = 0.05 to 0.2) crystallites were synthesized by two steps, solution free-mechanochemical method. In order to obtain photocatalyst of different morphology and crystallite size, calcination temperature was varied from 400 to 800æ%C. These photocatalysts are then characterized by XRD, XPS, SEM, EDX, FT-IR, PL and UV-Visible spectrophotometer. The minimum possible calcination temperature at which $Cd_xZn_{1-x}O$ materialize from corresponding precursor is determined by TG-DTA analysis. X-ray diffraction data suggest that the obtained $Cd_xZn_{1-x}O$ crystallites are of wurtzite

structure and the XRD data of these samples matches to that of JCPDS card No. 36-1451. The XPS study supports incorporation of Cd^{2+} in Cd-doped ZnO samples. UV-visible spectra imply lowering of band gap energy of Cd- doped ZnO as compare to bare ZnO. The lowering of band gap energy helps to absorb more photons which lead to generation of more electron–hole pairs. The PL spectra suggest that the more number of oxygen vacancies exist in $Cd_xZn_{1-x}O$ as compare to that in pure ZnO. Photocatalytic activity of $Cd_xZn_{1-x}O$ was checked by means of oxidative photocatalytic degradation (PCD) of Rhodamine 6G under irradiation of sunlight in a batch photoreactor. The PCD efficiency was found to be dependent on crystallite growth rate and morphology of $Cd_xZn_{1-x}O$. The PCD efficiency of $Cd_xZn_{1-x}O$ was found to decrease with increase in calcination temperature as the particle size was increased. In addition to effect of calcination temperature, the influence of various other parameters such as photocatalyst amount, initial concentration of Rhodamine 6G and pH was also examined for maximum PCD of Rhodamine 6G.

AO-04 : Radon and Thoron Study in Some Dwellings of Nagaland State with DTPS and DRPS

Dipak Sinha*

Department of Chemistry, Nagaland University, Lumami-798627, Nagaland
E-mail : dipaksinha@gmail.com

There has been an increasing concern regarding exposure to radon (^{222}Rn), thoron (^{220}Rn) and their progeny due to their detrimental effects on human health. In fact, out of 98% of the average radiation dose received from natural sources, about 52% is due to breathing of radon, thoron and their progeny present in dwellings. There have been several studies on radon and thoron measurements by several authors using passive methods. It had been the usual practice to calculate both the Radon and Thoron progeny concentration from the measured gas concentration using an assumed equilibrium factor. However, this process of progeny concentration estimation involves a lot of uncertainty especially in the case of thoron progeny. Thus in order to provide a realistic assessment of these species in the indoor environment, it is necessary to conduct direct measurements of radon and thoron progeny, since inhalation doses are predominantly due to decay products of radon and thoron, and not due to the gases themselves. With the development of Direct Thoron Progeny Sensor (DTPS) and Direct Radon Progeny sensor (DRPS), one can measure the progeny concentration directly with these detectors. These are

passive solid state nuclear track detectors (SSNTDs) mounted with energy degrader foils of suitable thicknesses so as to selectively register the alpha particles emitted from deposited progeny atoms (developed by Radiological Physics and Advisory Division of BARC). Present paper is an initial report about the study carried out in some dwellings of Nagaland. The measurement shows that the mean Radon progeny concentration ranges in between 1.85 Bq/m^3 to 10.68 Bq/m^3 and for thoron progeny, the concentration varies in the range 0.06 Bq/m^3 to 2.67 Bq/m^3

AO-05 : Elemental Content and their Bioavailability of Honey Sample from Different Floral Origin

S. M. Hande and Dattatray Phadtare

Department of Chemistry, Haribhai V. Desai College, Pune-411002
E-mail : drsunilhande@gmail.com

In the present work, elemental content and bioavailability of different honey samples were determined. Honey is a natural viscous, aromatic sweet product prepared by honeybees from living parts of plants and is used as food and medicinal purposes. The mineral content in honey may represent the quality of honey.ICP-AES technique was used for the determination of elemental content.The bioavailability of various elements was determined using in vitro method.The physical properties such as pH, colour, conductivity etc. were also determined. The potassium was the most abundant mineral and it showed the concentration from 2.45 to 88.77 ppm. The other elements Na, Mg and Ca are present in moderate amounts whose concentration ranges from 2.80 to 13.06 ppm, 0.56 to 1.77 ppm and 2.57 to 15.55 ppm respectively. During the gastric and gastrointestinal digestion, Na and Ca found to be more bioavailable than K and Mg.This preliminary research provided the groundwork for further studies of Indian honey using other techniques like HPLC, FTIR.

AO-06 : Graphene and Graphene Oxide : Applications and Future Perspectives

Ranjita Das, Atul Wankhade and Anupama Kumar

Chemistry Department, Visvesvaraya National Institute of Technology, Nagpur-440010.
E-mail : drkumaranupama@rediffmail.com; atulwa2006@yahoo.co.in

Graphene is one of the most promising nano-materials because of its unique combination of excellent properties, which opens a way for its exploitation in a wide spectrum of applications in the fields of physics, chemistry, biotechnology, material science as well as medical science. Graphene is the mother element of graphite,

fullerenes and carbon nanotubes. Graphene oxide (GO) is the functionalized form of Graphene with oxygen-containing chemical groups. Graphene and GO exhibits a wide range of unique physico-chemical properties such as good electrical and thermal conductivity, mechanical flexibility, low thermal expansion coefficient and optical transparency. These versatile features have added a revolutionary discovery in the field of both academics and industries showingwide range of applications in energy production and storage, nanocarrier in drug delivery, wastewater treatment, and adsorptive remediation for emerging pollutants and also used in electronics, sensors and bio devices. Present work reports the recent advances of Graphene based nano-composites, its synthetic aspects and its applications in the field of environmental science. These materials are useful in removing the environmental pollutants which is an emerging key issue in wastewater treatment.The recent trends in Graphene research along with its applications and future directions in which the field is also reported.

AO-07 : Enhance Ultrasonic, Photocatalytic and Sonophotocatalytic Degradation of Safranine by using Nb_2O_5 Nano Catalyst

Gunvant H. Sonawane

Department of Chemistry, Kisan Arts, Commerce and Science College, Parola, Dist-Jalgaon-425111 (M.S)
E-mail : drgunvantsonawane@gmail.com

The ultrasonic, photocatalytic and sonophotocatalytic degradation of Basic Red-2 accompanied by Nb_2O_5 nano catalysts were studied. The structure and morphology of synthesized Nb_2O_5 nano catalyst was investigated using scanning election microscopy (SEM), Electron dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD).The effects of various experimental parameters such as the Basic Red-2 concentration, catalyst dose, pH and addition of H_2O_2 on the ultrasonic, photocatalytic and sonophotocatalytic degradation were investigated. Photocatalytic and sonophotocatalytic degradation of Basic Red-2 was strongly affected by initial dye concentration, catalyst dose, H_2O_2 addition and pH. Basic pH (pH-10) was favored for the ultrasonic (US), photocatalytic (UV+ Nb_2O_5) and sonophotocatalytic (US+UV+Nb_2O_5) degradation of Basic Red-2 by using Nb_2O_5 nano catalyst. The ultrasonic degradation of Basic Red-2 was enhanced by the addition of photocatalyst. Then, the effect of Nb_2O_5 doseon photocatalytic and sonophotocatalytic degradation were studied, and it was found that increase in catalyst dose increase in the percentage degradation

of Basic Red-2. In addition, the effects of H_2O_2 on ultrasonic, photolytic, photocatalytic and sonophotocatalyticdegradation was also investigated, and it was found that H_2O_2 enhances the % degradation of Basic Red-2. The possible mechanism of ultrasonic, photocatalytic and sonophotocatalytic degradation of Basic Red-2 reported by LC-MS shows generation of different degradation products.

AO-08 : Spectrophotometric Determination of Trace Amount of Paraquat Herbicide in Environmental and Biological Samples

Madhurani Shukla and Kishore K. Tiwari*

Government Nagarjuna P.G. College of Science, Raipur-492010 (C.G.)
E-mail : kishoretiwari2003@yahoo.com

A highly sensitive spectrophotometric method is developed for the determination of trace amount of broadly used herbicide paraquat using mild reducing agent D-galactose is described. Paraquat is reduced with D-galactose in an alkaline medium and produces a blue radical ion. The absorption maximum of this blue radical ion is measured at 600nm. The colour system obeys Beer's law in the range of 0.04-0.4 µg ml^{-1} of paraquat. Sandell's sensitivity and molar absorptivity for the method were found to be 0.00041µg cm^{-2} and 6.23×10^5 L $mol^{-1}cm^{-1}$ respectively. The analytical parameters such as time, temperature etc. have been optimized for obtaining complete colour reaction. This method is free from the commonly used pesticides interferences. The proposed method was successfully applied for the determination of paraquat in various environmental and biological samples.

AO-09 : Effect of Furfuraldehyde on the Polymerization of Acrylonitrile Initiated by Benzoyl Peroxide

Gyan Singh and R. K. S. Dhakarey*

University Department of Chemistry, Institute of Basic Sciences, Khandari, Agra.
E-mail : singhsinghgyan@gmail.com

Polyacrylonitrile is a synthetic, semicrystalline organic polymer resin, with the linear formula $(C_3H_3N)_n$. PAN is one of the versatile polymers that is widely used for making membranes due to its good solvent resistance property. It has been used as a substrate for nanofiltration (NF) and reverse osmosis (RO). The thermosetting characteristic offered by PAN makes it suitable as a carbon membrane precursor. It usually does not liquefy or soften during any stage of pyrolysis and preserves its morphology upon the

pyrolysis. 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.

AO-10 : Effects of Different Chemicals and Probiotic on the Blood Biochemistry Profile of Living Species

Raj Ranjan Jha

P. G. Deptt. of Chemistry, Ranchi University, Ranchi (Jharkhand)
E-mail : rajranjanjha@yahoo.co.in

In recent years the inorganic constituents in biological system have been receiving increasing attention. One of the major roles played by metallic element in biochemistry is in metaloenzymes and in the enzyme catalysis. The role of the metal atoms in enzymic catalysis is currently an active subject of research. The trace elements unquestionably play an important role in Pathology and Physiology of biological system. Therefore, the effect of probiotic bacterial culture and mineral mixture individually or in ‘combination was studied in 30, apparently healthy weaned rabbits of 6 weeks of age. At 6^{th} week of age, all the rabbits were randomly divided into five groups. Each group was having 6 rabbits. Group G_1 was considered as control group maintained on basal diet without probiotic and mineral mixture. G_2 and G_3 groups were supplemented with 2% and 4% mineral mixture, respectively along with basal diet. Group G_4 was supplemented with 60g probiotic along with basal diet whereas G_5 group was supplemented with 60g probiotic and 2% mineral mixture along with basal diet. The present results showed that rabbits of G_5 and G_4 groups had significantly higher total serum protein values compared with the other dietary treatments. Glucose level was observed highest in the G_5 group followed by G_4 group. The total serum cholesterol level was reduced significantly in treatment groups as compared to control group suggesting that these feed supplements may reduce the cholesterol level and may be helpful in preventing atherosclerosis or other cardiac diseases. The highest level of lipid in blood of rabbit was observed in G_5 group. They were in their physiological level indicating that supplementation of probiotics/ yeast culture and mineral mixture did not change the ratio of these minerals in the blood. It further supported that these feed supplements have no adverse effect on kidney. The rabbits of G_3 group had higher body weight than G_2& G_1 groups during experimental period.

AO-11 : Geochemical Examination of Groundwater in Amaravathi River Basin of Karur District (Tamilnadu) and Removal of Pollutants by GO Nanoparticles

K. Loganathan[1] and A. Jafar Ahamed[2*]

[1]Department of Chemistry, Vivekanandha college of Arts and Sciences for Women (Autonomous) Affiliated to Periyar University, Tiruchengode – 637 205, Tamilnadu
[2]Post Graduate and Research Department of Chemistry, Jamal Mohamed College (Autonomous) Affiliated to Bharathidasan University, Tiruchirappalli – 620 020, Tamilnadu
E-mail : agjafar@yahoo.co.in, chemistrylogu@gmail.com

Groundwater resources support many urban, rural and remote communities around India. Aquifers are a source of water for drinking, irrigation, stock supply, bottling and many other uses. Monitoring provides data on groundwater quantity and quality and is an integral aspect of groundwater management. Twenty-four groundwater samples were collected, processed, and analyzed for various physico-chemical parameters such as pH; electrical conductivity; total dissolved solids; total hardness; cations such as calcium, magnesium, sodium, and potassium; anions such as bicarbonate, chloride, sulfate, fluoride, nitrate, and phosphate in the laboratory using the standard methods given by the American Public Health Association. Specifically, we investigated trace metals like cadmium (Cd), lead (Pb), copper (Cu), zinc (Zn), manganese (Mn), nickel (Ni), iron (Fe), and chromium (Cr) using Atomic Absorption Spectrophotometer (Perkin Elmer A analyst 400). The plan of nanostructured adsorbents with controlled functionalities offers new possibilities to tackle the low adsorption capacity or efficiency problems because of their high specific surface areas and enhances active sites. Adsorption capacity of graphene oxide (GO) nanoparticles was confirmed by XRD, SEM, FTIR and EDS techniques. The treatment process of the groundwater sample using carbon nanomaterial (in mg) show a positive result for reducing the excess metal ions (Cd and Pb), in addition to various other water quality parameters.

AO-12 : A Module Designed-Arsenic Removal Filter for Rural Community

Kalpna Kumari

Deptt. of Chemistry, B.P.S. College Desari, B. R. A. Bihar University, Muzaffarpur.
E-mail : kalpna.chemistry@rediffmail.com

The problem of arsenic intoxication by contaminated drinking water emerged in the past two decades, when surface water and

ground water from open dug Wells and tube well formerly used to cover the drinking water supply in rural areas of many tropical regions. As documented chromic arsenic exposure can lead to severe health problems such as hyperkeratosis, Melanesia, skin cancer and cancer of internal organs. Arsenic pollution of ground water has been recognized in the ganga region of bihar. The ground water of numerous households in this region is not only contaminated by arsenic but it also contains high iron concentration. Arsenic removal is necessary in urban and communal water as well as in areas pumping ground water through family based tube well. Therefore I have investigated the arsenic removal household filter for rural communities. The arsenic bio-sand filter (ABF) comprises of two removal unit a) the arsenic removal unit consists of the metal diffuser box, citrus sinensis skin powder and a polyester cloth b)the pathogen removal unit consists of sand and gravel layers. Arsenic removal is governed by the precipitation of iron (hydr) oxides, which forms a coating on the sand's surface. Arsenic then adsorb to the iron (hydr)oxides and forms complex compound with citrus sinensis skin which forms a coating on polyester cloth filter and also sand surface. The arsenic removal efficency of (ABF) filters was examined from 10 samples collected from 10 sampling stations. Arsenic removal efficiency of 80% was achieved in ground water containing 10-21(ppb)and iron 0.75 to 3.50 mg/l. High iron concentration clearly enhance arsenic removal .ABF filters use locally available materials and are operated without chemicals can treat a reasonable amount of ground water within a short time and can be easily replicated by the affected communities.

AO-13 : Synthesis of La_2O_3 Nanoparticles using Glutaric Acid and Propylene Glycol for Future CMOS Applications

Amanullakhan A. Pathan, Kavita R. Desai and C.P. Bhasin*

Department of Chemistry, Hemchandracharya North Gujarat University,Patan- 384265.
E-mail : cpbhasin@yahoo.com

This Research paper deals with the preliminary studies on synthesis and characterization of lanthanum oxide (La_2O_3) nanoparticles by Pechini method but using different reactant (Glutaric acid and Propylene glycol). FTIR spectroscopy was done for observing the presence of La-O bond. The synthesized lanthanum oxide nanoparticles were characterized by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) for morphological and particle size determination. The average particle size was shown near 56-60 nm. Thermals

analysis was done by TG-DSC Analyzer. Lanthanum oxides exhibit some important applications such as luminescent devices, sensors, up-conversion materials, and catalytic fields. The research focuses now on so- called “higher-ê” materials with a dielectric constant of above 30 in order to satisfy the demands for future CMOS applications.

AO-14 : Efficient Energy Storage in Te-rGO Medium

Ashiwni Alegaonkar and Satish Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
E-mail : skpar@chem.unipune.ac.in

We report on efficient energy storage medium character of Te-rGO having specific capacitance around 300F/g. Initially reduced graphene oxide (rGO) was prepared by modified hummer’s method following this Tellurium (Te) was incorporated into rGO. These samples were subjected to various characterization techniques such as Raman, XPS, SEM, and TEM. Analysis revealed that Te has been incorporated successfully in rGO. The obtained samples were subjected to electrochemical analysis. Te-rGO electrode was developed and capacitance voltage (CV) measurement was performed over different scan rates. In addition the measurements were performed for fix number of cycles. Analysis revealed that specific capacitance of Te-rGO attained high value around 320 F/g at scan rate of 10mv/s. As a result Te-rGO seems to be potential candidate for electrolytic cell application.

AO-15 : 2,4 Dihydroxy -5-Iodo-α-Phenyl Acetophenone Oxime [DHI-α-PAO] as an Analytical Reagent : Studies on Co(II) Chelate

Nitinkumar B. Patel

Shree Jayendrapuri Arts & Science college, Bharuch (Gujarat)
E-mail : nitinkumarpatel.324@gmail.com

2,4-Dihydroxy-5-Iodo-α-phenyl acetophenone oxime has been used as an analytical reagent for the gravimetric and spectrophotometric determination of Co(II) at pH 9.0. The Beer's law is obeyed up to 31.12 ppm of Co(II) ion at 510 nm. The molar absorptivity of complex at 510 nm is found to be 4.37 x 10^2 lit $mol^{-1}cm^{-1}$ and Sandell’s sensitivity is found to be 0.1347 µg/cm^2. Job’s method of continuous variation and Yoe and Jones mole ratio method had reveal the metal:ligand ratio in the complex to be 1:2. The stability constant determined spectrophotometrically and Gibb’s free energy change for complex formation reaction also been

calculated and found to be 3.63 x10^9 and -13.124 k.cal/mol respectively. From TGA studies, the energy of activation for the decomposition step has been calculated using Broido method. It was found to be 10.70 & 11.40 k.cal/mol for step-I & II respectively. The reagent has been characterized on the basis of elemental, IR, UV and NMR spectral studies. The reagent has been successfully applied to the determination of Co(II) in cobalt metal sample.

AO-16 : 2,4 -Dihydroxy -5-Bromo Hexaphenone Oxime (DHBHPO) as an Amperometric Reagent : Simultaneous Determination of Cu(II) and Ni(II) in Alloy

Pratesh J. Shah

Shree Jayendrapuri Arts and Science College, Bharuch (Gujarat)
E-mail : pratesh.shah@gmail.com

Cu(II) and Ni(II) forms coloured 1:2 (metal : ligand) complex with DHBHPO at pH 4.5 and 8.5 respectively. Half wave potential was found to be -0.118 v (Vs SCE) at 4.5 pH for Cu(II) and -1.05 v (Vs SCE) at 8.5 pH for Ni(II). Half wave potential for the reagent DHBHPO was determined for both the pH and found -1.3 v (Vs SCE) at pH 4.5 and -2.3 v (Vs SCE) at pH 8.5. Thus it was possible to titrate Cu(II) at -0.4v(Vs SCE) and Ni(II) at -1.5v (Vs SCE) with standard ethanolic solution DHBHPO , amperometrically.Cu(II) aliquots containing 1.589 to 7.79 mg and Ni(II) aliquots containing 1.470 to 5.870 mg was determined with fair accuracy. Interference of foreign ions was studied.The German Silver alloy was analysed for Cu(II) and Ni(II). Weighed sample was dissolved in nitric acid and diluted to 250 ml. A 5 ml aliquot of the stock solution was pipette out in polarographic cell. To this 20 ml acidic buffer and 1.5 ml 0.2% gelatine solution was added. This solution was deoxygenated by passing nitrogen gas. The current was measured at -0.4v (Vs SCE) and standard solution of ligand was added in 0.5ml increment. The titration was continued until the current reading remained constant, indicates equivalent point for Cu(II). Then the cell voltage was raised to -1.5v (Vs SCE) and pH of the solution was raised about 8.5. Titration continued after deoxygenation, until the constant current reading obtained. Cu(II) and Ni(II) content found , agreed well with the results obtained with standard gravimetric method.

AO-17 : Antibacterial Activity of Nano Mixture of W-ZnO and W- $Zn_5(OH)_6(CO_3)_2$ with Ordinary Saliva Samples

Vinutha H. R, Malathi Challa*, Sweekruthi, V. Sravanthi and Lakshmi Narayani. R.

Department of Chemistry,MSRIT, Bangalore
E-mail : maalathichalla@gmail.com

A novel nano mixture of doped W- ZnO and W- $Zn_5(OH)_6(CO_3)_2$ has been synthesized using a simple combustion method where in $Zn(NO_3)_2$. $6H_2O$ is used as a precursor and sodium tungstate as a dopant , Lycopersiconesculentum (tomato extract) as a fuel of V\W% of F\O which have been taken in the ratio of 20:1.The Characteristics peaks of W-ZnO and W- $Zn_5(OH)_6(CO_3)_2$ mixture has been studied using powder X-rd spectrophotometer. The peaks at angle (2è) of 31.7° ;34.4° ; 36.2° are corresponding to (100) (002) (101) along with other peaks47.5°, 56.6°, 62.9°, 66.4°, 67.9°, 72.7° and 77.0° correspond to (102), (110), (103), (200), (112), (201), (004) and (202) planes which are all good agreement with JCPDS-05-0664 [28-31] of nano ZnO. The existing additional peaks, 21.8°; 24.69°; 38.2°; 40.45°; 41.25°; 51.89°; 53.85° and 64.9° correspond to (111) (310) (020) (401) (021) (510) (312) (330) (810) (023) planes respectively have showed good agreement with JCPDS (19-1458) of nano $Zn_5(OH)_6(CO_3)_2$. The irregular particles size of nano W-ZnO and W- $Zn_5(OH)_6(CO3)_2$ mixture from X-rd peaks and SEM is 30-45 nm. The antibacterial activity of this nano mixture with a variation of dopant concentraton, has been tested with a saliva samples along with negative gram bacteria as a reference in different interval times. It is observed that a drastic increment in antibacterial activity of nano mixture from 11.5 to 17.5 mm of zone of inhibition, when dopant tungsten percentage increases by 0.2 in nano mixture.

AO-18 : Application of New Biosorbent from Abutilan Indicum Leaf Powder in the Removal of Ni(II) Ions from Aqueous Medium : Kinetics and Equilibrium Studies

Ramesh Naik, N.V. Sandeep Kumar, K. Imran, N. Sathish Kumar and K. Seshaiah*

Inorganic and Analytical Chemistry Division, Department of Chemistry, Sri Venkateswara University, Tirupati – 517 502
E-mail : seshaiahsvu@gmail.com

A new biosorbent, iron nanoparticles loaded ash (nFe-Ash) of Abutilan indicum leaf was prepared and studied its application in the removal of Ni (II) ions from aqueous solution. The adsorbent

was characterised by some instrumental techniques like FT-IR, SEM, TEM and XRD. Experimental parameters such as pH, dose, contact time, concentration and temperature were evaluated in batch mode. Maximum biosorption of Ni(II) ions on to the biosorbent was achieved at pH 6.0. The adsorption studies included both equilibrium adsorption isotherms and kinetics. Equilibrium data fitted very well with the Langmuir isotherm model. Kinetics studies showed better applicability for pseudo-second-order model for the adsorbent. The maximum adsorption capacity showed by the biosorbent was 76.12 mg g^{-1}. Desorption and regeneration of the biosorbent was carried out by dil. HCl solution and regeneration studies proved that the biosorbent have promising regeneration potential.

AO-19 : Synthesis, Characterization of Divalent and Trivalent Metal Ions Doped Bismuth Oxide and its Application for Dye Degradation Using Visible Light

N. J. Karale[1], P. A. Nagawade[1], G. S. Gugale[2], M. G. Chaskar[3] and A. K. Nikumbh[1*]

[1]Department of Chemistry, Savitribai Phule Pune University (Formerly University of Pune), Pune 411 007.*
[2]Department of Chemistry, H. V. Desai College, Pune- 411 002
[3]Department of Chemistry, PDEA's Baburaoji Gholap College, Sangavi, Pune – 411027
E-mail : aknik@chem.unipune.ac.in

The undoped and doped oxide such as Bi_2O_3 and $Bi_{1.9}Sm_{0.038}Cu_{0.062}O_3$ are synthesized by tartarate method using their respective salt solutions. The tartarate precursors are then systematically characterized by micro analytical method, infrared spectroscopy and TGA/DTA analysis. The obtained precursors are then decomposed at 650^{0}C for two hour to convert into respective semiconductor oxides and then investigate their structural, electrical and photocatalytic activity. The composition of undoped and doped bismuth oxides is determined by XRF and EDAX spectroscopy method.X-ray diffraction pattern possess single phased with monoclinic structure. The morphology and particle sizes are determined by XRD and SEM measurements, which confirmed the nanosized oxides are formed. The electrical conductivity is increased with increasing temperature. The activation energy found to be extrinsic surface defect migration in the whole temperature range. Thermoelectric power measurements showed n-type semiconductor. In the present investigation, the photodegradation of Victoria blue-B solution by using undoped and doped bismuth oxides under sunlight are studied. The effect of initial dye concentration, amount of oxides, pH, contact time etc. are also investigated.

AO-20 : Adsorption of Methyl Orange from Waste Water by Spent Tea Leaves

Sweety J. Patel and C. P. Bhasin

Department of Chemistry, Hem. North Gujarat University, Patan-384265 (Gujarat)
E-mail : cpbhasin@yahoo.com

The aim of present work was to investigate the ability adsorption of methyl orange dye from wastewater using low-cost adsorbent, spent tea leaves (STL), in batch isotherm adsorption technique. The adsorption experiments were carried out under different conditions of initial dye concentration (50-500) mg/l, STL dose (0.05-1) g, pH solution (2-11), and contact time (10-180) min under constant temperature of 30 C. The results were indicated that the optimum conditions were adsorbent dose was 0.43 g per 100 ml dye solution, pH=7. The equilibrium isotherms have been analyzed using the Langmuir and Freundlich models. The experimental results were best described by the Freundlich isotherm model with maximum monolayer adsorption capacities found to be 62.2 mg/g with the high value of correlation coefficient. The results suggested that STL has high potential 98% to be used as effective adsorbent for MB dye removal.

AO-21 : Adsorptive Removal of Methylene Blue Dye from Artificially Contaminated Water using Cucumissativus Peel Waste as a Low Cost Adsorbent

Abu Nasar*

Department of Applied Chemistry, Faculty of Engineering and Technology
Aligarh Muslim University, Aligarh-202 002
E-mail : abunasaramu@gmail.com

In the present work the applicability of cucumissativus peel (CSP) waste as a low-cost adsorbent for the removal of hazardous methylene blue dye from wastewater was studied. The efficacy of dye removal of the adsorbent is determined by investigating the various parameters such as adsorbent dose, contact time, initial dye concentration, particle size, pH and temperature. The isotherm analysis reveals that the adsorption process can be better described by Freundlich adsorption isotherm indicating the heterogeneous nature of adsorbent surface. Adsorption kinetics was found to obey pseudo-second order kinetics. Thermodynamic data reveals that the adsorption process is spontaneous and exothermic in nature. The values of $\Delta H°$ and $\Delta S°$ have been found to be negative which indicate that the feasibility of process decreases with increasing temperature. The adsorbent regeneration was found to be best obtained in hydrochloric acid. The results indicate that CSP is an efficient low-cost adsorbent for the removal of methylene blue dye from wastewater.

AO-22 : PVC Based Polyaniline/Poly(3,4-Ethylenedioxythiophene) : Polystyrene Sulfonate Zirconium(IV) Phosphate Bending Actuator Membrane

Inamuddin

Department of Applied Chemistry, Faculty of Engineering and Technology, Aligarh Muslim University, Aligarh, Uttar Pradesh-202002

A polyvinyl chloride (PVC) based poly(3,4-ethylenedioxy-thiophene):polystyrene sulfonate zirconium(IV) phosphate (PVC-PEDOT:PSS-ZrP) composite cation exchange membrane was synthesized by solution casting technique and polyaniline (PANI) was coated on the surface of membrane by oxidative chemical polymerization of aniline monomers. The synthesized PANI/PVC-PEDOT:PSS-ZrP composite cation exchange membrane was characterized for physico-chemical properties by various techniques such as thermogravimetric analysis/differential thermal analysis/ differential thermo gravimetry (TGA/DTA/DTG), scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive X-ray (EDX) analysis and Fourier transforms infrared (FTIR) spectroscopy. The membrane was also characterized for ion exchange capacity, proton conductivity, water uptake, water loss and cyclic voltammetry studies. The tip displacement analysis of PANI/PVC-PEDOT:PSS-ZrP composite cation exchange membrane was also carried out. The results showed that fabricated composite cation exchange membrane was able to produces generative forces (tip forces) and hence produced remarkable displacement. Therefore, the proposed composite cation exchange membrane was found appropriate for actuation which will provide an effective and promising platform for micro robotic applications.

AO-23 : Ferric Chloride Catalysis in the Bromination of 2,4-Dinitrophenol and 5-Chlorosalicylic Acid in (90 : 10% v/v) Acetic Acid, Water Mixture Medium

D. Dasharath and Y. B. Vibhute*

Department of Chemistry, Kits for Women, Nizamabad-503002
**Department of Chemistry, Yeshwant Mahavidyalaya, Nanded*

Ferric chloride catalysis in the bromination of 2,4-dinitrophenol and 5-chlorosalicylic acid is investigated in (90 : 10% v/v) acetic acid : water mixture medium at 303°K, keeping the concentration of phenol (0.02M) and bromine (0.02M) constant with and without anhydrous $Fecl_3$. In the absence of any catalyst the reaction is second order, when the concentration of Ferric chloride in the

mixture in increased (From 0.02 to 0.06m) there was a steady increase in the observed k_2.

AP-CYSA-01 : Identification and Mapping of Major and Trace Elemental Pollution in Soil Evolving from Municipal Solid Waste in Dhapa, Kolkata with the Application of X-Ray Fluorescence Spectrometry

P. K. Jee[*1], A. Das[1], D. K. Bandyopadhyay[1] and A. P. Chattopadhyay[2]

[1]Geological Survey of India, Central Headquarters, Kolkata.
[2]Department of Chemistry, Kalyani University, West Bengal.
E-mail : pravasjee@gmail.com

Dhapa area, is part of the famous Kolkata Wetlands, has been the main municipal solid waste (MSW) disposal site for more than 100 years for the entire Kolkata Municipality where more than 95% of the total waste generated is disposed. The soil in this area is expected to be evolving from several layers of dumped waste through many decades and a significant part of the waste is illegally used as compost in adjacent farming activities. In the present study, topsoil samples (depth: about 5-10cm) from twenty different locations were collected for quantitative determination of ten major and minor and sixteen trace elements. Samples were studied using PANalytical PW 2400 WDXRF Spectrometer with certified reference materials as calibration standards for elemental quantification. Potentially high values (max, min, average in ppm) of the metals were found, more particularly Pb (29,980,466); Cr (107,595,304); Zn (189,3071, 1001) and Cu (76,465,330). The relative abundance of the metals are Zn >Mn >Pb >Cu >Cr > Ni. Significant correlation was observed between Pb and Ni (r = 0.85), Cu and Ni (r = 0.94), Cu and Co (r = 0.88) and Pb and Cu (r = 0.86). High values occur particularly where the top soil had evolved with several layers of the raw MSW, whereas lower values were found where conventional agricultural practise is still in use.

AP-CYSA-02 : A Study on Distribution and Bio-Chemical Properties of Aerosols Over the Indo-Gangetic Basin

Shalini Singh and Ranjit Kumar[*]

Department of Chemistry, Faculty of Science, Dayalbagh Educational Institute (Deemed University) Dayalbagh, Agra-5
E-mail : rkschem@rediffmail.com

Atmospheric microbial components are diverse in nature and there is wide variation in their taxonomy, physical, ecological,

behavioral and pathogenic characteristics. The airborne microorganism affects climate and has significant health implications. The culturable airborne microorganism also varies widely and is influenced by meteorological parameters such as temperature, relative humidity, wind speed, solar radiation, time, nutrients and species. The effects of aerosols get exacerbated in the presence of chemical constituents. The concentration of microbial components also depends upon the concentration of particulate matter and sizes. The respirable suspended particulate matter (RSPM) concentration is higher than fine particles ($PM_{2.5}$) while the microbial constituentis high in PM_{10} than $PM_{2.5}$. The bacterial and fungal concentration, characterization/identification and their distribution reveal the presence of pathogenic microbes in the aerosol samples. The bacterial concentration is higher than fungal concentrations in PM_{10} and $PM_{2.5}$ both. Biochemical analysis has been performed to characterize and identify the bacteria. Elemental analysis has revealed the level of heavy metals viz., Pb, As, Co, Ni, Cu and Zn in aerosols which exacerbates the allergenic effects of aerosols. A correlation between microbial components and heavy metals has been also established.

AP-CYSA-03 : Mitigation of Particulate Matter Bound Airborne Microorganisms by Natural Polymer Based Nanofiber

Ritwika Roy[1], Rohi Jan[1], Suman Yadav[1], Sachin Chavan[2] and P. Gursumeeran Satsangi[1*]

**[1]Department of Chemistry, Savitribai Phule Pune University, Pune*
[2]Department of Mechanical Engineering, Bharati Vidyapeeth Deemed University, Pune
E-mail : pgsatsangi@chem.unipune.ac.in, rroyt1988@gmail.com

Indoor particulate pollution is becoming a serious public health concern at global scale and considerable attention has been developed for decreasing the environmental contaminants during last few years. Bio-aerosols which include bacteria, fungi and virus contribute to about 5-34% of indoor air pollution and are linked with various infectious diseases, respiratory diseases and cancer. In this regard nano fibers are an exciting new class of material which becomes very effectual for remediation of microbial contaminants. Therefore, in present study, nano fibers prepared from biodegradable natural based polymer was used for mitigating the microbes present in air. Electro spinning method was used to prepare both CS-PVA and CS-PVA-MMT (3%) nano fibers. The morphological studies of the electro spun mats revealed that uniform bead-free nano fibers were formed with an average diameter of 436 ± 148 and 231 ± 110 nm in CS-

PVA and CS-PVA-MMT. FTIR and XRD results showed the complete and successful blending of the polymers with each other and complete exfoliation of nano clays (MMT) in CS-PVA mixture, as indicated by the absorption peaks corresponding to 469 and 512 cm^{-1} observed in the spectrum of pure MMT and CS/PVA MMT respectively. The mechanical properties of the CS-PVA nano fibers were highly improved by addition of only 3wt% MMT. Antimicrobial activity of both CS-PVA and CS-PVA-MMT assessed by optical density and disc diffusion method showed significant antibacterial properties. Apart from this CS-PVA-MMT showed more antibacterial properties due to the presence of MMT as it enhances the antimicrobial effect of CS. The prepared nano-fibers can be put on windows of offices, schools, buildings, and even in vehicles for remediation of biological components of PM. Therefore, these nano-fibers can be useful for the purpose of mitigating environmental contaminants.

AP-CYSA-04 : The Role of Environmental Epidemiology in Public Health

Kulsoom Koser*, Laxmi Singh and Ajay Taneja

Department of Chemistry, Dr B.R Ambedkar University, Khandari Campus, Agra -282002
E-mail : kulsoom786koser@gmail.com

Environment pollution is the major horrific environmentalism to which we are living today. In case of environment all living being are creating the environmental destructions. Environmental pollution is a major contribution in our daily life, such as air, water, and land. The progress in science and technology is chief to pollute the environment and damage the natural balances. There are so many different pollutions in the environment, these includes water pollution, thermal pollution, land pollution, pesticides pollution, radiation pollution, noise pollution & air pollution. so epidemiology effects our public health such as respiratory diseases in case of respiratory diseases these includes chronic bronchitis, pulmonary emphysema, and bronchial asthma and another is lung cancer, pneumonia, also skin diseases, allergy etc. so the word epimedemiology comes from the Greek epic means “upon” and demos meaning people it is an infectious disease the word epidemiology a word can be used epidemic & endemic should be used to describe disease occurrence in all host species. Epidemiology findings contribute to preventing and controlling health related states or events by providing useful information for directing public health policy & planning about adverse health behavior. When

epidemiology effects our health its primarily evidence is related deaths such as aggravated asthma bronchitis emphysema, lung & heart epidemiological disease evidences indicate that approximately 130000 lung cancer deaths every years. Caused by chronic depiction radioactive gases & deaths. Its symptoms are including change in size, shape, color, or elevation of a mole. Epidemiology finding contribute to preventing & controlling health related states or events by providing useful information for directing health policy & planning as well as information for directing health policy & planning individuals about adverse behavior.

AP-CYSA-05 : Removal of Chromium from Contaminated Water Using Iron Oxide Nanoadsorbent

Dhanraj S. Shirsath and V. S. Shrivastava

Nanochemistry Research Laboratory, G. T. Patil College, Nandurbar-425412, (M.S.)
E-mail : dhanrajshirsath111@gmail.com, drvinod_shrivastava@yahoo.com

The heavy metals pose a serious water pollution problem especially contamination of potable groundwater with heavy metals that cause health hazards also its concentration is high in industrial and sewage wastewater. The main focus of this study to remove heavy metal chromium from contaminated water by using synthesized Iron Oxide Nanoadsorbent (ION). The batch adsorption study was conducted for the removal of chromium along with different parametric studies such as Initial concentration of chromium metals, adsorbent dose, pH, contact time and temperature. The employed ION gives positive results, the adsorption of chromium is very rapid and most of fixation occurs at first 30 minutes. The adsorbent was characterized before and after treatment of Chromium contaminated water, by various techniques such as SEM-EDS, XRD and FTIR. The adsorption kinetics obeys second order kinetic. The result suggests that ION can be beneficial in chromium removal from the contaminated water.

AP-CYSA-06 : Toxicity of Trace Metals Present in Smokeless Tobacco Products

Daud Hussain and R.K.S. Dhakarey

University Department of Chemistry, Institute of Basic Sciences,
Dr. B.R.A. University, Khandari, Agra
E-mail : daudchouhan162@gmail.com

Increase use of Tobacco Products is associated with many health problems; hence there is need for research into the heavy metals

contents of smokeless tobacco products. In this study ten brands of smokeless tobacco products (STPs) commonly used were investigated. Samples collected were analysed for heavy metals concentration by AAS. Over the years the research was focused only on toxic organic components while a little attention is given towards the toxic effects of heavy metals. There is no doubt that organic toxins are responsible for myriads problems effecting human's health but the clinical effects caused by heavy metals in tobacco use cannot be ignored when humans are easily exposed to tobacco products. When these trace metals are present in higher concentration in human body then they causes a number of diseases like oral, lungs, larynx, pharynx, oesophagus, breast, stomach and kidney cancer. This is the leading cause of death in developing countries. Trace metals such as Cr, Cd, Pb, Ni, and Hg were analysed and the concentration of these are above permissible limits. The conc. of these metals i.e. Cr (0.216-0.845), Cd (0.00-0.644), Pb (0-0.522), Ni (0.614-2.014) and Hg (0.031-0.064). The concentration of Chromium and Nickel are above the permissible limit in all the samples.

AP-01 : Electrochemical Synthesis and Evalution of Antioxidant Activity of Copper Oxide Nanoparticles

Pallavi D. Shelke[*1, 2] and Anjali S. Rajbhoj[2]

[1]Department of Chemistry, New Arts, Commerce and Science College, Ahmednagar (MS).
[2]Department of Chemistry, Babasaheb Ambedkar Marathwada University, Aurangabad (MS).
E-mail : anjalisrajbhoj@gmail.com

Copper oxide nanoparticles synthesized by electrochemical reduction method and characterized by XRD, EDX and HRTEM. The resulted particles are long straw and particle size in the range of 5-8 nm. The antioxidant behavior of synthesized CuO nanoparticles was evaluated by scavenging free radicals of 2, 2-diphenyl-1-picrylhydrazyl hydrate (DPPH). The free radical scavenging activity of CuO nanoparticles was monitored by UV–visible spectrophotometer. CuO nanoparticles showed efficient antioxidant activity effect.

AP-02 : Assessment and Impact of Coal Fired Plant Effluents on the Water Quality Around Kanti Thermal Power Station Muzaffarpur

Vijay Kumar

Department of Chemistry, L.S.College, Muzaffarpur, Bihar-842001
E-mail : kvijay2259@gmail.com

Water is a basic need of living beings. Among all their needs,

drinking water gets first priority. Normally if water is fit for drinking, it will be suitable for all purposes. But the coal fired power plant landfills and other disposal practices pollute water quality despite all of their precautionary measures & living beings near power plant face a health risk higher than health standard. The water pollution is harder to recognize until after illness has occurred. In the present work, we have studied quality of water samples from different sampling stations around & inside the thermal power stations. Ten water samples were collected and analyzed for the parameters such as pH, DO, BOD, COD, Chloride, Sulphate, TDS, Na, K, Ca, Mg, Fe etc. To assess the quality of water, each parameter was compared with the standard desirable limit of parameter in drinking water as prescribed by WHO & ISI. Some of the parameters have been found to be in permissible range while some of them were higher than permissible limit. The study indicates that majority of water is Ca-Mg-Fe-Chloride & Sulphate types.

AP-03 : Optimization of Preparative Scale TLC Development

Pawar S. P.[1], Adhyapak M. S.[1], Lingampalle D. L., Nayna Pahade and Ubale S. B.[2]

[1]Department of Chemistry, Vivekanand College, Aurangabad
[2]Department of Chemistry, Deogiri College, Aurangabad
E-mail : adhyapak@vivekanandcollege.edu.in

Preparative Thin Layer Chromatography is widely used for purification of isolated desired species. Satisfactory and reproducible results may not be obtained, specially, for new species. This article describes some findings about the optimization steps practiced for purification of certain medicinal plants. These findings would be useful for other researchers dealing with chromatographic purification procedures.

AP-04 : Adsorption Studies on Granular Activated Carbon for the Removal of Some Selected Pharmaceuticals and Personal Care Products

G. Archana[1], Rita Dhodapkar[2] and Anupama Kumar[1]

[1]Chemistry Department, Visvesvaraya National Institute of Technology, Nagpur[440010
[2]WWT Division, National Environmental Engineering Research Institute, [CSIR], Nagpur[440020
E-mail : drkumaranupama@rediffmail.com, rs_dhodapkar@neeri.res.in

Water contamination by pharmaceuticals and personal care products (PPCPs) has been an environmental issue for the last decade. Most PPCPs accumulate in the environment through human

consumption and excretion, and are often removed ineffectively by wastewater treatment plants which are not designed to manage them. Ultimately these contaminants enter into surface water and rivers, causing environmental water pollution [1]. Amongst the various methods available for removal, adsorption is preferred because it is simple and cost effective. In addition, adsorption does not result in any secondary toxic pollutant which can be more harmful than the parent compound [2-5]. Present study reports the use of commercially available Granular Activated Carbon (GAC) for removal of five finger print PPCPs (acetaminophen ciprofloxacin, caffeine, irgasan and benzophenone). The surface area and iodine value for GAC was 675 m2gm-1 and 725.71 mg g-1respectively. Scanning Electron Microscopy (SEM) analysis indicated rough morphology and microporous nature of GAC with pore diameter between 170.3-250.8(nm) and wide pore size distribution. The % removal for Ciprofloxacin was 46%, for caffeine it was 53%, for acetaminophen it was 80%, 53% for Benzophenone and 74% for Irgasan at optimised dose and time of 25 mg/g and 90 minutes respectively. The study indicates that the use of GAC as tertiary treatment stage in sewage treatment plants (STP) can be an effective and economical way of removing PPCPs.

AP-05 : Analysis of Physico-Chemical Characteristics of Surface Water Samples Collected from West Zone of Central India

Arvind Prasad Dwivedi[1] and Indra Prasad Tripathi[2]

[1]Department of chemistry, Govt. Sanjay Gandhi Smrati College, Sidhi M.P.
[2]Faculty of Science and Environment M. G. C. G. V. Chitrakoot,
Satna-485780 (Madhya Pradesh)
E-mail : adarvindchitrakoot@gmail.com

In the present study we are intended to find out the diffuse chemical pollution in central India on the basis of surface water bodies. We have designed twenty sampling stations district for this study in east zone i.e. Rewa, Satna, Sidhi, Singrauli, Shahdol, Umaria, Katni, Panna, Chhatarpur, Jabalpur ,Mandala, Dindori, Siwani, Chhindwara, Narsinghpur, Hosangabad, Betul, Damoh, Sagar and Bhopal. Various water quality parameters such as temperature, pH, turbidity total hardness, TDS, DO, BOD, COD, nitrate, sulphate and phosphate were determined using standard analytical methods . All the values were compared with the WHO Standard. Seventy five percent (75%) samples of BOD and COD were observed higher than the permissible limit during three different season set by WHO. Temperature, TDS, nitrate, sulphate and phosphate were

found well within the prescribed limit. The access of contamination may be the outcome of high human, industrial and agricultural activities in their locality. Proper Monitoring is needed to avoid anthropogenic contamination.

AP-06 : Synthesis, Structural and Electrical Properties of Rare Earth Transition Metals Perovskite-type Oxides Prepared by the Dicarboxylate Precursor Method

M. D. Sangale, A. K. Deshmukh, K. B. Gavhane and R. R. Pawar

Department of chemistry, R.B.Narayanrao Borawake.College, Shrirampur.
E-mail : mdsangale@gmail.com; sangalemohan@yahoo.com

The homogeneous co-precipitation of dicarboxylate (i.e tartarate, oxalate) of transition metals (Mn^{2+}, Co^{2+} and Ni^{2+}) and rare earths (La^{3+}, Sm^{3+}, Gd^{3+}) are obtained from chloride solutions. The thermal decomposition (TGA, DTG, and DTA) of these precursors showed first dehydration and then decomposition to carbonates followed by rare-transition metal perovskite-type oxides. The formation of the pure rare earth-transition metal perovskite-type oxides is further characterized by chemical analysis, elemental analysis, EDAX analysis, X-ray powder diffraction, d. c. electrical conductivity ,X-ray diffraction patterns for all oxides show a single phasic material with orthorhombic structure except $LaCoO_3$ and $LaNiO_3$. The data of temperature variation of the d.c. electrical conductivity showed a definite kink in the temperature range 464-573 K. The conduction mechanism from 573-760 K are interpreted by a semi metallic type behavior.

AP-07 : Physicochemical Studies on Major Pollutants in Drinking Water in Parola Taluka

P. M. Yeole

Centre for PG Research in Chemistry, Department of Chemistry, R. L. College, Parola-425111.
E-mail : pravinyeole.707@rediffmail.com

In present study the samples of bore wells and wells from various areas of Parola were collected and analyzed to assess the physico- chemical characteristics for drinking water quality.

Water is one of most important components of the environment and it sustains life on the earth. The use of water by human, plant and animals is universal. It is essential for life, health and sanitation. Now days it has become an essential commodity for the development of industries and agriculture. The water required for domestic consumption should posses a high degree of purity and it should

be free from suspended and dissolved impurities; bacteria etc. Due to industrialization, urbanization and agricultural activities and growth of population all the sources of water are either polluted or contaminated. The main sources of water pollutants are uncontrolled disposal of sewage, other liquid wastes arising out of domestic, industrial, agricultural and animal husbandry schemes, deliberate application of insecticides / pesticides. It is therefore necessary that the quality of water should be monitored at regular intervals.

AP-08 : Role of Copper Hexacyaoferrate (II) as a Photocatalyst for Degradation of Erythrosine-B

Paras Tak and Pinki B. Punjabi

Department of Chemistry, PAHER University, Udaipur-313003 (Raj.)
E-mail : parastak2011@gmail.com

It is well known that ferrocyanide ion show photo-labile property. The ferrocyanide ion generates electron on exposure of light, which may be utilized for the photoreduction of dye. In the present work, photo-labile nature of ferrocyanide ion was used for the photocatalytic degradation of Erythrosine B dye. Here, copper hexacyanoferrate (II) was synthesized and further used for this degradation of the dye. Effect of different parameters like pH, concentration, light intensity etc. was studied on the rate of reaction. On the basis of observation, a suitable mechanism for the photocatalytic degradation of Erythrosine dye has been proposed.

AP-09 : Environmental Geochemistry of Sateli Satarda Mine in Sindhudurg District, Maharashtra (India)

Dhananjay N. Kokil and Vikas A. Thakur*

**PG Research Centre, Rayat Shikshan Sanstha's Mahatma Phule A.S.C.College, Panvel. (Affiliated to University of Mumbai)*
E-mail : tha.vikas@yahoo.com

Environmental Geochemistry is the new application of geochemistry to the welfare of human kind is closely related to pollutant hydrogeology and geochemistry. Mineralogical studies of mines are important for understanding the environment because most of ores and minerals are very sensitive to changes in environmental conditions, especially to temperature, humidity and pH. Mining is considered to be one of the major causative activities of environmental degradation. Mining involves removal of soils and extraction of minerals resulting in environmental pollution which degrade the surrounding environment. The effect can be more

detrimental when it results in spreading of hazardous elements. The mine chosen by us as a case study is Sateli-Satarda mines (15^{0}14'30":73"40'00') located in Sindhudurg district . This mine can extract million of tonnes of Iron and manganese ore annually. We carried out analysis with classical methods, advanced instruments including spectral studies to understand geological phenomenon before and after mining. It was observed that Soils are slightly neutral to highly basic (pH 7.5 to 10.0) while water samples are acidic to slightly basic (pH 5.2 to 7.5) . Some of the representative results of analysis ICP-AES are: Soil inside Mine shows (%) Al- 2.79-6.39, Cr- 0.019-0.057, Fe- 64.42-82.87, Mn- 0.356-6.224, Cu-0.002-0.008,Ni-0.009-0.013,Zn-0.005-0.008 and S-0.02-0.04. Water analysis shows (ppm), Al- 2.92-81.753, Cr-0.09-0.357, Cu- 0.234-2.088, Fe- 7.796-37.292, Si-0.751-8.006, ; Mn-0.166-7.45, Ni-0.06-0.242, Pb- 0.374-1.823, Zn- 0.563-22.84 and S-12.343-45.314. In Spectral studies, X-Ray Fluroscence technique have shown the presence of Fe, Si, Al, Mn, Ni, Pb, Cr, Cu, Zn and S. FT-IR spectroscopic investigation carried out in the range of 4000-500 cm^{-1} and Far IR in the range of 600-100cm^{-1} confirm the presence of haematite ($2Fe_2O_3$), and pyrolusite($2MnO_2$) . Therefore the studies carried indicate significant effect of heavy and toxic metals on the surrounding environment of Sateli-Satarda mines.

AP-10 : The Study on Physico-Chemical Parameters of Ground Water of Coastal Villages of Olpad and Choryasi Taluka of Surat District, Gujarat (India)

F. T. Patel*, G. M. Malik and A. S. Patel

Department of Chemistry,Navyug Science College,Rander Road Surat-395009(Gujarat)
E-mail : falupatel49@yahoo.in

Ground water samples were collected from different sampling stations of coastal villages of Olpad and Choryasi Taluka of Surat district,Gujarat(India).The Ground water samples from 20 sampling stations of coastal villages of Olpad and Choryasi Taluka for their physico-chemical properties were evaluated. The study for the period of May 2015 to April 2016 was carried out. The analysis of samples for pH, colour, odour, temprature, alkalinity, sulphate, COD, DO, TS, TSS, TDS, hardness, Ca hardness, Mg hardness, Ca^{++},Mg^{++}, chloride, phosphate, bicarbonate, silica was performed. The results on comparing with water quality standards put down by ICMR and WHO were considered for the study. The high values of parameters may have health implications and therefore these need attentions.

AP-11 : Antibacterial Activity of Biologically Synthesized Silver Nanoparticles from Medicinal Plant

Hiral Vaghela[1*], Rahul Shah[2] and Kokila Parmar[1]

[1]Department of Chemistry, HNG University, Patan- 384265,Gujarat
[2]Pacific University, Udaipur-313003, Rajasthan
E-mail : hiralvaghela152@gmail.com

Plant mediated biologically synthesized of nanoparticles is gaining importance due to its eco-friendliness. The synthesized metal nanoparticles is an expanding research area due to the potential applications for the development of novel technologies and very less toxic applications. In our research work, we describe a cost effective and environment friendly technique for green synthesis of silver nanoparticles and evaluate their antibacterial activity. Synthesis and characterization of silver nanoparticles was carried out by using bark extract of Moringa ptergo sperma plants reducing agent as well as capping agent. The synthesized nanoparticles were characterized with UV-Visible spectrometry (UV-Vis), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM) and X-ray diffraction spectroscopy (XRD).The antibacterial activity of silver nanoparticles has been observed.

AP-12 : A Study of Physical and Chemical Properties of Soil

Sharayu M. Thorat

Department of Chemistry, Shri Shivaji College, Akola-444001 (M.S.)
E-mail : mamtasangole@rediffmail.com

Soil analysis is a set of various chemical processes that determine the amount of available plant nutrients in the soil, but also the chemical, physical and biological soil properties important for plant nutrition or “soil health . Hence , aims of soil analysis are to determine the level of availability of nutrients or the need for its introduction, to predict the increase in yields and profitability of soil ,to provide the basis for calculating the required fertilizing of each crop, to evaluate the status of each nutrient element and simultaneously determine the compensation plan (nutrient management).The study was include measuring pH and soil moisture in the field, measuring soil temperature, measuring bulk density and soil moisture, measuring organic matter content, measuring total soil water holding capacity, measuring organic matter content and measuring soil texture.

AP-13 : Sustainable Agriculture a Must for Mankind

K. Yadav[*] and Anita Kumari[1]

[*]P. G. Deptt. of Chemistry, Samastipur College, Samastipur LNMU-Darbhanga
[1]Research Scholar, University Deptt. of Chemistry LNMU-Darbhanga
E-mail : yadv.kusheshwar@yahoo.com

Sustainable agriculture provides high yield undermining the natural systems and resources that productivity depends on. This approach comprises of natural processes and uses the best of current knowledge and technology to avoid the unintended consequences of industrial and chemical based agriculture. Here farmers minimize their use of pesticides and fertilizers thereby saving money and protecting future productivity as well as the environment. Key goals of sustainable agriculture are to achieve weed-control, pest-control, disease-control, erosion-control and high soil quality by adopting the techniques like crop-rotation, cover crops, soil-enrichment, natural pest predators and bio-intensive integrated pest management. Growing different crops in succession in the same field is one of the most powerful techniques of sustainable agriculture. It is a key element of the permanent and effective solution to pest problems because many pests have preferences for specific crops only. Hence by adopting crop-rotation pest control may be achieved. Having plants growing in the soil at all times helps farmers to achieve the basic goals of preventing soil erosion, suppressing weeds and enhancing soil quality. Appropriate cover crops reduce the need of chemical inputs like herbicides, insecticides, pesticides and fertilizers. Good soils can improve yields and produce robust crops. Soil-enrichment can be done by leaving crop residues in the field after harvest, plowing under cover crops or adding composted plant materials or animal manure.

AP-14 : Physico-Chemical Analysis of River Bed Sediments of Ganga and its Tributaries in Vaishali and Muzaffarpur Districts

Kalpna Kumari[1] and Madhup Raj[2]

[1]Dept. of Chemistry, BPS College Desari,BRA Bihar University, Muzaffarpur
[2]Post Graduate and Project Fellow, SERB (DST), Dept. of Chemistry, BPS College Desari,
E-mail : kalpna.chemistry@rediffmail.com, manu.raj03@gmail.com

People on globe are under tremendous threat due to undesired changes in the physical , chemical and biological characteristics of air, water and soil. These are relative to animal and plants and finally affecting on it. High levels of pollutants mainly organic matters in river beds cause an increase in BOD,COD,TDS, Total

Suspended Solids, pH ,alkanity ,hardness and other characters. They make water unsuitable for drinking, irrigation or any other use. In present investigation, different parameters has been analysed from different sites. Sediments collected from river beds showed slightly acidic pH at site 1, 3, 5, 11. All other sediments showed slightly alkaline pH ranging from 6.9 to 7.53. Electrical conductivity ranged from 252.37 to 497.61 micro siemens. TDS content was observed higher at site 4 by value of 278.61 mg/l. Organic carbon content was higher at site 4 and is the indication of higher fertility of the sediments. On the sites showed good amount of organic carbon content.

AP-15 : Synthesis, Characterization and Photocatalytic Activity of Cadmium Sulphide Nanoparticles

Kavita R. Desai, Amanullakhan A. Pathan and C. P. Bhasin*

Department of Chemistry, Hemchandrachary North Gujarat University, Patan-384 265 (Gujarat)
E-mail : kavita.desai139@gmail.com

A wide range of methods have been implemented for the removal of synthetic dyes from wastewater to decrease their impact on the environment. Photocatalytic degradation is proved to be the most popular and effective technique for the removal of dyes from aqueous solution. Therefore, we synthesized Cadmium Sulphide nanoparticles using thiourea as a source for Sulphide ion in the presence of Cadmium nitrate. The prepared nanoparticles were characterized by FTIR spectroscopy, x-ray diffraction, SEM & TEM. The photocatalytic activity of CdS nano particles was tested for degradation of Congo red dye. The degradation of Dye was fast in the presence of nano CdS than amorphous form.

AP-16 : A Chemical and Physical Analysis of Soil for Monitoring Changes in Soil Productivity

Mamata T. Sangole

Department of Chemistry, Shri Shivaji College, Akola-444001 (M.S.)
E-mail : mamtasangole@rediffmail.com

Soil is a complex, living, changing and dynamic component of the agroecosystem. It is subject to alteration, and can be either degraded or wisely managed. A thorough understanding of the ecology of the soil ecosystem is a key part of designing and managing agroecosystems in which the long-term fertility and productive capacity of the soil is maintained, or even improved. This understanding begins with knowledge of how soil is formed in a

given ecological region, and includes integration of all the components that contribute to the structure and function of the entire soil ecosystem. A great many biological, chemical and physical factors determine soil quality. By measuring some of these components and determining how they respond to management in an agricultural context, a foundation for assessing the health of the soil can be established. Ultimately, indicators of sustainability can be grounded in the assessment of soil conditions and how they change as a result of the choices a farmer makes in managing the agroecosystem. Proposed indicator include Measuring pH and soil moisture in the field, Measuring soil temperature, Measuring bulk density and soil moisture, Measuring organic matter content, Measuring total soil water holding capacity, Measuring organic matter content and Measuring soil texture. So the goal of this study was to assess the effectiveness and use of simple chemical, biological, and physical soil quality indicator tests that can be on-site.

AP-17 : Synthesis and Characterization of Hausmannite (Mn_3O_4) at Different Temperatures by Combustion Method

Lakshmi Narayani. R, Malathi Challa and Anu Sukhdev

Department Chemistry, MSRIT, Bangalore-54.
E-mail : rkrishlakshmi@gmail.com; maalathichalla@gmail.com; anusukhdev@yahoo.co.in

A novel method of synthesis is empolyed in preparation of Hausmannite nano particles using natural fuel extracted from green vegetable Alliem cepa at different temperatures of 300^0C and 500^0 C by combustion process. In this combustion method, the precursor $MnNO_3$ and fuel Alliem cepa are used as F/O in the ratio of 1:2 . The XRD peaks of Mn_3O_4 at an angle (2è) of 18.0935^0 ; 29.3252^0; 32.8438^0; 36.0800^0; 44.2705^0 correspond to (101); (112); (103); (202); (220); (224) planes and exhibited good agreement with JCPDS card (# 024-0734) but 59.8236^0 peak appeared in XRD spectrum of Mn_3O_4 prepared at higher temperature of 500^0 C. It is observed that the crystallinity of nano powder is increased when temperature increases from 300^0-500^0 C. The irregular particle size of nano compound from XRD and FESEM is 20-25 nm at 300^0 and increases to 30-50 nm at 500^0 C. The EDX result also confirms the formation of hausmannite Mn_3O_4.

AP-18 : Antifungal Compounds from Lactic Acid Bacteria to Protect Against Fungal Spoilage in Vegetables and Fruits

Pragati S. Abhyankar[1] and Balu P. Kapadnis[2]

[1]Department of Microbiology, Haribhai V Desai College, Pune
[2]Department of Microbiology, SPPU, Pune
E-mail : apragati10@gmail.com

The most important microorganisms involved in deterioration of agricultural produce are fungi. Fungicides are a primary means of controlling postharvest diseases. Public and scientific concern about the presence of synthetic chemicals in our food supply and in the environment has been increasing in the past decade. The use of lactic acid bacteria to combat fungal decay of agricultural produce is a promising solution. The study and application of antifungal LAB has evoked a considerable interest in recent years. Significant progress has been reported on the isolation and characterization of antimycotic compounds, which include various organic acids, cyclic dipeptides and fatty acids. Lactic acid bacteria are Gram-positive, nonmotile, nonspore forming, rod and coccus shaped organisms. They produce lactic acid as the major end product of carbohydrate fermentation. Significant progress has been reported on the isolation and characterization of antimycotic compounds, which include various organic acids, cyclic dipeptides and fatty acids. The “generally recognized as safe” (GRAS) status of LAB, offers the potential to use these bacteria as biological control agents in post-harvest produce to prevent fungal growth and reduce the health hazards associated with mycotoxins. Animal toxicity studies have shown non toxic nature of their use.

AP-19 : Fabrication of SnO_2 Coupled with ZnO Nanorod with Enhanced Photocatalytic Performance

Prakash K. Labhane[1], Lalchand B. Patle[1] and Gunvant H. Sonawane[*]

[1]MGSM's, Arts, Science and Commerce College, Chopda, Jalgaon (M.S.)
[*]Kisan Arts, Commerce and Science College, Parola, Jalgaon, (M.S)
E-mail : drgunvantsonawane@gmail.com

The SnO_2 coupled ZnO nanorod was prepared using the coprecipitationroutein the presence of Triton- X as a surfactant and characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM)and UV-Vis spectroscopy. XRD results confirmed the simultaneous presence of hexagonal ZnO as well as tetragonal SnO_2 phase. The crystallite size of prepared samples was evaluated by Debye Scherrer's and Williamson- Hall analysis.The

photocatalyticactivities of SnO_2 decorated on ZnO nanorod was evaluated using the photodegradation of methylene blue dye. The photodegradation proceeds much more rapidly in the presence of SnO_2 decorated ZnO photocatalyst compared to pure ZnO and SnO_2 nanoparticles. The enhancement of the photocatalytic activity could be due theformation ofhetero-junctions ZnO-SnO_2. The results demonstrates that photostable SnO_2 decorated ZnO nanorod is very promising to fabricate highly efficient photocatalyst.

AP-20 : Removal of Nickel (II) from Synthetic Effluent Water by Activated Carbons Prepared from Marine Algae Sargassum vulgare.sp

Suresh Jeyakumar R. P. and Nagoormeeran M.

Department of Chemistry, Vivekananda College of Arts and Sciences for Women (Autonomous) Tiruchengodu-637205, Tamilnadu
E-mail : sureshjoseph3@yahoo.co.in

The adsorption technique is found to be an effective method for the treatment and removal of nickel ions from aqueous solution. The activated carbons of marine algae have been reported to have high adsorption capacities for a number of heavy metal ions. In this investigation, the efficiency of marine algae Sargassum vulgare activated carbons and commercially activated carbon (CAC) were studied for removing Ni (II) ions from synthetic effluent water. Batch adsorption experiments were carried out as a function of pH, contact time, initial nickel concentration and adsorbent concentration. The percentage adsorption of Ni by CCSC, SSSC, and CAC are 90.57%, 98.29%, and 80.25% respectively. Adsorption data were fitted with the Langmuir, Freundlich and Temkin models. Two kinetic models pseudo first order and pseudo second order were selected to interpret the adsorption data. Maximum adsorption capacity of active carbon was calculated 30.46 mg/g for CCSC, it was calculated 37.52 mg/g for SSSC and 24.71 mg/g for CAC respectively.

AP-21 : Physico-Chemical Studies, Detection and Identification of Organics from Industrial Wastes

Subhash D. Khairnar and Vinod S. Shrivastava*

Nano-Chemistry Research Laboratory, G. T. Patil College, Nandurbar-425412
E-mail : drvinod_shrivastava@yahoo.com

In this work pysico-chemical studies of industrial waste water samples and detection, identification of organics for this purpose the Industrial effluents waste samples were collected from GIDC Surat (Gujarat).The physico-chemical parameters were analyzed by

following the APHA methods and collected samples are subject to analyzed physico-chemical analysis such as pH, Chemical Oxygen Demand (COD), Hardness, Electrical Conductivity (EC) and Total dissolve solid (TDS).The main principle of this study is to find out organics moieties in industrial effluents by GC-MS and FTIR techniques. For the detection and identification of organics from these samples were extracted by using dichloromethane (DCM) and analyzed by using GC-MS, FTIR techniques at SICART Vallabh Vidyanagar Gujrat.

AP-22 : Studies on Pyrazolone Azo Dye as Analytical Reagent

Rimpal Sawant* and Ketan Desai

SIR P. T. Sarvajanik College of Science, Surat-395007, Gujarat.
E-mail: rimpalsawant@yahoo.in

Some azo compounds were prepared by coupling the diazonium salts of amines with 2,4-dimethylphenol The structure of azo compounds were determined on the basis of elemental analyses, spectroscopic techniques. Complexes of nickel (II) and copper (II) have been synthesized and characterized. The composition of complexes has been established by using UV-Vis spectroscopic methods as well as conductivity magnetic susceptibility measurements. The nature of the complexes formed were studied following the mole ratio and continuous variation methods, Beer's law obeyed over a concentration range (1×10-4 - 3×10-4 M). High molar absorptivity of the complex solutions was observed. Analytical data revealed that all the complexes exhibited 1:2 metal-ligand ratios. On the basis of physicochemical data tetrahedral geometries were assigned for the complexes. Biological activity of the ligand and complexes were screened. In addition, the dyeing performance of the prepared ligands and their complexes were applied on cotton fabric.

AP-23 : Photocatalytic Degradation of Eosin-Y by using TiO_2 and Ag Doped TiO_2 Nano Catalyst

Sunil G. Shelar and Gunvant H. Sonawane*

Department of Chemistry, S.R.N.D Arts, Commerce and Science College, Bhadgaon, Jalgaon- 424105 (M.S)
**Department of Chemistry, Kisan Arts, Commerce and Science College, Parola, Jalgaon- 425111 (M.S)*
E-mail : drgunvantsonawane@gmail.com

TiO_2 and Ag doped TiO_2 were synthesized by Sol gel method. Structure and morphology of synthesized Ag doped TiO_2 nano catalyst was investigated using scanning election microscopy (SEM),

Electron dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD). The photocatalytic activity of Ag doped TiO_2nano catalyst was investigated by degradation of Eosin-Y solution under visible light radiation. The effects of various experimental parameters such as the Eosin-Y concentration, catalyst dose,Effect of pH on the photocatalytic degradation were investigated. The kinetics study shows that the reaction follows first order kinetics.Among the different amounts of dopant that like 1, 2, and 4wt% Ag-doped TiO_2nanocatalyst?It was observed that 4 wt % Ag doped TiO_2 shows highest degradation with visible light radiation for Eosin-Y solution than Pure TiO_2 nano catalyst. The particle size, morphology and separation of photo induced electron–hole pair are the main factors which influence photocatalytic activity.

AP-24 : Effective Photocatalytic Removal of Eosin Y dye using Bi_2O_3-Bentonite Nanocomposite

Sandip P. Patil[1] and G. H. Sonawane[2]*

[1]Nano-chemistry Research Laboratory, G. T. Patil College, Nandurbar-425 412 (M.S.)
[2]Dept. of Chemistry, Kisan Arts, Commerce and Science College, Parola-425 111 (M.S.)
E-mail : drgunvantsonawane@gmail.com

The Bi_2O_3-bentonite is used for the photocatalytic removal of Eosin Y (EY) in presence of visible light irradiation. Bi_2O_3-bentonite shows enhanced photocatalytic efficiency than pure Bi_2O_3 due to intercalation with bentonite clay. After visible light irradiation for 60 min the removal of EY via photocatalytic degradation achieved by Bi_2O_3, bentonite and Bi_2O_3-bentonite 53.8, 47.7 and 92.3% respectively for 1 gL^{-1} photocatalyst at pH 4. It is observed that increase in light absorption and decrease in electron-hole recombination enhances photocatalytic efficiency. Photocatalytic degradation of EY by Bi_2O_3-bentonite proceeds via advanced oxidative process. Adsorption kinetics proceeds via pseudo-second-order kinetics while, adsorption isotherm found to follow Langmuir isotherm. The separation factor R_L in the present study reveals favourable adsorption process.

AP-25 : Adsorption of Dyes from Textile Effluents by using Activated Carbon Prepared from Sugar Cane Bagasse

T. V. Nagalakshmi[1*]and K. A. Emmanuel[2]

[1]Department of Chemistry, LakiReddy BaliReddy College of Engineering, Mylavaram -521230, A.P.
[2]Department of Chemistry, Sir C. R. Reddy Autonomous College, Eluru-534 007, A.P.
E-mail : mannava_laxmi@yahoo.co.in

An activated carbon was developed from Sugar Cane Bagasse

(SCB), characterized and used for the removal of Direct Black38 (direct) and Reactive BMR (reactive) dyes from wastewater successfully. The pore structure of the resulting carbon was analyzed using N_2 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. Batch mode experiments were conducted to know the adsorption capacity of prepared activated carbon for the removal of selected dyes. Equilibrium isotherm equations used to describe experimental adsorption data were Freundlich, Langmuir, Temkin and Dubinin- Radushkevich. Basing on correlation co-efficient and chi-square analysis, it was observed that Langmuir isotherm provides the best correlation for experimental data. In adsorption process of selected dyes, fitting of the kinetic data demonstrate that the dynamics of sorption could be better described by pseudo-second-order model indicating a chemisorptive rate-limiting.

AP-26 : Comparative Study of Fluoride and Chloride in Ground Water Samples in Jalgaon District

V. C. Badgujar[1] and P. M. Yeole[2]

[1]Department of Chemistry, Pratap College, Amalner-425401
[2]Centre for PG Research in Chemistry, Department of Chemistry, R.L. College, Parola-425111
E-mail : pravinyeole.707@rediffmail.com

In present study determination of fluoride and chloride from ground water in Jalgaon district. Fluoride becomes toxic to animals and human beings when present at concentrations >1mgl-1 in drinking water and injurious to crops when present at >10mgl-1 in soil solution. Some of these waters are unsuitable for drinking and if used for irrigation may be accumulated at concentrations in fodder crops injurious to cattle. The physico-chemical analysis of ground water sample from various places in Jalgaon district. The analysis of pH, EC, fluoride, chloride etc. was carried out as per standard method. The results were compared with the values stipulated by WHO standards. The results indicate that the fluoride in some samples was found above standard probably due to seasonal variable and salt water contamination. Some samples can be used for irrigation purpose.

AP-27 : Removal of Rose Bengal dye using Natural Algerian Montmorillonite

Shailesh J. Vajapara and C. P. Bhasin*

Department of Chemistry, Hemchandrachary North Gujarat University, Patan – 384 265 (Gujarat)
E-mail : shaileshvajapara91@gmail.com

Adsorption of rose bengal using an Algerian montmorillonite has been investigated. The influences of several parameters such as contact time, adsorbent dose, pH and temperature on the adsorption of the above dye has been tested. The results showed that nearly 40 min of contact time are found to be sufficient for the adsorption to reach equilibrium. The residual concentration of the dye is determined using UV/Vis Spectrophotometer at wavelength 545 nm. Langmuir and Freundlich isotherm models were used to describe adsorption data. Adsorption kinetics was best described by the pseudo-second order model.

AP-28 : Photocatalytic Degradation of Cobalt Picrate in the Presence of Semiconductor

J. J. Vora[1], L. S. Bhutadiya[2] and V. R. Shukla[2]

[1]Department of Chemistry, Hemchandracharya North Gujarat University, Patan -384265
[2]Sheth M N Science College, Patan-384265
E-mail : jabali_vora@hotmail.com

This study investigated the degradation of aqueous Co-picrate using advanced oxidation process. The occurrence of photocatalytic reaction at different time intervals has been observed spectrophotometrically. Various kinetic parameters of metal picrate were studied such as effect of concentration, amount of semiconductor, pH, light intensity etc. Important conclusion were drawn and structured with photo catalytic degradation.

AP-29 : Synthesis of Biogenic Silver Nanoparticles from Medicinal Plant and its Antibacterial Activity

Rahul Shah*[1], Hiral Vaghela[2] and Kokila A. Parmar[2]

[1]Pacific University, Udaipur-313003, Rajasthan
[2]Department of Chemistry, HNG University, Patan- 384 265, Gujarat
E-mail : rahulshah1691@gmail.com

Biological synthesis of nanoparticles from medicinal plant is gaining importance due to its eco-friendliness. The synthesis of metal nanoparticles is a broad research area due to the potential applications for the development of different novel technologies. In our research work, we have described a cost effective and eco-

friendly technique for the green synthesis of silver nanoparticles and evaluated their Antibacterial activity. Synthesis and characterization of silver nanoparticles was carried out by using Crateva religiosa plant bark extract as reducing agent as well as capping agent. The Synthesized nanoparticles were characterized with UV-Visible spectrometry (UV-Vis), Fourier Transform Infrared Spectroscopy (FT-IR), Scanning Electron Microscopy (SEM) and X-ray Diffraction Spectroscopy (XRD). The antibacterial activity of silver nanoparticles has been observed.

AP-30 : Analysis of Water Samples Collected from Pune Area

Gulab S. Gugale*, Ankita. R. Basarikatti and Adhik. H. Godse

**Department of Chemistry, Haribhai V. Desai College, Pune -411 002*
E-mail : gsgugale02@gmail.com

Water is one of the main sources through which pollutants gets into human system. With the advances in analytical science in determination of micro level constituents in water and lot of clinical data being made available more and more chemicals found in aquatic system are being labeled as “toxic”. In the present investigation water samples were collected from eight different places from Pune area (Maharashtra state, India) in October 2015 and were analyzed for major ions (Ca, Mg, Na, K, Cl, PO_4 etc.) and water parameters (pH, conductance, Total hardness, alkalinity etc.). The physico-chemical characteristics revealed that in general water samples collected from Appa Balwant Chowk, Katraj and Wagholi, increased the Total hardness, calcium and magnesium which were very high well exceeding the tolerance limits. Their occurrence due to human activities. The chemical constituents of other area of Pune were found to be well below the prescribed limits. Recommendations have been made for water quality upgrading.

AP-31 : Irrigation of Waters and their Suitability for Different Crops at District Agra-A Study

Prem Prabhaker

Deparment of Chemistry Paliwal (P.G.) College, Shikohabad,
Distt-Firozabad (205 135), (U.P.)
E-mail : brpremprabhakar34@gmail.com

About 65% of India’s population lives in villages and most of them depend upon agricultural practices for their livelihood. Previously, they depended upon the rainfall for the irrigation purposes, which was quite uncertain. They, then, started using underground water of wells, tubewells, ponds, rivers etc. This

study has been done in order to find out the means of measuring the amounts of different chemical constituents (pesticides and herbicides) by various techniques such as FT-IR, UV-Visble and Gas chromatography in different irrigation waters and soils of nearby villages of district Agra to find out the suitability for different crops and their varieties. For the improvement of this particular science of agriculture has always been a concern of mankind.

AP-32 : Physico-Chemical Study of Ground Water of Various Places in Agra

Amit K. Agarwal* and Sandhya Agarwal

Department of Chemistry Agra College, Agra-282002 (U.P.)
B. R. Ambedkar University, Agra
E-mail : akagarwal.chem@gmail.com

Today the demand of pure water is continuously increasing due to massive increase in population and human activities. For the study, different samples of groundwater have been collected from the various places of Agra (UP). The results of this study were compared with the water quality standards of ISI and WHO. In this study different physico-chemical parameters like conductance, turbidity, pH, color, odour, temperature, chemical oxygen demand, total dissolved solids and concentrations of ions like sulphate, phosphate, Mg^{++}, Ca^{++}, Cl^{-}, F^{-}, etc. were determined 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 odours, quality characteristics.

AP-33 : Comparative Study of Sonocatalytic, Photocatalytic and Sonophotocatalytic Degradation of Dyes by using Semiconducting Materials

Sunil D. Marathe and Vinod S. Shrivastava

Nano Chemistry Research Laboratory, G.T.P. College, Nandurbar 425412
E-mail : drvinod_shrivastava@yahoo.com

In this work a comparative study of sonocatalytic, photocatalytic and sonophotocatalytic degradation of three dyes i. e. rose bengal, reactive blue 59 and eosin Y was carried out. The effect of different operational parameters like initial dye concentrations, the amount of catalyst, contact time and pH were studied to determine the optimized conditions for degradation. The sonocatalytic experiments were carried out in an ultrasonic bath (Systronics 6.5 L) which acts as a source of ultrasound radiations.

AP-34 : Wet Chemical Method of Analysis of Geological Samples (Classical as Well as Other Instrumental Techniques)

Raj Ranjan Jha

Department of Chemistry, Ranchi University, Ranchi
E-mail : rajranjanjha@yahoo.co.in

The chemical transformation of any ore/mineral sample into a desired form so as to facilitate analysis of its constituents is known as opening of the sample. Hence, conversion of an ore or mineral sample into desired soluble or insoluble species. In simple words, opening of an ore is its dissolution in suitable solvent or flux depending upon the aim of analysis. Thus, opening of a sample is a very vital and important step in ore/mineral analysis. The separation of soluble and insoluble species should be near 100%. The exact choice of method for opening of an ore depends on the nature of the ore, the element of interest and its chemical properties. The selection of the appropriate method of sample decomposition is very important for correct analysis. To achieve this, an analyst should carefully take into account the chemical properties of various minerals present in the sample. Owing to the variable characteristics of the ore, it is not possible to have any one set procedure applicable to all samples. It is often necessary to combine two or more methods to effect the dissolution of an ore. There are mainly two methods to open an ore. They are (1) wet method & (2) dry method. Wet method constitutes the digestion of an ore sample with an acid or a mixture of acids to convert the complex ore minerals into simple chemical compounds. The action of an acid or a mixture of acids is supplemented by heat and pressure. Heat and pressure hasten the dissolution rate. This is normally preferred over dry method due to its simplicity and it requires less attention, moreover, the vessel used is less affected by the dissolving media. Before entering into the further details of use of wet methods and dry methods, it is necessary to categorize the ore samples. On the basis of their chemical composition and chemical properties, the categorization makes the opening of an ore easy and logical.

AP-35 : Synthesis and Biochemical Characterization and Characterization of Some Lanthanide Complexes

H. D. Chaudhari[1], Haresh R. Patel[2] and J. J. Vora[*]

[1]Adarsh Science College, Radhanpur, Banaskantha. India
[2]Department of Chemistry, Sankalchand Patel University, Visnagar
[*]Department of Chemistry, Hemchandracharya North Gujarat University, Patan
E-mail : jabali_vora@hotmail.com

Lanthanide ions are possessing typical characteristic for example

Lanthanide contraction fluorescence, Magnetic Properties etc. The combination of Lanthanide ions with complexing or chelating biologically important ligand to form coordination compound is an important area of current research. Less explored biologically important ligand are allowed to react with solution of lanthanides perchlorates and attempt has been made to synthesize solid complexes. These complexes are subjected to U.V Visible Spectroscopy, IR Spectroscopy, and Elemental Analysis of these compounds has been evaluated by Standard methods and attempts have been made to correlate structural characteristic with properties of these complexes.

AP-36 : Synthesis and Biochemical Characterization of Some Ground Water Sample of Visnagar

Riddhi Dave, Chandrika Chaudhary, Komal Luhariya and J. J. Vora*

Department of Chemistry, Hemchandracharya North Gujarat University, Patan
E-mail : jabali_vora@hotmail.com

The Visnagar city is copper city. The city is very big and very pollutant affecting in this city. The water sample was analysis. These parameters are subjected to pH, carbonate, bicarbonate, total hardness Analysis, C.O.D and B.O.D Analysis of these compounds has been evaluated by Standard methods and attempts have been made to correlate characteristic with properties of these ground water of Visnagar.

AP-37 : Use of Canna Lily Flower as Photosensitizer in Dye Sensitized Solar Cell

Suprabha S. Sahoo, H. M. Pathan and Sunita Salunke-Gawali*

Department of Chemistry, Savitribai Phule Pune University, Pune 411007
E-mail : sunitas@chem.unipune.ac.in

Use of naturally abundant flora and faunas as biggest source for generation of renewable energy in the field of photovoltaics plays a significant role to meet global energy demands and rapidly depleting fossil fuels. Despite of clean, ecofriendly, long-lasting and easily availability of solar energy cost-effectiveness and low performance of PV devices lead DSSC to come into public domain. Dye sensitized solar cells are the best alternatives than other types of Thin film technologies. Recent investigation conducted with a naturally available Canna (Canna Lily) flower extract in ethanol as a dye and sensitizing TiO_2 metal oxide as a photo anode. The device was fabricated with nano structured TiO_2 paste by doctor blade method followed by sintering at 450 °C for one hour

in vacuum. The efficiency of the device was studied with the natural dye present in canna flower by varying its concentration, time of dye loading and changing reductive electrolytes. After 5 hours of dye loading we got power conversion efficiency of 0.019% which can be further improvised by optimising the parameters. Characterization of the film by UV-Visible, FT-IR spectroscopy, CV, SEM, X-ray diffraction studies has been done.

AP-38 : Geochemical and Spectral Studies of Bauxite Mines of Western Ghat in Maharashtra (India)

Raghunath J. Katkar and Vikas A. Thakur*

Rayat Shikshan Sanstha's Mahatma Phule A. S. C. College Panvel, Navi Mumbai, Maharashtra

E-mail : tha.vikas@yahoo.com.

Mining is considered to be one of the major causative activities of environmental degradation. However exploration of minerals is must in the developmental world and metals is required for industry and even for energy production. Mining involves removal of soils and extraction of minerals resulting in environmental pollution which degrade the surrounding environment. The effect can be more detrimental when it results in spreading of hazardous elements. The mine chosen by us as a case study are two bauxite mines at ringewadi plateau mine ($16^0$51' N: $73^0$52'E) and Dhangarwadi($16^0$562 N: $73^0$532 E) located in Kolhapur. The estimated reserve is15.65 million tonnes at Dhangarwadi mine and 1.06 million tonnes at Girgaon. These mines can extract million of tonnes of Aluminium and titanium ore is annually. We carried out analysis with classical methods, advanced instruments including spectral studies to understand geological phenomenon before and after mining. It was observed that Soils are acidic to slightly basic (pH 4.9 to 7.7) while water samples are acidic to basic (pH 5.9 to 8.9). Some of the representative results of analysis ICP-AES are: Composition of high grade ores(%): Al- 14.47, Ti- 2.68, Fe 8.54, Cr- 0.065, P- 0.06; low grade ore (%), Al- 21.14 -31.42, Ti-: 1.20-2.68, Fe- 12.90-14.64, P -0.07-0.08 ; Soil inside Mine shows(%) Al- 18.39-19.99, Ti-1.01-1.34, Cr- 0.03-0.07, Fe- 18.35-20.62, Mn- 0.01-0.05, P- 0.12-0.15; Soil in surrounding mine shows (%) Al- 13.63-15.96, Ti- 1.17-2.25, Cr- 0.02-0.03, Fe- 14.82-21.71, Mn- 0.02-0.34, As- 0.001-0.004, P- 0.01-0.34, S- 0.01-0.02, Water analysis shows (ppm), Al- 2.52-6.18, Ti-0.08-0.22, Ca- 51.14-405.9, Cr- 0.1-0.21, Cu- 0.137-1.497, Fe- 5.905-14.035, Si-0.751-8.006, ; Mn- 0.126-1.531, Ni-0.04-0.125, Pb- 0.279-0.745, P- 0.25-2.76,Sr- 0.142-1.025, Zn- 0.632-3.059 and S-14.061-32.894. In Spectral studies, X-Ray Fluroscence

technique have shown the presence of Zr, Nb, Sr,Rb, Th,As, Pb, Zn, Ga, Cu, Ni, Co, Fe, Cr, Ti, Ca, K, Si, Al, Mg, Na. FT-IR spectroscopic investigation carried out in the range of 4000-500 cm^{-1} and Far IR in the range of 600-100cm^{-1} confirm the presence of Alumina(Al_2O_3) and haematite ($2Fe_2O_3$), Therefore the studies carried indicates significant effect of heavy and toxic metals on the surrounding environment of Dhangarwadi and Ringewadi-Girgaon Plateau Mine.

AP-39 : Ferric Chloride Catalysis in the Bromination of 2, 4-Dinitrophenol and 5-Chlorosalicylic Acid in (90 : 10% v/v) Acetic Acid, Water Mixture Medium

D. Dasharath[1] and Y. B. Vibhute[*]

[1]Department of Chemistry, KITS FOR WOMEN, Nizamabad-503002
[*]Department of Chemistry, Yeshwant Mahavidyalaya, Nanded
E-mail : tha.vikas@yahoo.com

Ferric chloride catalysis in the bromination of 2, 4-dinitrophenol and 5-chlorosalicylic acid is investigated in (90 : 10% v/v) acetic acid : water mixture medium at 303°K, keeping the concentration of phenol (0.02M) and bromine (0.02M) constant with and without anhydrous $FeCl_3$. In the absence of any catalyst the reaction is second order, when the concentration of Ferric chloride in the mixture is increased (From 0.02 to 0.06m) there was a steady increase in the observed k_2. The rate equation for the $FeCl_3$ catalysis may be represented as follows,

$-d[Br_2]/dt=K[ArH]\ [Br_2] + Kc[ArH]\ [Br_2]\ [FeCl_3]_n$, $k_2=K+Kc\ [FeCl_3]_n$

Where, k_2 is the observed second order rate constant K and Kc are the rate constants for catalyzed and unanalyzed reactions, respectively and 'n' the order for $FeCl_3$.

AP-40 : Environmentally Ecofriendly Synthetic Approach for Bio-Compatible Macrocycles

Ashu Chaudhary

Department of Chemistry, Kurukshetra University, Kurukshetra-136119.
Email : ashuchaudhary21@gmail.com, achaudhary21@hotmail.com

The varied nature of the chemical world requires various greener pathways in our quest towards attaining sustainability. Green chemistry has come a long way since its birth in 1991, growing from a small grassroots idea into a new approach to scientifically-based environmental protection. The emerging area of green chemistry envisages minimum hazard as the performance criteria while designing new chemical processes. Rather than end-of-the-

pipe remediation approach, which involves cleaning up of waste after it has been produced, the main objective is to avoid waste generation in the first place. There are different shades of greener processes being developed as we continue exploring alternatives to conventional chemical synthesis and transformations. The desired approach will require new environmentally benign syntheses. The chemistry of macrocyclic complexes has witnessed an outline by individual scientific backgrounds and individual interest due to their analytical, industrial, agricultural and medicinal. The anticancer properties of square-planner platinum compounds have fueled an interest in the chemistry of all the metal complexes. Keeping all these factors in mind we aimed to synthesize and characterize macrocyclic compounds with N_4–tetraamide ligands. The main emphasis has been given on in vivo studies on male rats by performing biochemistry and fertility test. The aim is also to prevent the toxic effect or abnormal observations of the pesticides and antifertility agents. Good antimicrobial complexes have been selected for antitumour activity. The positive findings will be discussed in detail.

AP-41 : Microbial Degradation of Xenobiotic Compounds and Heavy Metals

Bijoy S Goswami[1], Charmin Sultana[1] and Manoj Barthakur[2]

[1]Department of Chemistry, B. Borooah College, Guwahati-781007
[2]Department of Botany, B. Borooah College, Guwahati-781007
E-mail : bijoysgoswami@gmail.com

The present study is undertaken with the objectives (i) Isolation of microorganism from oil contaminated sludge (ii) biodegradation potential of the isolates bacteria towards aromatic hydrocarbons like naphthalene, toluene and some heavy metals like Cu, Pb, Cd. In this study the sludge (Oil Contaminated) is collected from Guwahati Refinery, Noonmati and the Bacteria is isolated by using serial dilution methods. The isolated Bacterial strain is finally identified as Nocardiopsisalba.

In this study, the UV- Visible Spectrophotometric Study Shows that all the samples have some definite Optical Density which proves that Nocardiopsisalbabacteria degrade the Naphthalene and Toluene solution at different concentrations. 60 ppm treated for Naphthalene has the highest optical density. The IR study shows that the control sample contains the peak of -Alkane, Aromatic hydrocarbon, Nitro groups, -CH (bending) while the treated sample contains the peak of $-CH_3$ and $-CH_2$ in anti -symmetric and symmetric, Carboxylic acid (O-H stretching), -CH (bending) etc.

GC Study shows that the Retention Time indicates that the Nocardiopsisalba bacteria can degrade the Naphthalene and Toluene into some other compound. GC- Mass Studies indicates that the degraded products are identified as acids and Diols like 1-pentacosanol, Tetracontane 1,40 diol, Acetic acid.Nocardiopsis albabacteriacan degrade the Cu metal at different concentration while it cannot degrade the Pb& Cd metal. Thus we can conclude that Nocardiopsisalba bacteria can degrade the Naphthalene and Toluene into some other compounds which are less toxic and hence it is considered as an efficient microbial degradation bacteria.

AP-42 : Electrochemical Properties of Polyacrylonitrile/ Polypyrrole Composite

Mohammad Faraz Ahmer

Department of Electrical Engineering, Mewat College of Engineering, Mewat
E-mail : farazahmar@rediffmail.com

Polyacrylonitrile/polypyrrole (PAN/Ppy) composite was prepared by sol gel method. It was characterized by using X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM) and energy dispersion X-ray analysis techniques. For the determination of capacitance, cyclic voltammetry was used. The SEM images demonstrate granular surface morphology. The specific capacity of synthesized material was 222 F g^{-1}. This study will open the way to develop green energy systems. The appearance of the peaks in FTIR spectrum revealed the formation of PAN/Ppy composite by the combination of PAN and Ppy as components.

AP-43 : Metal Speciation and Mobility Index Study in Soils near Deepar Beel Bird Sanctuary of Guwahati in Assam

Bijoy S. Goswami and Manash P. Choudhury

Department of Chemistry, B. Borooah College, Guwahati-781007
E-mail : bijoysgoswami@gmail.com

The prime objective of this study is to characterize and map the spatial distribution and mobility of heavy metals present in top soil layer at Boragaon, Guwahati; the latter being known as the garbage dumping site of GMC, situated near DeeporBeel Bird sanctuary. In this context, metal speciation and it's mobility is considered to be an effective tool to check the level of toxicity and to study the mobility of various metals in that area.

Baragaon is located to the south-west of the Guwahati city, in Kamrup (metro) district of Assam, India. This area is about 500

meters from the DeeporBeel which a bird Sanctuary. DeeporBeellies at latitude $26^{0}05^{/}$-$26^{0}11^{/}$ N and longitude: $91^{0}35^{/}$-$91^{0}43^{/}$ E and occupies 4,014 km^2 (1,550 sq mi) of total area. The speciation study is used to separate the five fraction, viz. adsorptive and exchangeable (F1), Bound to Carbonate Phase (F2), bound to reducible phase (iron and manganese oxides) (F3), Bound to Organic matter and sulfides (F4) and residual or lattice metals (F5) for working out the chemical associates of metals such as Cu, Zn, Pb& Cd in the surface soil samples from the locations.

The present study showed that soil have higher concentration of Zinc (Zn), Lead (Pb) while Cadmium (Cd) is present in very little amount. Lead (Pb), Cadmium (Cd) associated with the exchangeable fraction bound in considerably high amount in this work. A large portion of Zn is found in organic fraction bound matter and Cu is found in residual fraction in the study.With respect to mobility, of all the four metals, Lead (Pb) has highest mobility fraction value and is most mobile and Copper (Cu) is found to be least mobile. The Mobility Index Study indicates that the Pb is in a state of high mobility and its availability to biological system will be high while Cu is the least mobile metal. The mobility index in the present work is in the order of Pb> Cd > Zn > Cu.

AP-44 : Drinking Water Quality Study with Special Emphasize on As, Fe and F content of Morigaon District in Assam

Munmi Sarma[1], Bijoy S. Goswami[1] and Manoj Barthakur[2]

[1]Department of Chemistry, B. Borooah College, Guwahati-781007
[2]Department of Botany, B. Borooah College, Guwahati-781007
E-mail : bijoysgoswami@gmail.com

Water quality assessment is one of the prime concern and a major challenge in all over the world. Needless to say water quality criteria is directly related to the health factors. Drinking water has a vital role in public health and this is a major driver for the development of standard to ensure the safety of drinking water and to safeguard public health.

The present study is undertaken with the principal objectives such as (i)Characterization of water quality with respect to the following physic – chemical parameters – pH, Conductance, Total Dissolved Solids, Hardness (ii)Analysis of Major Anions and Cations – Sulphate, Phosphate, Nitrate, Fluoride, Chloride, Calcium, Magnesium, Sodium, Potassium (iii) Distribution of Toxic Metal Content with respect to Arsenic (As), Iron (Fe),Copper (Cu), Lead

(Pb), Manganese (Mn) (iii) To detect the Coliform group of bacteria from water samples (iv) To determine water quality index

In this present study water samples are collected from 23 Locations from Morigaon District, Assam. Out of 23 samples 16 samples are collected from tube well, 5 from ring well and 2 from supply water.

In this present investigation, it has been observed that the pH values ranges from 6.1- 7.4 while Conductance ranges from 1.002 mS/cm to 1.149 mS/cm. Total dissolved solids ranges 62.2 to 633 ppm. Hardness ranges 44- 364 mg/L. Sulphate ranges4.4 mg/L - 64mg/L and Nitrate ranges 0.012 mg/L to 1.051mg/L. Fluoride ranges 0.98 mg/L to 4.2 mg/L. Iron ranges from 0.002 mg/L to 5.2 mg/L. Manganese values ranges from 0.006 mg/L to 3.78 mg/L .Arsenic values ranges from 2.22 µg/L to 19.77 µg/L. The Co-relation study also shows that there is a good positive correlation between various parameters. The water Quality Index study shows that out of 23 samples 11 samples have values between 75 and 100 which indicates these samples are in very poor quality status. 52.17% water samples were classified under “unsuitable for drinking” category in accordance with their WQI values. Thus there is an instant need to take ameliorative steps in this region to prevent the population from adverse health effects.

AP-45 : Removal of Methylene Blue and Pb from Aqueous Solution Using Bio-adsorbents

Surabhi Lahkar and Bijoy S. Goswami

Department of Chemistry, B. Borooah College, Guwahati-781007
E-mail : bijoysgoswami@gmail.com

Contamination of surface and groundwater with industrial effluents is becoming a major threat to human health as well as aquatic life. Among the various hazardous materials that contaminate water, dyes released from textile, photographic and dyestuff industries, and heavy metals released either naturally through a variety of geochemical processes or by direct discharge of municipal and industrial wastes, are of particular environmental concern. There has been increasing scientific concern about the hazardous effects of colored dyes. The main objective of this present study to investigate the feasibility of Bio-adsorbent Bokul (Mimusopseleng) leaf powder (BLP), Bokul leaf ash(BLA) and Banana pseudo-stem ash(BSA) as an efficient adsorbent for the removal of methylene blue dye and Pb(II) from water. The present study is carried out with respect to Characterization of Bioadsorbents,

Batch studies in terms of pH, Agitation, Concentration, Time, Isotherm Model and Kinetic Studies.

In this present investigation the predominant findings are, pH of bokul leaf powder, bokul leaf ash and banana pseudo stem ash are found to be 5.6, 9.6 and 10.0 respectively. The surface areas of BLP, BLA & BSA are found to be 26.2 m^2/g, 45.4 m^2/g, and 227.8 m^2/g respectively. The bulk densities of BLP, BLA & BSA are found to be 0.24 g/cm3, 0.41 g/cm3 and 0.23g/cm3 respectively. In the batch studies it has been observed that pH has significant influence on adsorption. It is observed that the optimum pH for Methylene Blue removal is 4,12,2 for BLP,BLA,BSA respectively, and optimum pH for Pb(II) removal is 2,8,10 for BLP,BLA,BSA respectively.The equilibrium time obtained for adsorption of Methylene Blue onto BLP,BLA, and BSA adsorbents are 90,90,120 min respectively and the equilibrium time for the adsorption of Pb(II) onto BLP,BLA,BSA adsorbents are 60,75,75 min respectively. The adsorption of both Methylene Blue and Pb(II) onto Bokul leaf powder, Bokul leaf ash and Banana pseudo-stem ash follows second order kinetics. It can be concluded that the Methylene Blue and Pb(II) are efficiently removed from the aqueous solutions by adsorption process using Bokul leaf powder, Bokulleaf ash, and banana pseudo-stem ash.

AP-46 : Philosophy of Chemistry : An Emerging Field

Chetan Prabha Singh[1] and R. K. S. Dhakarey[2]

[1]Department of Philosophy, Agra College, Agra-282002
[2]Department of Chemistry, I.B.S. Khandari, Dr. B.R.A. University, Agra - 282002
E-mail : cp.singh25april@gmail.com

Chemistry is the study of the structure and transformation of matter. In the 21st century, chemistry has become the largest scientific discipline, producing over half a million publications a year ranging from direct empirical investigations to substantial theoretical work. However, the specialized interest in the conceptual issues arising in chemistry, hereafter Philosophy of Chemistry, is a relatively recent addition to philosophy of science.

Philosophy of chemistry has two major parts. In the first, conceptual issues arising within chemistry are carefully articulated and analyzed. Such questions which are internal to chemistry include the nature of substance, atomism, the chemical bond, and synthesis. In the second, traditional topics in philosophy of science such as realism, reduction, explanation, confirmation, and modeling are taken up within the context of chemistry.

Modern chemistry is thoroughly atomistic. All substances are thought to be composed of small particles, or atoms, of the Periodic Table's elements. Yet until the beginning of the 20th century, much debate surrounded the status of atoms and other microscopic constituents of matter. As with many other issues in philosophy of chemistry, the discussion of atomism begins with Aristotle, who attacked the coherence of the notion and disputed explanations supposedly built on the idea of indivisible constituents of matter capable only of change in respect of position and motion, but not intrinsic qualities.

An idea about Philosophy of Chemistry will be discussed.

INORGANIC CHEMISTRY SECTION

Sectional President's Address

Studies on Multifunctional Schiff Bases Derived from 4-Aminoantipyrine and their Metal-Co-ordination Compounds of Biological and Medicinal Relevance

Ram K. Agarwal

Former Head, Department of Chemistry, LajpatRai Postgraduate College (C.C.S. University), Sahibabad-201005 (Ghaziabad)
E-mail : ram_agarwal54@yahoo.com

Multifunctional ligands have found applications at the forefront of all areas of biological and medicinal inorganic chemistry. Heterocyclic compounds are widely distributed in nature and essential to many biochemical processes. Pyrazolones *e.g.,* antipyrine/4-aminoantipyrine (N-hetrocyclic compound) is an active moiety as a pharmaceutical ingredient, especially in non-steroidal anti-inflammatory agents used in the treatment of arthritis and other musculoskeletal and joint disorders. Schiff bases have played an important role in the development of coordination chemistry as they readily form stable complexes with transition/inner transition/ main group metal ions. They show interesting properties *e.g.*, their ability to reversibly bind oxygen, catalytic activity in hydrogenation of olefins and transfer of an amino group, photochromic properties and other biological properties *e.g.*, antibacterial, antineoplastic, antimalarial and antiviral behaviours. Studies of new kinds of chemotherapeutic Schiff bases are now attracting the attention of biochemists.

Synthetic drug chemistry started with the German Chemist Ludovic Knorr who synthesized in 1884, the first drug with fever and pain release effect, *i.e.* antipyrine. A large anount of antipyrine derivatives have been isolated for different medical purposes and compounds with analgesic and anti-inflammatory effects, antiviral,

antibacterial, antitumoral and herbicidal activities. A variety of derivatives can be obtained when the proton at the position 4 is substituted. The antibacterial activity of Schiff bases of 4-aminoantipyrine were tested against *Staphyloccus aureus, Klebsilla pneumonia, Salmonella typhi, Pseudomonas aeruginosa* and *Bacillus subtilis.* The metal complexes showed higher inhibitory activity than the ligands and have higher activity than ampicillin except for *Klebsilla pneumonia* and *Pseudomonas aeruginosa.* Many transition metal [Cu(II) and VO(IV)] complexes of Schiff bases of 4-aminoantipyrine exhibited higher bactericidal activity towards *E.coli* and *A.boumanii* . The efficiency of metal-based therapeutic agents changes considerably by making small changes in the Schiff base ligands attached to the metal.

Other than Schiff bases *e.g.* semicarbazones or thiosemicarbazones derived from 4-aminoantipyrine are reported as potential chemotherapeutics. The Schiff base type compounds (e.g. thiosemicarbazones) are noted for their pharmacological properties, particularly as antiparasitic, antibacterial and antitumoral agents. As anticancer agents, it is believed that their mechanism of action is through the inhibition of ribonucleoties reductase. So far suggested that DNA is the primary intracellular target of anticancer drugs because the interaction between small molecules and DNA can cause DNA damage in cancer cells blocking the division of cancer cells and resulting in cell death. The thiourea moiety present in thiosemicarbazone contains several donor atoms and is thus capable of acting as a multifunctional ligand toward a metal. It is believed that the metal chelating abilities partially account for their biological activities and many studies on the biological activity of thiosemicarbazone-metal complexes are performed. The biological and medicinal activities of these compounds suggest that the molecular features essential for such activities must be ascertained by designing synthetic routes to modify, replace or substituted the derived thiosemicarbazone ligands. From our laboratory, we have reported a large number of Schiff bases of 4-aminoantipyrine e.g., N,O-donors, N,N,O-donors and N,N,S-donors and their metal-coordination compounds and evaluated their biological and medicinal properties.

IIL-01 : Exploration of DNA Interactions and Biocidal Activity of Cu(II) Complexes of Schiff Bases : Synthesis and Spectral Characterization

Shivaraj

Department of Chemistry, Osmania University, Hyderabad, Telangana State-500007
E-mail : shivaraj_sunny@yahoo.co.in

The present work focuses on the preparation of Schiff bases by both, conventional method and microwave-assisted condensation of 3, 5-dimethyl-4-amino isoxazole / 2-amino-6-(trifluoromethoxy) benzothiazole / 6-amino benzothiazole with substituted salicylaldehydes and their Cu(II) complexes. These Schiff bases and their complexes have been structurally characterized by elemental analysis, magnetic susceptibility measurements, spectral techniques and TG-DTA. The ligands and their metal complexes have been crystallized by slow evaporation / diffusion methods for X-ray diffraction studies. Based on the analytical and spectral data square planar geometry is assigned for binary complexes. The ligands and their complexes have been screened for antimicrobial activity against bacteria (Escherichia coli and Pseudomonas aeruginosa) and fungi (Aspergillus niger and Rhizopus oryzae) by paper disc method. It is observed that the Cu(II) complexes showed more activity than corresponding Schiff bases. Binding studies of these complexes with Calf thymus DNA (CT-DNA) have been investigated by UV spectra and Viscocity measurements. It is found that these complexes are binding through intercalation to CT-DNA. Further DNA cleavage experiments have also been investigated by agarose gel electrophoresis on pBR322 and it is observed that these Cu(II) complexes are capable of cleaving supercoiled plasmid DNA in the presence of H_2O_2 and UV light. In vitro antitumor activity of some Cu(II) complexes on Human Cervical Carcinoma Cells (HeLa) have been measured using the MTT assay, it is found that some Cu(II) complexes exhibited good antitumor activity on HeLa cell lines.

IIL-02 : Effects of Different Chemicals and Probiotic on the Blood Biochemistry Profile of Living Species

Raj Ranjan Jha

P. G. Deptt. of Chemistry, Ranchi University, Ranchi (Jharkhand)
E-mail : rajranjanjha@yahoo.co.in

In recent years the inorganic constituents in biological system have been receiving increasing attention. One of the major roles played by metallic element in biochemistry is in metaloenzymes and in the enzyme catalysis. The role of the metal atoms in enzymic

catalysis is currently an active subject of research. The trace elements unquestionably play an important role in Pathology and Physiology of biological system. Therefore, the effect of probiotic bacterial culture and mineral mixture individually or in ‘combination was studied in 30, apparently healthy weaned rabbits of 6 weeks of age.

At 6^{th} week of age, all the rabbits were randomly divided into five groups. Each group was having 6 rabbits. Group G_1 was considered as control group maintained on basal diet without probiotic and mineral mixture. G_2 and G_3 groups were supplemented with 2% and 4% mineral mixture, respectively along with basal diet. Group G_4 was supplemented with 60g probiotic along with basal diet whereas G_5 group was supplemented with 60g probiotic and 2% mineral mixture along with basal diet.

The present results showed that rabbits of G_5 and G_4 groups had significantly higher total serum protein values compared with the other dietary treatments. Glucose level was observed highest in the G_5 group followed by G_4 group. The total serum cholesterol level was reduced significantly in treatment groups as compared to control group suggesting that these feed supplements may reduce the cholesterol level and may be helpful in preventing atherosclerosis or other cardiac diseases. The highest level of lipid in blood of rabbit was observed in G_5 group. They were in their physiological level indicating that supplementation of probiotics/ yeast culture and mineral mixture did not change the ratio of these minerals in the blood. It further supported that these feed supplements have no adverse effect on kidney.

The rabbits of G_3 group had higher body weight than G_2 & G_1 groups during experimental period.

IIL-03 : Development of Copper(II)-Based Homogeneous Catalysts for the Synthesis of 1,2,3-Triazoles and Symmetrical Biaryls

Devendra D. Pathak, Samaresh Layek and Bhumika Agrahari

Department of Applied Chemistry, Indian Institute of Technology (Indian School of Mines), Dhanbad-826004, Jharkhand
E-mail : ddpathak@yahoo.com

Copper(II) compounds have long been used as catalysts in a variety of organic reactions such as Ullmann, Diels-Alder, Suzuki, Kharasch-Sosnovsky and Castro-Stevens coupling. Copper(I) catalyzed Azide-Alkyne Cycloaddition (CuAAC) reactions are the premise of “Click Chemistry”.[1] In continuation of our recent interest

in transition-metal mediated organic synthesis, we report an easy synthesis of two new copper(II) complexes $[Cu(dppo)_2]$, **1**, (dppo = 1,3-diphenylpropane-1,3-dione) and $[Cu(cyhxn)_2(H_2O)_2][OTf]_2$, **2**, (cyhxn = *trans*-cyclohexane-1,2-diamine) from $CuCl_2.2H_2O$ and $[Cu(OTf)_2]$, respectively and the corresponding ligand in methanol. Both complexes have been isolated and characterized by various spectroscopic techniques and single crystal X-ray studies. The complex **1** has been found to be a versatile catalyst for the synthesis of 1,2,3-triazoles from an arylboronic acid, sodium azide and an alkyne at rt,[2] while complex **2** proved to be a promising catalyst for synthesis of symmetrical biaryls from arylboronic acids, without the use of a base or oxidant. The IR, UV, EPR and CV data on complexes will be discussed along with the catalytic applications of both complexes in C-C and C-N bond formation reactions.

IIL-04 : Design, Single Crystal Structures, Spectral and Electrochemical Properties of Binuclear Copper(II) Complexes as Possible Antioxidant Catalysts for Superoxide Dismutation

R. N. Patel

Department of Chemistry, A. P. S. University Rewa (M.P.) 486003
E-mail : rnp64@ymail.com

Binuclear complexes have been receiving considerable interest due to their biological and industrial relevance. Copper serves as co-factor in many biochemical reactions mediated by enzymes. These enzymes are involved in distinct process in living systems. The low molecular weight complexes with antioxidant superoxide dismutase (SOD) activity have been proposed for the treatment of a vast variety of diseases. Antioxidant SOD mimics could have distinct advantage over the natural enzymes as pharmaceutical agents, including the ability to access intercellular space, cellular permeability, the lack of immunogenanicity, a longer half-life time in the blood potential and oral delivery a lower lost goods. It has been a great interest to investigate the biomimetic activity of dicopper complexes using $O_2^{\cdot -}$ as a convenient model substrate for the identification of functional model for the metalloenzymes, in a biomimetic approach. On the basis of the proposed catalytic mechanism and the X-ray information available for antioxidant SOD activity, we have synthesized several copper(II) binuclear complexes having as a main requirement the presence of two copper centers in close proximity to permit the binding of the $O_2^{\cdot -}$ prior to the electron transfer reaction. Present complexes act as catalysts for Cu-CuSOD and are good examples of metal-substituted

derivative of Cu-ZnSOD. Studies of a metal substituted derivative could help in the evolution of mechanistic possibilities for enzymatic reaction. Antioxidant SOD activity of this types of derivative is interesting. The single crystal structures, properties and antioxidant superoxide dismutase activity of various binuclear copper(II) complexes will be highlighted.

IIL-05 : Recent Forontiers of Carbon Nanotubes

C. P. Bhasin

Department of Chemistry, Hem. North Gujarat University, Patan- 384 265 (Gujarat)
E-mail : cpbhasin@yahoo.c

Tremendous progress has been achieved during the past 25 years on not only improving the yields of carbon nanotubes and move progressively towards their mass production, but also on gaining a profound fundamental understanding of the nucleation and the growth processes. Parameters that influence the yield but also the quality (e.g., microstructure, homogeneity within a batch) are better understood. The influence of the carbon precursor, the reaction conditions, the presence of a catalyst, the chemical and physical status of the latter, and other factors have been extensively studied. The purpose of the present Review is not to list all the experiments reported in the literature, but rather to identify trends and provide a comprehensive summary on the role of selected parameters. The role of the catalyst occupies a central place in this Reviews a careful control of the metal particle size, particle dispersion on the support, the metastable phase formed under reaction conditions, its possible reconstruction, and faceting strongly influence the diameter of the carbon nanotubes, their structure (number of walls, graphene sheet orientation, chirality), their alignment, and the yield.

IIL-06 : Tetragonally Distorted Octahedral complexes of Cu(II)

Punam Verma and Shivadhar Sharma

Institute of Bio-Chemistry, Magadh University, Bodh Gaya

Some six coordinate complexes of Cu(II) have been synthesized with metribuzin as primary ligand and Cl^-, Br^-, NO^-_3, $CH_3{}^-COO^-$ and ClO_4^- as secondary ligands. They have been characterized by microanalysis, i.r. spectra molar conductivity, magnetic moment, electronic spectra and E.S.R. spectra. The values of the various crystal field parameters like $Dq_{(xy)}$, $Dq_{(Z)}$ Ds and Dt have been derived from their electronic spectra which suggest obvious distortion in their octahedral symmetry. The values of g_{II} and $g_{\wedge}$

derived from their E.S.R. spectra clearly show the presence of the unpaired electron in dx^2-y^2 orbital of Cu(II). The magnetic moment values of Cu(II) complexes show that they are magnetically dilute i.e. mononuclear complexes. Metribuzin is a well known herbicide. Hence the herbicidal character of Cu(II) complexes of metribuzin has also been studied and it has been observed that the herbicidal character of metribuzin is inhanced on complexation with Cu(II).

IO-CYSA-1 : Magnetically Retrievable Nickel Substituted Barium Ferrite ($Ba_{1-x}Ni_x Fe_2O_4$; x=0.0 0.2, 0.4, 0.6, 0.8, 1.0) Catalyst Synthesized by Citric Acid Auto Combustion Method for Efficient Reduction of 2-Nitrophenol

Chandu N. Potangale and Satish K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune
**E-mail : skpar@chem.unipune.ac.in*

This study deals with the scrutiny of mixed metal oxide of barium ferrite Ba_{1-x} $Ni_xFe_2O_4$ (x=0.0, 0.2, 0.4, 0.6, 0.8, 1.0) as catalysts for the reduction of 2-nitrophenol. The ferrite samples with uniform particle size are synthesized using the citric acid auto combustion technique. Barium nickel iron citrate precursors by TG-DTA, revealed the calcination temperature 800 ^oC. Powder X-ray diffraction patterns demonstrated the single phase formation of synthesized catalyst. The catalytic activity of synthesized ferrites is checked for reduction of 2-nitrophenol to 2-aminophenol in water where $NaBH_4$ is used as reducing agent. The effect of varying ratio of amount of catalyst and 2-nitrophenol is scrutinized. The enhanced reduction efficacy was observed with the introduction of Ni^{2+} in to the Barium ferrite lattice due to octahedral site preference of Ni^{2+} and synergistic effect of metal ions.

IO-CYSA-2 : Selective N-acetylation with Simultaneous S-oxidation of *o*-amino Thiol Over Ce Doped ZnO Nanocrystallites

R. M. Jagtap, Arun V. Bagade and S. K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
**E-mail : skpar@chem.unipune.ac.in*

The organic transformations with selectivity of the products have attracted a great attention of the researchers. ZnO is a renowned semiconductor due to oxygen vacancies including good transparency, high electron mobility and wide band gap (3.2 eV).

Along with electronic properties, the Lewis acidity of ZnO is imperative for catalysis and it can also be tuned by doping some metal like La, Ce, Al, Co, Ni etc.

In present work, we have synthesized Ce doped ZnO by simple co precipitation method. The hydroxide precursors calcined at 400°C to get 0 to 10% CeZnO spherical nanocrystallites. The synthesized materials were well characterized by IR, XRD and DRS spectroscopy. The sphere morphology, crystallite size and elemental analysis were confirmed by SEM-EDS analysis. The application of CeZnO as an efficient catalyst towards the selective acetylation of *o*-amino thiol at ambient temperature was studied in acetonitrile. The 7.5% CeZnO was found to be the best catalyst which achieved simultaneous dual transformations as selective N-acetylation and S-oxidation of *o*-amino thiol.

IO-CYSA-3 : Dual mode Emission-active Ratiometric and Intensity-based Zinc Probes for Cell Imaging

Krishna Naik and Vidyanand K. Revankar

Dept. of Chemistry, Karnatak University, Dharwad - 580003
E-mail : krishnanaik.kud@gmail.com, vkrevankar@rediffmail.com

Present study reports Zn^{2+} chemosensing potencies of two novel pyrazole based moieties, bis(2-hydroxybenzylidene)-1H-pyrazole-3,5-dicarbohydrazide(PHSA) and bis(2-hydroxy-3-methoxybenzylidene)-1H-pyrazole-3,5-dicarbohydrazide(PHOV). Despite structural similarities, the two chemosensors operate via two different dual mechanisms for Zn^{2+} sensing. Enhanced red shift in the emission of the ratiometric probe and minimized proton induced interferences in intensity based probes are observed. The probes exhibit dissociation constants 1.2156 and 4.7997nM for PHSA and PHOV respectively. The detection limit is in the range of 10^{-9} M. The probes demonstrate lower cytotoxicity levels against HeLa cells and selectively lethal to Leukemia cells. Further, both the probes successfully visualize intracellular Zn^{2+} in HeLa cells and Vigna radiata.

IO-CYSA-4 : Hydroxamic Acids - Co (II)/ Mo (VI) Complexes : Interaction Studies With DNA/RNA

Yamini Thakur and Rama Pande*

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur-492010, Chhattisgarh
E-mail: yamini.thakur2010@gmail.com

The present study embodies the detail of interaction of Co-N-p-tolylbenzohydroxamic acid (Co-N-TBHA) and Mo-N-phenyl-p-

methoxybenzohydroxamic acid(Mo-N-PMBHA) with Poly(A) and its consequences by UV-Visible absorption , fluorescence spectroscopy, viscosity measurements and molecular docking. Comparative binding studies were also performed with ct-DNA and t-RNA. Absorption studies of the interaction of Co-N-TBHA and Mo-N-PMBHA with Poly(A)/ct-DNA/t-RNA have indicated that these complexes can bind to nucleic acids and the binding constants were calculated. Fluorescence quenching spectra revealed strong binding of Co-N-TBHA and Mo-N-PMBHA to Poly(A)/ct-DNA/t-RNA. The relative viscosities of hydroxamic acid-Poly (A)/ct-DNA/t-RNA complexes have increased value as compared to Poly (A)/ct-DNA/t-RNA alone. The docked posture of Poly(A)/ct-DNA/t-RNA with Co-N-TBHA and Mo-N-PMBHA uncover the strong binding interactions as it has smaller value of binding energy. This study provides detailed insight into the binding specificity of Co-N-TBHA and Mo-N-PMBHA to Poly(A) over several other nucleic acid structures. The binding affinity follows the order of Mo-N-PMBHA > Co-N-TBHA suggesting its potential as a lead compound for RNA based drug targeting.

IO-CYSA-5 : In situ Oxidation Triggered Heteroleptically Deprotonated Cobalt(III) and Homoleptic Nickel(II) Complexes of Diacetyl Monoxime Derived Novel Trinitrogen Chelators; Anticancer Activity of the Most Active Complex

Vinayak Kamat and Vidyanand Revankar

Dept. of Chemistry, Karnatak University, Dharwad - 580003
E-mail : vinukamat@gmail.com, vkrevankar@rediffmail.com

Two novel trinitrogen chelating unsymmetrical Schiff base ligands, 3-(hydroxyimino)-2-butanone-2- (1*H*- benzothiazol- 2- yl) hydrazone and 3-(hydroxyimino)-2-butanone-2- (1*H*- benzimidazol- 2- yl) hydrazone are synthesized by the condensation reaction of diacetyl monoxime with 2-hydrazino-benzothiazole/benzimidazole. Ligands have shown ML_2 type octahedral coordination towards Ni(II) and in situ generated Co(III) ions. Ligands and complexes are characterized by various spectro-analytical techniques. Both the ligands have shown similar mode of ligation, but different mode of deprotonation with the metal ions. Ligands are left neutral and innocent in the case of nickel complexes while anionic and non innocent in the case of cobalt complexes. Further, in situ oxidation of Co(II) to Co(III) has triggered a different mode of deprotonation between the two ligands of the same cobalt complex. Out of the four complexes synthesized, three complexes are characterized by SC-XRD technique, to evidence the structural facts. A comparative account of bond lengths of two complexes of the

same ligand is presented. Structures of all the four complexes have been screened priminarily for their anticancer potencies. Further, one among the four, the nickel complex of benzothiazole core is used for one dose growth inhibition activity analysis against 53 different cell lines. The tested complex has shown highest growth inhibition over a Non-Small Cell Lung Cancer cell line EKVX.

IO-CYSA-6 : Hierarchical Synthesis of Silver Monoliths and Their Efficient Catalytic Activity for the Reduction of 4-Nitrophenol to 4-Aminophenol.

Mustri Bano[*] and Farid Khan

Nanomaterials Discovery Laboratory, Department of Chemistry, Dr. H. S. Gour Central University, Sagar – 470003
[*]E-mail : mustribano1@gmail.com;

A novel catalyst Ag/triton X-705/SiNPs is synthesized by modified sol-gel method without the use of acid or base as catalyst for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in presence of 0.1M $NaBH_4$ in aqueous media. The reduction time was 30-35 seconds is a function of concentration of 4-NP varied from 0.001M to 0.009M at a constant concentration of Ag/Triton X-705/SiNPs 0.006g. Fe_3O_4NPs, dextran, and trimethylbenzene (TMB) were added separately to Ag/ Triton X-705 hydrogel to modify their morphology and catalytic activities against the reduction of 4-NP to 4-AP. The as synthesized monoliths were characterized by FT-IR, TGA, PXRD Analysis, SEM, TEM and (BET) surface area analyzer. Pseudo first order rate constant (k), energy of activation (E_a), and thermodynamic parameters viz. activation enthalpy ($\Delta H^{\#}$), activation Gibbs free energy ($\Delta G^{\#}$) and entropy of activation ($\Delta S^{\#}$) have also been determined. The turn over frequency (TOF) of Ag/Triton X-705/SiNPs catalyst was 9.66×10^{20} molecules/sec and the catalyst used up to nine cycles successfully with greater efficiency claimed to be a potential and leading candidate for the industrial conversion of 4-NP to 4-AP. We claimed that the catalyst Ag/Triton X-705/SiNPs took almost minimum time for the reduction of 4-NP to 4-AP.

IO-CYSA-7 : DNA Interaction, Antimicrobial Studies of Newly Synthesized Copper (II) Complexes with 2-Amino-6-(trifluoromethoxy)Benzothiazole Schiff base Ligands

Aveli Rambabu and Shivaraj[*]

Department of Chemistry, Osmania University, Hyderabad, Telangana-500007
E-mail : shivaraj_sunny@yahoo.co.in

Four novel Schiff base ligands, **L**[1](1-((*E*)-(6-(trifluoromethoxy)

benzo[*d*]thiazol-2-ylimino)methyl)naphthalen-2-ol,$C_{19}H_{11}F_3N_2O_2S$), **L**^{2}(3-((*E*)-(6-(trifluoromethoxy)benzo[*d*]thiazol-2-ylimino)methyl) benzene-1,2-diol, $C_{15}H_9F_3N_2O_3S$),**L**^{3}(2-((*E*)-(6-(trifluoromethoxy) benzo[*d*]thiazol-2-ylimino)methyl)-5-methoxyphenol,$C_{16}H_{11}F_3N_2O_3S$) and**L**^{4}(2-((*E*)-(6-(trifluoromethoxy)benzo[*d*]thiazol-2-ylimino)methyl)-4-bromophenol, $C_{15}H_8BrF_3N_2O_2S$) and their binary copper(II) complexes **1**[Cu(L^1)$_2$], **2**[Cu(L^2)$_2$],**3**[Cu(L^3)$_2$] and **4**[Cu(L^4)$_2$]have been synthesizedand characterized by elemental analysis, ^{1}H-NMR, ^{13}C-NMR, ESI mass, FT-IR, ESR, UV-Visible, magnetic susceptibility, TGA, SEM and powder XRD studies. Based on spectral and analytical data, a square planar geometry is assigned for all Cu(II) complexes. The ligands and their Cu(II) complexes have been screened for antimicrobial activity against bacterial species*E. coli, P. aeruginosa, B.amyloliquefaciens*and *S. aureus*and fungal species *S. rolfsii* and *M. Phaseolina* and it is observed that all Cu(II) complexes are more potent than corresponding ligands. DNA binding (UV absorption, fluorescence and viscosity titrations) and cleavage (oxidative and photo cleavage) studies of Cu(II) complexes have also been investigated against calf thymus DNA (CT-DNA) and supercoiled pBR322 DNA respectively. From the experimental results, it is found that the complexes bind effectively to CT-DNA through an intercalative mode and also cleavage pBR322 DNA in an efficient manner.

IO-CYSA-08 : Exploration of DNA Interactions and Biocidal Activity of Incorporated Benzothiazole Schiff base Complexes : Synthesis and Validation

Narendrula Vamsi Krishna, Gali Ramesh and Shivaraj*

Department of Chemistry, Osmania University, Hyderabad, Telangana-500007
E-mail : shivaraj_sunny@yahoo.co.in

Using the novel Schiff base ligands, L_1=2-(-(benzothiazol-6-ylimino)methyl)-4-chlorophenol (BTEMCP), L_2=2-(-(benzothiazol-6-ylimino)methyl)-4-nitrophenol (BTEMNP) bivalent Cu(II), Ni(II) and Co(II) complexes have been synthesized and characterized by analytical and spectral methods like elemental analysis, Mass, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, IR, ESR, SEM, EDX and XRD. Considering magnetic moment and UV-visible spectral data square planar geometry has been proposed to all metal complexes. The interactions between the complexes and DNA have been investigated by means of electronic absorption, fluorescence spectroscopy, viscosity and agarose gel electrophoresis. The antibacterial activity of the Schiff

bases and their complexes have been studied and the data showed that the metal complexes have more potent biocidal activity than the parent Schiff base ligands.

IO-CYSA-09 : Spectroscopic Characterization and Antimicrobial Studies of Some Novel Complexes

Hardik D. Chaudhary[1], Jwalant J. Vora[1] and Jabali J. Vora[2*]

[1]M.G. Science Institute Ahmedabad, Gujarat
[2]Hemchandracharya North Gujarat University, Patan-384 265 Gujarat*

Coordination chemistry is a very rapidly growing branch due to its multidisciplinary characteristics. Biologically important molecules have tendency to form complex with natural receptor sites as well as coordinate compounds with biologically important metal ions. Furthermore, coordination compounds are found to be, sometimes, more physiologically active in comparison with the parent bioactive ligand. Furthermore, ligands with heterocyclic system and multiple functional groups are found to be much physiologically active. Therefore, similar kind of ligands have been taken in there complexes are prepared with Zn(II), Mn(II), Co(II), Ni(II), Cd(II), Cu(II) and Hg(II) These are characterized by spectroscopic methods and subjected to biochemical studies.

IO-CYSA-10 : Copper(II) Mono- and Binuclear Complexes : Biomimetic Synthesis, Antioxidant SOD Activity and DFT Calculations

Yogendra Pratap Singh and R. N. Patel[*]

Department of Chemistry, A.P.S. University, Rewa-486003 (M.P.)
E-mail : ypsingh777@gmail.com

Three new copper(II) complexes, viz., $[Cu(L)(NO_3)(H\text{-}_2O)]H_2O$ **1,** $[Cu(L)(H\text{-}_2O)_2]NO_3$ **2** and $[Cu_2(L)_2(pyrazine)](ClO_4)_2{\cdot}4H_2O$ **3** were prepared by the biomimetic synthesis strategy [HL = 4-chloro-2-{(*E*)-[2-(pyridin-2-yl)hydrazinylidene]methyl}phenol] Structural characterization revealed very different local geometries about to copper(II) ions, being square pyramidal for homonuclear complexes (τ_5 = 0.021 for **1** and τ_5 = 0.13 for **2**) and square planar for homobinuclear pyrazine bridged complex **3** (τ_4 = 0.06). The crystal structure of complexes **1-3** are formed by supramolecular structure by classical and non-classical hydrogen bonding. Magnetic measurements of bulk material **1, 2** and **3** revealed weak antiferromagnetic coupling in all complexes, however, of very different strengths. The epr spectra of **1, 2** and **3** complexes in polycrystalline state exhibited broad signals at g 2.15 due to spin-

spin interaction between two copper ions. The cyclic voltammograms of mononuclear complexes (**1** and **2**) in DMSO gave one Cu^{II}/Cu^{I} irreversible wave. On other hand, pyrazine bridged binuclear complex **3** exhibited two waves which correspond to $Cu^{II}Cu^{II}$ / $Cu^{II}Cu^{I}$ and $Cu^{II}Cu^{I}$ / $Cu^{I}Cu^{I}$ redox processes. Differential pulse voltammetry (DPV) experiments also exhibited the same reduction behavior. These complexes exhibited effective antioxidant SOD activity. On the basis of experimental and theoretical DFT studies, the structure-activity relationship of these complexes have also been discussed.

IO-01 : Establishment of A Novel Series of Soild State Charge Transfer Complexes Based on Non-Transitional Metal Juglonates

Mrudula Wadekar[1], P. S. Khandagale[2], B. M. Rawal[3] and S. S. Kadam[1]

[1]Y. M. College, Bharati Vidyapeeth University, Paud Road, Pune-411038
[2]Henkel Private limited, Hinjiwadi, Pune
[3]South Gujarath University, Surat, (Gujarath)
E-mail : m_p_wadekar@yahoo.co.in

Juglones are hydroxy derivatives of 1,4 naphthoquinone (I) in which the hydroxy group is placed at C_{-2}, C_3, C_5 or C_8 positions. While synthesizing their metal chelates with non transition metals, we have come across an interesting and attractive series of metal chelates which possess intense visible colours.The characteristic features of all these chelates are as follows (a) nature of these colours depends on the specific juglone derivatives as well as the central metal ion (b) these colours cover not only the entire visible spectrum but several of their intermediate shades (c) all these chelates are sparingly soluble in water and inert organic solvents, they are however relatively more soluble in donor organic solvents (d) the intense colours are quite stable in solid state over a very long period (e) the colour intensity diminishes to a large extent in their solution state (f) the particle size of many of these juglonates tends to nanometric level.

Up till now, we have synthesized more than 250 such metal Juglonates which constitute a novel series of **solid state charge transfer complexes**. This is a unique series of this type to be introduced in coordination chemistry. Through this communication, we would like to present a brief account of the nature, characteristic features and possible applications of this novel series.

IO-02 : Synthesis, Characterization and Biological Aspects of Co(II) and Ni(II) Metal Complexes of Schiff base 4-(2,5-dimethoxybenzylidene)-Amino-3-Mercapto-6-Methyl-5-Oxo-1,2,4-Triazine

Kiran Singh[*] and Ritu[1]

Department of Chemistry, Kurukshetra University, Kurukshetra-136119
[*]E-mail : kiransinghkuk@yahoo.co.in

Co(II) and Ni(II) metal complexes have been synthesized with Schiff base derived by condensation of 4-amino-3-mercapto-6-methyl-5-oxo-1,2,4-triazine with 2,5-dimethoxybenzaldehyde. All the newly synthesized compounds were characterized with the help of IR, NMR, electronic and magnetic moment measurements. Molar conductance data indicates the non-electrolytic nature of metal complexes.On the basis of above techniques octahedral geometries have been proposed around Co(II) and Ni(II) complexes. Agar well diffusion method was used to evaluate the biological activity of Schiff base and its metal complexes against various microbes named as: *Bacillus subtilis*, *Staphylococcus aureus,Pseudomonas aeruginosa*, *Escherichia coli,Candidaalbicans* and *Saccharomyces cerevisiae*. It has been observed that all the metal complexes exhibit better antimicrobial activity as compared to Schiff base.

IO-03 : Effect of Glycine on Optical, Dielectric and Second Harmonic Generation (SHG) of Bisthiourea Manganese Malonate : A New Semiorganic Non-Linear Optical Material

Malhari N. Raste and Satish K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
[*]E-mail : skpar@chem.unipune.ac.in

A new class of semiorganic nonlinear optical materials viz. bisthiourea manganese malonate (BTMnM) and glycine doped bisthiourea manganese malonate (BTMnM-Gly) has been synthesized by mechanochemical method. They are characterized by various techniques. Chemical composition was confirmed by chemical and CHNS analysis. Incorporation of glycine in pure compound was determined by FTIR and EDAX. FTIR studies also ascertained the coordination of metal ions to thiourea through sulphur atom. SEM images show BTMnM is crystalline with hexagonal shape and BTMnM-Gly, porous and agglomerated in nature. Thermal stability was investigated by TG and DTA showing BTMnM is more stable. Transmittance spectra reveal that lower UV cut-off wavelength of

BTMnM is 316nm and that of BTMnM-Gly, 295nm, thus both materials have good optical transmission in entire visible region. The dielectric measurements of material with varying frequencies at room temperature were also studied. Dielectric constant and dielectric loss decreases with increase in frequency. These lower values at high frequency enhance the second harmonic generation efficiency. The SHG measured by Kurtz-Perry powder technique was found to be higher for BTMnM-Gly than pure BTMnM. However it is 0.255 times lower to that of KDP which defines nonlinear optical nature of material and their suitability for NLO applications.

IO-04 : Synergism of Ba-Ca-Fe in $Ba_xCa_{1-x}Fe_2O_4$, Where $0.0 \leq X \leq 1.0$ Towards Catalytic Degradation of Toxic Rhodamine-6G under Ambient Light Condition

Ravindra Y. Pawar, Sangita N. Pund and Satish K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007

**E-mail : skpar@chem.unipune.ac.in*

The catalytic degradation of Rhodamine-6G (Rh-6G) has been investigated in aqueous solutions using barium substituted calcium ferrite (BSC), $Ba_xCa_{1-x}Fe_2O_4$, (where $0.0 \leq x \leq 1.0$) as catalyst which is synthesized by citrate gel combustion method and well characterized by various techniques. The experiments were carried out to investigate the factors that influence the Rh-6G catalytic degradation. A preferential degradation of Rh-6G dye was identified by spectroscopic method. The effect of various parameters like, chemical composition of the catalyst, pH of the medium, reaction temperature, concentration of dye, and catalyst amount on the degradation process were studied in detail. The experimental results show that, the degradation of Rh-6G is possible in absence of any external oxidizing agent like H_2O_2 and ambient light conditions. Degradation efficiency remains higher than 90% even when the catalyst $Ba_xCa_{1-x}Fe_2O_4$ is being used for 4 cycles. $Ba_{0.8}Sr_{0.2}Fe_2O_4$ was found to be a better catalyst amongst the series towards the degradation of Rh-6G in aqueous medium. It is due to the synergism between Ba, Ca and Fe ions in $Ba_{0.8}Ca_{0.2}Fe_2O_4$. Hence, taking into account the favorable catalytic properties and low leaching of iron ions, BSC ferrite is a promising catalyst for dye wastewater treatment.

IO-05 : Discrete Supramlecular Palladium Nano-Cages as Efficient Catalysts for C-C Coupling Reactions

Subhashis Pradhan and Rohith P. John*

Department of Applied Chemistry, Indian Institute of Technology (ISM), Dhanbad-826004, Jharkhand
E-mail : rohithjohn@gmail.com

Supramolecular metal–organic assemblies are widely studied for their architectural diversity, magnetic properties, molecular sensing and catalytic applications. In many such assemblies the key design strategy involves use of ligands of various podalities and metal ions as connecting nodes. In the design of discrete assemblies using ligands with N-terminal donor atoms, Cu, Pt and Pd are employed to provide square-planar connecting node. In this context, we have explored the potential for C-C coupling reaction by two such discrete palladium containing metal-organic assemblies, $Pd_2(L^1)_4$, **1**, and $Pd_6(L^2)_8$, **2**. L^1 is pyridine terminal dipodal ligand while L^2 is a tripodal ligand. The discrete Pd-assemblies were characterized by ESI-mass and ^{1}H-NMR analysis. The size of the assembly, **1**, was determined by HR-TEM measurements to be about ~2.2nm, and that of **2** was found to be ~2.8nm. The structure of the assembly **1** was optimized using HF calculations and STO-3G basis set, while that of **2** was carried using B3LYP functional and 3-21G basis set. The sizes of the optimized assemblies are in conformity with the experimentally obtained values. A series of Suzuki and Heck coupling reactions were carried out using assembly **1**. The compound catalyses Suzuki reactions heterogeneously in aqueous ethanol medium under mild and 'phosphine free' conditions, while Heck reactions homogeneously in DMF. The integrity of the catalysts was monitored using, FE-SEM/EDX analysis. Both the catalysts were found to catalyze upto 3rd cycle without losing significant activity. The assembly **2**, was found to catalyse Sonogashira reaction in water under copper free conditions.

IO-06 : Dioxomolybdenum (VI) Complexes with o-Phenylenediamine and 4-Methyl-o-Phenylenediamine Ligands

Sushma Sinha* and Ashwini Kumar[1]

**Department of Chemistry, M.S.K.B.College, Muzaffarpur*
[1]Department of Chemistry, S.N.S.College, Muzaffarpur
E-mail : sushmashinha52@gmail.com

Two new dioxomolybdenum (VI) complexes $[MoO_2(acac)LL2]$ (I) and $[MoO_2L_2L_23]$ (II)[L=$OC(CH_3)CHCOCH_3$, L2 =$NH_2C_6H_4NH_2$,

L3 = $NH_2C_6H_3CH_3NH_2$] with diamine o-Phenylenediamine (OPDA) and 4- Methyl-o-Phenylenediamine (4-Me-OPDA) ligands have been synthesized and characterized. Compounds (I) (61% yield) and (II) (62% yield) were obtained from the reactions of $MoO_2(acac)_2$ [acac=acetyl acetonato] with 1 equiv. of OPDA and 4-Me-OPDA. ^1H, ^{13}C NMR, IR spectral data indicated that the ligands acted as unidentate and structures of both compounds were six-coordinated. The dioxomolybdenum (VI) complexes (I) and (II) are efficient catalysts for oxidation of alcohols with H_2O_2 as an oxidant.

IO-07 : Studies on Fluoroboro-Bridged Macrocyclic Complexes of Cobalt(III)

Ashwini Kumar[*] and Anamika[1]

[*]Department of Chemistry, S.N.S. College, BRA Bihar University, Muzaffarpur, (Bihar)
[1]Department of Chemistry, Jamshedpur Women's College, Jamshedpur, Kolhan University (Jharkhand)
E-mail : ashwinikumar.chem@gmail.com

A series of fluoro-boro-bridged Co (III) macrocyclic complexes of the type CoCyB'X, where Cy represents the macrocyclic ligand, 1,8-diboro-2,7,9,14-tetraoxa-1,1,8,8-tetrafluoro-3,6,10,12-tetraaza-4,5,11,12-tetrafurylcyclotetradeca-3,5,10,12-tetraene, [bofafcyclene(14)], X represents halide ions and B' represents a nitrogen donor base as pyridine, β-picoline or γ-picoline, have been prepared by the reaction of boron trifluoride on oxime complexes of the type [Co(oxime H)$_2$B'X]. Structurally important IR bands, viz. $\nu_{C\text{-}N}$, $\nu_{N\text{-}O,}$ $\nu_{B\text{-}O,}$ and $\nu_{B\text{-}F,}$ have been identified. Some of the macrocyclic complexes shows the general features of the spectra of octahedral cobalt (III) complexes. While the spectra of others can be interpreted assuming a C_{4u} or D_{4h} symmetry. Ligand field splitting parameter 10 Dq and interelectronic repulsion parameter B have been calculated for the octahedral complexes. The tetragonal parameter (D_t) value for low symmetry complexes are all positive and are of the order of 600 cm^{-1}. Thermal studies indicate the stability to be found in the order : [Co bofafcyclene(14)pyX] < [Co bofafcyclene(14)β-picX] < [Co bofafcyclene(14)γ-picX].

IO-08 : Future Prospects of Nanotechnology

Anamika* and Ashwini Kumar[1]

[*]Department of Chemistry, Jamshedpur Women's College, Jamshedpur, Kolhan University (Jharkhand)
[1]Department of Chemistry, S.N.S. College, BRA Bihar University, Muzaffarpur, (Bihar)
E-mail : anni_a@rediffmail.com

Nanotechnology is the ability to manipulate material at a molecular level driving out novel and exciting properties. The

impact of nanotechnology is expanding and nothing will remain untouched. Applications are enormous and limitless. Nanotechnology enables in doing things better than conventional technology. The union of small molecules / ions like CO, H_2O, NH_3, N_2H_4 with cations such as H^+, Mg^{2+}, Fe^{2+} etc. on their own create supramolecules. Self assembly of these supramolecules form the material world. These assemblies union of scientific discipline is revealing the leading edge of Nanotechnology. Fullerenes, carbon nanotubes and atomic force microscopy were in their infancy. In less than a decade, material science and life science together are unraveling the mysteries of controlling, on a molecular level, the structure of matter. Nanotechnologies, major field of which include Nano manufacturing process, Nanomaterials, Nanodevices, and Nanomeasurement, are expected to become fundamental technologies for manufacturing in a wide range of industries. These new technologies are bound to have an impact on the chemical, energy, electronics and space industries. They will also have applications in medicine and health care, drug and gene delivery being important areas. This article brings the important facets of nanomaterials research, highlighting the current trends and future directions. Since synthesis, structure, properties and simulation are important element of nanoscience, materials chemists have a major role to play.

IO-09 : Synthesis, Spectroscopic, Molecular Structure, Electrochemistry and DFT studies of Some Oxidovanadium(IV) and Dioxidovanadium(V) Complexes

R. C. Maurya* **and P. K. Vishwakarma**

Coordination, Bioinorganic and Computational Chemistry Laboratory, Department of P. G. Studies and Research in Chemistry and Pharmacy, Rani Durgavati University, Jabalpur-482001 (M.P.) India

**E-mail : rcmaurya1@gmail.com, inorgpkv85@gmail.com*

This paper reports the synthesis, spectral, thermal, electrochemical and DFT studies of thiosemicarbazone derived ONS donor Schiff base oxidovanadium(IV) and dioxidovanadium(V) complexes. The interaction of bis(acetylacetonato)oxidovandium(IV), $[VO(acac)_2]$ with ONS-donor Schiff base ligands HL in 1:1 mole ratio [where, HL= dehydroaceticacid-N-thiosemicarbazone, Hdha-tsc **(I)**; dehydroaceticacid-N-4-methyl-3-thiosemicarbazone, Hdha-mtsc **(II)** or dehydroaceticacid-N-4-phenyl-3-thiosemicarbazone, Hdha-ptsc **(III)** in methanol for 15 minutes yields oxidovandium(IV) complexes of composition [VO(L)(acac)]. Aerial oxidation of

[VO(L)(acac)] for 5 days yields dioxidovandium(V) complexes of composition $[VO_2(L)(H_2O)]$. The Synthesized complexes were characterized by physicochemical analyses involving magnetic measurements, infrared, electronic, ESR, NMR spectral and thermal studies. Thermogravimetric (TG) curve was used to arrive at the insights of thermal stability of one of the synthesized complexes.

DFT studies have been carried out for the two representative complexes **3** and **6**. The molecular structures, infrared intensities, charge distribution and molecular orbital descriptions HOMO% LUMO, absolute electronegativity (χ_{abs}) and absolute hardness (η), non linear optical (NLO) properties, NBO, MESP, were obtained for molecule using the B3LYP density functional theory (DFT) with the standard B3LYP/LANL2DZ basis set. The nonlinear optical properties viz., dipole moment (μ), mean polarizability (α) total first hyperpolarizability (β_0) are also reported. The stability of the molecule arising from hyper-conjugative interaction and charge delocalization has been analyzed using NBO analysis. The combined experimental and calculated results justify the proposed octahedral geometry of the compounds.

IO-10 : Preparation and Characterization of Holmium Substituted Cobalt Ferrite Nanoparticles by Co-precipitation Method

Ramdas A. Pawar, Sujata S. Modhave and Manohar G. Chaskar

Department of Chemistry, PDEA's Baburaoji Gholap College, Sangavi, Pune– 411027
E-mail : rapawar@hotmail.com, rapawar9@gmail.com,

The ferrite nanoparticles with composition of $CoHo_xFe_{2-x}O_4$ (where x = 0.0 - 0.15) were prepared by chemical co-precipitation method, which allowed control of their composition and morphology. The preparation processes were monitored by thermal studies. The obtained ferries were characterized by XRD, TEM, d.c. electrical conductivity, thermoelectric power and Magnetic hysteresis measurements. The phase identification of the materials by X-ray diffraction reveals the single-phase nature of the materials. The lattice parameter increased with rare-earth content $x \leq 0.15$. The TEM photographs of these compounds were exhibit the average particle size in the range of 37.4 to 72.8 nm. The data of temperature variation of the direct current electrical conductivity showed definite breaks, which corresponds to ferrimagnetic to paramagnetic transitions. The thermoelectric power for all compound are positive over the whole range of temperature. The magnetic properties of rare-earth substituted cobalt ferrites showed a definite hysteresis loop at room temperature. The reduction of saturation

magnetization, ratio MR/MS and magnetic moments may be due to dilution the magnetic interaction.

IO-11 : Synthesis, Characterization, DFT Studies and Antioxidant Enzymatic Activity of Copper(II) Mono-, bi- and Polynuclear Complexes with N'-[(E)-Phenyl(pyridin-2-yl) Methylidene] Benzohydrazide

Yogendra Singh* and Ram N. Patel

Department of Chemistry, A.P.S. University, Rewa (M.P.) 486003
E-mail : ysapsurewa182@gmail.com

A series of five new copper(II) mono-, bi- and polynuclear complexes with *N*'-[(*E*)-phenyl(pyridin-2-yl)methylidene] benzohydrazide have been designed and synthesized as possible models for antioxidant superoxide dismutase mimics. All the synthesized copper(II) mono/binuclear complexes were characterized using various physicochemical techniques viz., microanalysis, FTIR, CV, UV, and EPR spectroscopy. The complexes are further characterized by single crystal X-ray methods. Variable temperature magnetic susptibility measurements have been carried out for binuclear complexes and shown an antiferromagnetic exchange interaction. The EPR spectra of these complexes exhibited broad signals centered g at g ≅ 2.74 due to the spin – spin interaction between or among the copper ions, while the EPR spectra of mononuclear copper(II) complexes (**1-3**) showed a signal which is characteristic of mononuclear square planar or trigonal bipyramidal (dz^2 ground state) copper(II) complexes. The cyclic voltamogramms of homo binuclear complexes (**4** and **5**) in DMSO gave the reversible waves which corresponds to Cu(II)——Cu(II) / Cu(I)——Cu(I) and Cu(II)——Cu(I) / Cu(II)——Cu(I) redox process. in addition all the complexes showed antioxidant superoxide anion free radical activity of biological pH.

IO-12 : Synthesis, Structural, Thermal and Computational Studies of Cu(II) and Zn(II) Complexes with N,O Donor Schiff base Ligand 2-chloro-6-{[(4-hydroxy-3-methoxyphenyl) methylidene] Amino}-4-Nitrophenol

A. P. Mishra* and Brajendra S. Kusmariya

Department of Chemistry, Dr. H. S. Gour Central University, Sagar-470003
E-mail : apmishrasagar@gmail.com, kusmariya@gmail.com

We report here two mononuclear Cu(II) and Zn(II) complexes of general formula $[M(L)_2].xH_2O$; {M = Cu^{II} & Zn^{II}} derived from

bidentate 2-chloro-6-{[(4-hydroxy-3-methoxyphenyl) methylidene] amino}-4 nitrophenol ligand (**HL**). These compounds were synthesized and characterized by elemental analysis, FT-IR, uv-vis, ^{1}H-NMR, molar conductance, thermal, PXRD and SEM-EDX studies.

The PXRD and SEM analysis shows the amorphous/ nanocrystalline nature of Cu(II)-complex and crystalline nature of Zn(II)-complex. The diffraction peak broadening was explained in terms of domain size and the crystallite lattice strain. Thermogravimetric analysis in the range of 300-1172K has been performed to determine the thermal stability of synthesized compounds. The non-isothermal kinetic parameters of degradation process were calculated using Coats-Redfern (C-R), Piloyan-Novikova (P-N) and Horowitz–Metzger (H-M) methods assuming first order degradation and proposed a random nucleation mechanism of thermal decomposition for both compounds. To support the experimental findings theoretical calculations by means of DFT and TD-DFT at B3LYP level were incorporated. In addition; frequency calculations, HOMO-LUMO, energy gap (ÄE), molecular electrostatic potential (MEP), spin density and crystal packing were also computed at the same level of theory.

IO-13 : Determination of Formation Constants and Free Energies of Same Mixed Ligand Complexes and Kinetic Parameters of Binary Complexes from TG Curves

Ravi Prakash and K.C. Gupta

Deptt. of Chemistry, B.S.A. College, Mathura – 281004
E-mail : kc.gupta78@gmail.com, drravichem@gmail.com

The Formation of 1:1:1 mixed ligand metal (M) complexes by Cu (II) and Ni (II) with Iminodiacetic acid (IDA) as a primary ligand (A) and L-Histidine and L-Cysteine as a secondary ligand (B) have been studied potentiometrically by employing the modified Irving and Rossotti method. The formation constants (log K^{MA}_{MAB}) were determined at (25± 1°C) in aqueous solution at μ = 0.2M ($NaClO_4$)

The free energies of formation ("F°) were calculated from the following equation.

$$\Delta F^{\circ} = -RT \ln K_{MBA}$$

The binary solid complexes of Cu (II) and Ni (II) with L-Cysteine were isolated from the equimolar solutions of metal per chlorates and ligands. The probable formulae were assigned on the

basis of elemental analysis which were supported by TG Curves. Kinetic parameters like activation energy (E_a), order of reaction, frequency factor (log Ƶ) and activation entropy (S^o) were calculated from the TG curves.

IO-14 : Stability Constants of Mixed Ligand Transition Metal Complexes

Bhoopendra Singh

Department of Chemistry, Agra College, Agra
E-mail : bhoopendrakkdc@gmail.com

Mixed ligand complexes of some transition metal viz., $Cu^{(II)}$, $Ni^{(II)}$, $CO^{(II)}$ and $Zn^{(II)}$ have been investigated Potentiometrically with 2-Hydroxy-benzalidine-anthranilic acid (HBBA), Pyridine-2,6-dicarboxylic acid (PDA) and Furan-2 carboxylic acid (FCA) in aqueous solution at temp. 25± 1^0C and 40 ± 1^0C at an ionic strength of 0.1 mol dm^{-3} (KNO_3). The stability constants of these 1:1:1 ternary complexes have been evaluated by the computational methods. The relative order of stability has been observed to be $Cu^{(II)}$ > $CO^{(II)}$ > $Zn^{(II)}$ > $Ni^{(II)}$. Which is in accordance with the increasing (ϕ) = charge / radius ratio. The change in thermodynamic parameter (Free energy change ΔG°, Enthalpy ΔG° and Entropy ΔG°) have also been calculated under the same conditions.

IO-15 : Synthesis and Characterisation of Magnesium, Zinc and Copper Metal Oxide Nanoparticles and Their Photocatalytic Application

Deepali and Manisha

In the present study different metal oxides (Magnesium, zinc and copper) nanoparticles were synthesized using two different methods wet chemical method and hydrothermal method.

In the preparation by wet chemical method the nitrates of the respective metals were dissolved in 100 ml of water to which NaOH Solution was added dropwise leading to generation of metal hydroxides. These hydroxides are calcined in furnace at 600 and oxide nanoparticles were obtained. In the hydrothermal method acetate salt of the metal dissolved in methanol was reacted wih sodium hydroxide in a Teflon lined sealed autoclave and heated at 100 under pressure for 6 hours.

These Nanoparticles were characterised using FESEM, EDAX and XRD to investigate their structural and morphological studies. The particles were tested for their antimicrobial and photocatalytic activity.

XRD data was used to calculate the particle size using Scherrers formula and it was found in the nanorange. SEM analysis showed metal oxide particles in the nanorange with varying morphology. Zinc oxide nanoparticles were in the range 70-150nm with spherical shape, whereas for MgO most of the nanoparticles are in the range 10-20 nm with spherical morphology. CuO nanoparticles showed rodshaped/ellipsoid morphology. EDAX confirms the presence of metals zinc, Mg and Cu in the samples. The photocatalytic activity of ZnO,MgO and CuO nanoparticles were investigated by the degradation of methylene blue dye in aqueous medium under natural sunlight. Results indicate that MgO nanoparticles having better photocatalytic efficiency under natural sunlight irradiation than ZnO and CuO nanoparticles. (may be due to smaller particle size.) Antibacterial study was carried using E coli and S aureus. Thus a very simple, cost-effective technique for development of nanoparticles was used. No specific conditions need to be maintained.

IO-16 : Green Synthesis of ZnO Nanoparticles using Plant Extracts

Sunil D. Kumbhar, Sunil B. Patil, Mahesh G. Kukade and Anita J. Bodake*

Department of Chemistry, Rajaram College, Vidyanagar, Kolhapur-416004 (MS)

Development of green nanotechnology is generating interest of researchers toward eco-friendly synthesis of nanoparticles. In the present study, stable zinc nanoparticles are synthesized using plants extract of Holarrhena pubescence seeds and Acanthocereus tetragonus leaves extract. The nanoparticles are characterized using X-ray diffraction, Fourier Transformed Infra-Red spectroscopy, Scanning Electron Microscopy, UV-Visible spectroscopy and Energy Dispersive Spectroscopy. The comparative results of synthesis were reported as H-ZnO and A-ZnO. It is observed that the morphology is well controlled in H-ZnO as compared to A-ZnO. Percentage composition of Zn and O in H-ZnO and in A-ZnO is studied by EDS analysis.

IO-17 : Green Synthesis, Characterisation, X-ray Studies and Supramolecular Associations of Organotellurium Compounds

Sangeeta Bajpai

Amity School of Applied Sciences, Amity University, Lucknow
E-mail : sbajpai1@amity.edu

The important aspect of Green chemistry for chemical synthesis

is to maximize the desired products and to minimize the by-productswhich acts as contaminants/ pollutants. Chemical wastes have a significant impact on our lives today. Though industrialization has played a pivotal role in solving many problems of the society but in this process environmental balance has been compromised up to great extent. Green color signals to proceed and green chemistry signals to sustain. In this context, some Organotellurium compounds (R2TeX2) (R = Alkyl, X = Halogens, Nitrates, Hydroxides etc) were synthesized by going green. The X-ray suitable crystals were grown in ecofriendly environment. These compounds were characterized by spectroscopic - and single X-ray diffraction studies. Supramolecular associations in these compounds are also discussed.

IO-18 : Optimization of the Rheological Properties of Silicon Carbide Slurries in Ceramic Processing Applications

A. S. Deshpande[1], P. A. Nagawade[1], P. V. Adhyapak[2] and A. K. Nikumbh[1*]

[1]Department of Chemistry, Savitribai Phule Pune University (Formerly University of Pune), Pune-411 007*
[2]Centre for Materials for Electronics Technology (C-MET), Panchawati, off Pashan Road, Pune-411 008
[*]E-mail : aknik@chem.unipune.ac.in

Casting behaviour and rheological properties are studied in order to define the appropriate conditions under which to prepare slips (i.e. slurries) for the production of high temperature ceramics. Various commercial Silicon carbide powders from different manufacturers were used. The compositional analysis of the powders was carried out by Energy dispersion X-ray analysis (EDAX). Phase purity of these powders was determined by X-ray powder diffraction patterns (XRD) which showed the single phase silicon carbide with cubic or hexagonal structure. The particle morphology and size were characterized using scanning electron microscopy (SEM) which showed a variation in shape and particulate size for these carbides. The surface area of these powders was measured by BET method and particle size distribution analysis was done using a laser granulometer. The particle size distribution and SEM measurements show that the silicon carbide powder (SC_2) was suitable for slip casting. The rheological properties were studied to define appropriate conditions for slip preparation. The slips (i.e. slurries) of this silicon carbide (SC_2) with different solid contents were prepared at different pH with deionized water and distilled ethanol as dispersing medium with and without dispersants. Polyethyleneimine (PEI) and Ammonium polyacrylate (Darvan C)

were used as dispersing agent. Investigations into rheology i.e. the dependence of viscosity and shear stress on shear rate were performed. HNO_3 and tetramethyl ammonium hydroxide were used for controlling the pH. The minimum viscosities were observed at pH = 7.9 for 80 wt% SiC powder (SC_2) and 20 wt% deionized water along with 0.2 wt% PEI dispersant system. The slip, green and sedimentation bulk density were measured.

IO-19 : Use of Canna Lily Flower as Photosensitizer in Dye Sensitized Solar Cell

Suprabha S. Sahoo, H. M. Pathan and Sunita Salunke Gawali*

Department of Chemistry, Savitribai Phule Pune University, Pune-411007
E-mail : sunitas@chem.unipune.ac.in

Use of naturally abundant flora and faunas as biggest source for generation of renewable energy in the field of photovoltaics plays a significant role to meet global energy demands and rapidly depleting fossil fuels. Despite of clean, ecofriendly, long-lasting and easily availability of solar energy cost-effectiveness and low performance of PV devices lead DSSC to come into public domain. Dye sensitized solar cells are the best alternatives than other types of Thin film technologies. Recent investigation conducted with a naturally available Canna (Canna Lily) flower extract in ethanol as a dye and sensitizing TiO_2 metal oxide as a photo anode. The device was fabricated with nano structured TiO_2 paste by doctor blade method followed by sintering at 450 °C for one hour in vacuum. The efficiency of the device was studied with the natural dye present in canna flower by varying its concentration, time of dye loading and changing reductive electrolytes. After 5 hours of dye loading we got power conversion efficiency of 0.019% which can be further improvised by optimising the parameters. Characterization of the film by UV-Visible, FT-IR spectroscopy, CV, SEM, X-ray diffraction studies has been done.

IO-20 : Synthesis and Physicochemical Properties of Substituted Pyrochlore-Type Nanooxides

M. B. Khanvilkar[1*], R. A. Pawar[2], M. D. Sangale[3], S. K. Pardeshi[4] and A. K. Nikumbh[4]

[1]Department of Chemistry, K. M. C. College, Khopoli, Dist-Raigad-410203.*
[2]Department of Chemistry, PDEA's Baburaoji Gholap College, Sangavi, Pune-411027
[3]Department of Chemistry, R.B.Narayan Borawake, College, Shrirampur, Dist-A.Nagar-413709.
[4]Department of Chemistry, Savitribai Phule Pune University, (Formerly Universityof Pune) Pune-411007.
[*]E-mail: mb.khanvilkar@gmail.com, aknik@chem.unipune.ac.in

Nanosized $Dy_{1.9}Yb_{0.1}Mn_{1.95}Cu_{0.05}O_7$ and $Y_{1.8}Pr_{0.2}Ru_2O_7$ pyrochlore oxides were synthesized under controlled condition by tartarate precursor method. The thermal analysis of these precursors shows that the decomposition of organic content was completed up to 650°C. The precursors were calcined at 700°C for two hour to form respective nanoparticles. The formation of pyrochlore oxides has been confirmed by X-ray powder diffraction and FT-IR studies. Transmission electron microscopy (TEM) confirms the particle size with a low agglomeration and nanosized. From TEM imaging, the particle size is determined to be 14 to 63 nm.

The data of the temperature variation electrical conductivity showed that both pyrochlore oxides were semiconductor. Thermoelectric power measurements showed n-type semiconductor for $Y_{1.8}Pr_{0.2}Ru_2O_7$, whereas p-type semiconductor for $Dy_{1.9}Yb_{0.1}Mn_{1.95}Cu_{0.05}O_7$ pyrochlore oxide. The variation of dielectric constant with frequencies (50Hz to 1MHz) showed initially interfacial polarization up to 275 KHz and beyond which shows domain wall motion.

IP-CYSA-01 : Photocatalytic Splitting of H_2S under Visible Light Radiation using Cadmium Sulphide Nano Composite Glass

Omkar Gugale[1*], Abhishek Jadahav[1], P. N. Dange[1], S. K. Apate[2] and B. B. Kale[2]

[1]All India Shri Shivaji Memorial Societies Collage of Engineering, Pune-411001*
[2]Centre for Materials for Electronics Technology (C-MET), Panchawati, off Pashan Road, Pune-411 008,
E-mail : omkargugale@gmail.com

The photo catalytic hydrogen generation from sulphide compound is one of the photo catalytic processes that have been of interest recently for hydrogen production. In the present study, Cadmium sulphide (CdS) nanocomposite glass was synthesized by using simple melt quenching technique. The optical and morphological studies of this compound were performed by using X-ray powdered diffraction (XRD), UV-Visible spectrophotometer and transmittance electron microscopy (TEM). Considering the band gap of this glass is well within the visible region. We have studied the photocatalytic activity for hydrogen generation from H_2S splitting under visible light irradiation.

IP-01 : 3d-Transition Metal Complexes of Dicyandiamide : Synthesis, Characterization and Antimicrobial Study

Jabali J.Vora[1], Manish P.Brahmbhatt[2] and Kuntal Prajapati[2]

[1]Department of Chemistry, Hemchandracharya North Gujarat University, Patan
[2]Sheth M.N. Science College, Patan

Some 3d-transition metal complexes with biologically importantliganddicyandiamide(N-Cyanoguanidine) have been synthesized in aqueous solution and characterization of the complexes have been deduced from UV-Visible, TGA, C H N analysis, FT-IR and Mass spectra. All the complexes and ligand have been subjected for antimicrobial study.

IP-02 : Alkaline Earth Chelates of 3 Chloro 5 Nitro Lawsone

R. B. Mhaske[1], Pratibha Jadhav[2], P. S. Khandagale[3] and D. G. Kanase[4]

[1]Hutatma Rajaguru Mahavidyalaya, Rajagurunagar
[2]Venutai Chavan Polytechnique, Sinhagad Road, Pune
[3]Henkel Private Ltd, Hinjewadi, Pune
[4]Dr. Patangrao Kadam Mahavidyalaya, Sangli
E-mail : shivaji_takale@yahoo.co.in

Lawsone (I) is an important naturally occurring ligand which is also the active constitute of *lawsonia alba*. It is the parent member of a number of its derivatives obtained by substitution at C3, C5 and C8 positions by electron donating as well as electron withdrawing substitutes. All these derivatives are typical ligands whose coordination chemistry is important both from fundamental and applied point of view. 3 chloro 5 nitro lawsone (II) is one of such derivative which is of specific interest for examining the effect of strong electron withdrawing substituent on the properties of lawsone.

In the present work, this derivative is prepared from dichlone by using literature method. It's chemical identity is established through elemental analysis and purity checked through m.p (258^0C) and paper chromatography. It's alkaline earth chelates with Mg (II), Ca(II), Sr (II) and Ba (II) are prepared by the methods established in our laboratory. Their molecular composition is determined from elemental analysis and thromogravimetry. All these chelates are pink to brown coloured. The structural investigation are done using thermogravimetric and spectroscopic techniques. The geometry of all these chelates having molecular composition $ML_2 2H_2O$ is trans octahedral.

IP-03 : Synthesis, Spectroscopy and Antimicrobial Studies of Some Transition Metal Ion Complexes of A New Pyrazole-based Schiff Base Ligand

Nitis Chandra Saha

Department of Chemistry, University of Kalyani, Kalyani-741 235, Nadia, West Bengal
E-mail : nitis.saha@gmail.com

A new pyrazole containing 'NNO' tridentate Schiff base ligand has been synthesized and characterized by elemental analyses, mass, IR, ^{1}H-NMR spectral parameters and X-ray crystallography. The versatile coordination modes of the ligand have been predicted by complex formation with Co(III), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II) salts. The synthesised complexes are characterized by different physico-chemical and spectral parameters. The ligand contains in its structure the coordination function of the tertiary nitrogen atom of pyrazole ring, the azomethine nitrogen and the phenolic oxygen atom, suitably spaced for chelation with a metal ion and acting as a 'NNO' tridentate donor ligand. *In vitro* antimicrobial activity of the reported ligand and the metal ion complexes are screened and the mode of action is also studied by scanning electron microscopy (SEM) against some pathogenic bacteria.

IP-04 : Studies on Synthesis Schiff'S Bases Derived from Ortho-phthalaldehyde and Their Pd (II) Complexes

Sreenivas V.[1], Aruna M.[2] and Prasanna B.[*]

[*]Department of Chemistry, Chaitanya PG College (Autonomous), Hanamakonda, Warangal, Telengana State-506 001
[1]Department of Chemistry, Kakatiya Govt. College, Hanamakonda, Warangal, Telengana State-506 001
[2]Department of Chemistry, Pingali Govt. Degree College (W), Waddepally, Hanamakonda, Warangal, Telengana State-506 001
E-mail : prasschem@gmail.com

Schiff bases are derived from aromatic carbonyl compounds and have been widely studied in connection with metalloprotein models and asymmetric catalysis, due to versatility of their steric and electronic properties. Schiff bases and their biologically active complexes have been often used as chelating ligands in the coordination chemistry of transition metals, radiopharmaceuticals for cancer targeting, agrochemicals, model systems for biological macromolecules, catalysts and as dioxygen carriers.

A simple and efficient method has been developed for the synthesis of tetra dentate Schiff base ligands are obtained from condensation of phthalaldehyde and 2-amino benzyl alcohol, 2-

amino-2-methyl-1-propanol and 2-aminobenzohydrazine respectively. These ligands were reacted with $PdCl_2$ in methanol to form corresponding Pd metal complexes like [Pd(BDMAB)], [Pd(BDMAT)] and [Pd(BDMAZ)]Cl_2. The synthesized ligands and complexes are characterized by elemental analysis, IR, ^{1}H-NMR and mass spectral studies.

IP-05 : Influence of Streric Bulk of Ligands on the Electronic Spectra of Metal Complexes of Cu (II)

Sumit Kumar Sinha, Chandra Mauleshwar Chandra and Shivadhar Sharma

P.G. Deptt. of Chemistry, Magadh University, Bodhgaya

The spectra of transition metal complexes are greatly influenced by the stereo chemical factors of ligands. Recently Chem-sen Liu and co-workers have reported that the steric bulk of anthracene ring plays an important role in the formation of metal complexes which may offer effective means for constructing unique co-ordination architecture will tailored properties by the steric hindrance of bulky skeleton keeping this fact in mind schiff"s bases of 2-formyl pyridine and 6 –methyl- 2- formyl pyridine have been prepared with different aliphatic amines like n- propyl ammine, iso–propyl ammine and tert. butyl ammine. These ligands have been used for comlexation with Cu (II) ion. It has been observed that d-d transition band shifts to lower frequency with increasing steric bulk near the donor side of ligands. The ESR parameters like $g_\perp$, $g_{||}$, $A_\perp$, $A_{||}$ and g, however, are not found to be influenced appreciably by the steric bulk of the ligands. The order of the values of ESR parameters i.e. $g_{||} < G > g_\perp$ is indicative of tetragonal distortion in octahedral symmetry of Cu (II) complexes.

IP-06 : Spectroscopic Characterization of Metal Complexes with Tetradentate Ligand

Sahdeo Kumar, Pawan Kumar Pandey and Shivadhar Sharma

University Deptt. of Chemistry, Magadh University, Bodhgaya-824234.

Some complexes of N,N-bis (3-hydroxy quinoline) 2- carboxidine-1,8-diammine naphthalene, abbreviated as NBHCN with Co (II) and Ni(II) metal ions have been synthesized. The comparison of infrared spectra of metal complexes with that of NBHCN (ligand) indicates the co-ordination of ligands through two azomethine nitrogen and two deprotonated hydroxy groups. Thus the ligands act as tetradentate join through four points to the metal ions. On the basis of element analysis and molar conductivity the complexes have been formulated as [$M(NBHCN)_2X_2$] where X stands for water,

pyridine and α-picoline which act as sec. ligands. The magnetic moment of Co(II) has been found to be 4.62-4.68 BM which is greater than three unpaired electrons in spin free octahedral complexes of Co (II) . The slightly excess value of Co (II) complexes from μs- 3.87 BM may be attributed to $4T_{1g}$ ground state of 4F term of d^7 system in octahedral symmetry Which being orbitally triply degenerate make sufficient contribution to the magnetic moment of complexes . The octahedral symmetry of Co (II) complexes has been further confirm by their electronic spectra which display three bands due to $4T_{1g} \rightarrow 4T_{2g}$, $4T_{1g} \rightarrow 4A_{2g}$ and $4T_{1g} \rightarrow 4T_{1g}$ (p) spin allowed transitions .The v_2/v_1 value also support the octahedral symmetry of Co(II) complexes. The magnetic moment and electronic spectra of Ni (II) complexes supports distorted octahedral symmetry.

IP-07 : Alkaline Earth Metal Complexes of Dicyandiamide : Synthesis, Characterization and Antimicrobial Study

Jabali J. Vora[1], Manish P. Brahmbhatt[2] and Pravin Prajapati[2]

[1]Department of Chemistry, Hemchandracharya North Gujarat University, Patan
[2]Sheth M. N. Science College, Patan

The more versatile alkaline earth metal complexes in their biological activity, were synthesized in aqueous solution by using biologically important dicyandiamide (N-Cyanoguanidine) as ligand. Synthesized complexes were characterized by UV-visible, IR, Mass spectra, TGA analysis and Elemental analysis. All the complexes and ligand have been screened for antimicrobial study.

IP-08 : Synthesis and Thermal Behavior of Schiff Base Transition Metal Complexes of [1-(5-chloro-2-hydroxyphenyl) Ethanone-2-(4-methylphenyl)-2-phenyl Ethylamine]

Rahul B. Mohod,* Abdul Wajid and Sukhadeo K. Bhagat

P. G. Department of Chemistry, Shri Shivaji College of Arts, Commerce and Science, Akola -444 001(M.S.)
E-mail : rahul_mohod@rediffmail.com

In view of the fast growing interest of Schiff base metal complexes on account of the structural, analytical and biological importance of their metal complexes, the synthesis of 1-(5-chloro-2-hydroxyphenyl)ethanone-2-(4-methylphenyl)-2-phenylethylamine [CHPEMPA] and its metal chelates with Cr(III), Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) have been carried out. The ligand and the complexes have been characterized on the basis of analytical, electrical conductance, molecular weight, IR and electronic spectra,

magnetic susceptibility measurements and thermogravimetric analysis. The thermogravimetric study indicates all the complexes are stable up to 60-70°C. Using standard equations, thermodynamic parameters such as ΔS and ΔG are calculated.The similarity in the values of kinetic parameters indicates a common decomposition reaction mode in all the complexes. The thermal activation energy of all the complexes has been calculated by Freeman-Carroll and Sharp-Wentworth methods.

IP-09 : Preparation of Rare Earth Metal Complexes with N-salisaldehydehyde Anthranilic Acid Ligand

Jabali J. Vora[1], Laxaman S. Bhutadiya[2] and Hitesh K. Patel[2]

[1]Department of chemistry, Hemchandracharya North Gujarat University, Patan-384265
[2]Sheth M. N. Science College, Patan-384265
E-mail : jabali_vora@hotmail.com

Lanthanide complexes are widely prepared because of their biologically active and biological importance. Lanthanide complexes ware synthesized with N- salisaldehyde anthranilic acid ligand. Synthesized complexes were characterized by UV-visible, IR, Mass spectra, TGA analysis and Elemental analysis. All the complexes and ligand have been subjected to antimicrobial study.

IP-10 : Synthetic and Thermal Studies of Some Schiff Base Complexes of [1-(5-Chloro-2-Hydroxy-3-Nitro-phenyl)Ethanone]-4-(2-Aminoethyl)Phenol

Jaishri Bavane* and Rahul Mohod

P. G. Department of Chemistry, Shri Shivaji College of Arts, Commerce and Science, Akola-444 001 (M. S.)
E-mail : jaishrisonawne@gmail.com

Complexes of Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Cd(II) ions withSchiff base ligand derived from1-(-5 chloro-2- hydroxyl-3 nitro phenyl)ethanone and 4-(2-aminoethyl)phenol have been prepared. From the analytical data, the complexes shows 1: 2 (metal:ligand)stoichiometry.The prepared Schiff base ligand and their complexes have been structurally characterized by analytical, FT-IR, diffused reflectance, magnetic susceptibility measurements and thermogravimetric analysis. The thermal dehydration and decomposition of these complexes were studied kinetically using both Freeman-Carroll and Sharp-Wentworth methods. The kineticparameters such as the order of the reaction and the activation energy have been determined.It was found that the thermal decomposition of the complexes follow first order kinetics. The thermodynamic parameters such as change in enthalpy(ΔH),

change in entropy (ΔS) and apparent entropy (S^*) have also been calculated.

IP-11 : Computer Assisted Determination of Relative Stabilities of Binary and Ternary Complexes of Cu (II) with Neurotransmitters and Substituted Amines in Aqueous Medium

S. R. Sonone and T. K. Chondhekar

Department of Chemistry, Dr. Babasaheb Ambedakar Marathwada University Aurangabad-431004
E-mail : srsonone@yahoo.com, tkc_chem@yahoo.com

The relative stabilities of binary and ternary complexes interms of β_{111}, β_{20}, β_{o2},K_l,K_R,Kr and Δlog k values for C_u(II) ion with l-DOPA,Gaba, cupramine Tryptophan, Mercapto Succinic acid (MSA) were determine using SCOGS Computer Programme. The calvin-Bjerrum titrations of l-DOPA as primary ligand and GABA, C_U pramine, tryptophan, tryptamine, MSA as secondary ligands were performed in aqueous medium at 300k maintaining ionic strength (μ) 0.1 M $Naclo_4$, using $_P$H-metric technique. The Δlog k values revealed that mixed metal-ligand complexes are less favoured than binary complexes. The l-DOPA,GABA and substituted amines used in the present study, coordinated to Cu(II) through $–NH_2$, -COOH, -OH and –SH groups. The ternary complexes contained chemical species ML_1, ML_2, MLH, ML_2H & ML_2H_2 for Cu(II) ion in aqueous medium. The relative stability constants have been determined using SCOGS programme. The trends in variation of relative stability constants explained on the basis of electrostatic and non-electrostatic forces, difference in bond type and geometrical structures.

IP-12 : Apoptosis Potential of Copper Complexes Containing b-Ketamine Derivatives in Human Breast Cancer Cells

V. Latha, C. Balakrishnan, S. Chithiraikumar and M. A. Neelakantan*

Chemistry Research Centre, National Engineering College, K. R. Nagar, Kovilpatti-628503,Thoothukudi District, Tamil Nadu
E-mail : drmaneelakantan@gmail.com

New symmetrical binuclear copper complexes (1 and 2) of β-ketamine derivatives were synthesized and characterized by elemental analysis and various spectral methods. The structure of the complexes in the ground and excited states were elucidated through the spectral and computational methods. Electrochemical

studies were carried out for the complexes. Cytotoxic effect of 1 and 2 on human breast cancer cells (MCF-7) was investigated. The dose-dependent inhibition of growth of cancer cells of the complexes was assessed by MTT assay. The nuclear fragmentation, membrane integrity and morphology of apoptotic cells were examined by using DAPI staining. The qualitative analysis of mitochondrial disruption with inhibitory concentrations of 1 and 2 were observed using FITC green and reactive oxygen species (ROS) generation through DCFH-DA staining analysis. Further apoptosis was confirmed by AO/EtBr dual staining. This suggests that the complexes induce apoptosis by the intrinsic pathway.

IP-13 : Rare Earth Metal Complexes of Schiff Base : Synthesis, Characterization and Antimicrobial Study

Jabali J. Vora[1], Manish P.Brahmbhatt[2] and Toral Yadav[2]

[1]Department of Chemistry, Hemchandracharya North Gujarat University, Patan
[2]Sheth M. N. Science College, Patan

The more biologically important lanthanide rare earth metal complexes were synthesized by using biologically important Schiff base as ligand. Synthesized complexes were characterized by UV-visible, IR, Mass spectra, TGA analysis and Elemental analysis. All the complexes and ligand have been screened for antimicrobial study.

IP-14 : Crystal Structure of 2-Anilino-N'-[(1E)-1-(2-Hydroxyphenyl)Ethylidene]Acetohydrazide(Hahea) and Synthesis, Spectral and Thermal Investigation of its Transition Metal Complexes

Vidyadhar C. Havanur[1] and Kalagouda B. Gudasi[2*]

[1]Department of Chemistry, KLE Technological University, Hubli, Karnatak
[2]Department of Chemistry, Karnatak University, Dharwad
[*]E-mail : kbgudasi@gmail.com

A new phenyl glycine hydrazide, 2-anilino-N'-[(1E)-1-(2-hydroxyphenyl) ethylidene]acetohydrazide (Hahea), was formed by the condensation of phenyl glycine hydrazide with 2-hydroxyacetophenone. The formation of Hahea is confirmed by elemental analysis, IR, ^{1}H-NMR. spectra and single crystal X-ray diffraction studies. Copper(II), nickel(II), cobalt (II), manganese(II), zinc(II) and cadmium(II) complexes of this ligand have been synthesized and characterized by elemental analyses, conductance measurements, magnetic susceptibilities, spectroscopic (IR, NMR, UV, EPR) and thermal studies. Molar conductance studies indicate non electrolytic behavior for these complexes. IR spectra indicate

that Hahea acts as a tridentate ligand coordinating through carbonyl oxygen, azomethine nitrogen and deprotonated phenolic oxygen. TG and DTA studies indicate that the complexes are stable up to 100°C and contain uncoordinated water molecules. The complexes have been formulated as $[M(ahea)_2]\cdot 3H_2O$ where M = Cu(II), Ni(II), Co(II), Mn(II), Zn(II) and Cd(II).

IP-15 : Elucidation of Thermodynamic Functions for APase Model Compound Using Thermal and Electrochemical Studies

Khursheed Ahmed*, Priti Singh Shuveksh and Srinivasulu Enamula

Department of Chemistry and Post Graduate Research Center,
Abeda Inamdar senior College, Azam Campus, Camp, Pune-1
**E-mail : khursheed92@rediffmail.com*

Four model compounds of Acid Phosphatase metalloenzyme (EC 3.1.3.2) viz. 1, 2, 3 and 4 having estimated formulae [μ-OH-Fe_2 (II,III) (o-NQox) (o-$NSQox)_2$ (CAT) H_2O], [μ-OH-μ-(OAc)Fe_2(II,III) (o-NQox) (CAT) (OH)], [(CAT) (o-NQox) Fe^{+3}-μ(OH) Fe^{+2} (o-NSQox) (o-NQox)] and [Fe^{+3} $(NQox)_3$] respectively have been synthesized. The electronic structures of compounds were confirmed from CHN Analysis, IR spectroscopy, TGA and electrochemical studies. In IR spectroscopic data, distinct peaks at 1278 cm^{-1} in 1, 1583 cm^{-1} in 2, 1535 cm^{-1} in 3 indicate presence of ligand in its semiquinone form. Activation energies of coordinated naphthoquinone ligand in various redox forms such as (o-NQox), (o-NSQox), (CAT) are calculated from TGA data as 42.42 KJ/mole, 23.65 KJ/mole and 67.7 KJ/mole respectively. These different redox forms of ligand are also confirmed from electrochemical peaks at -0.2 V, -0.75 V and -1.03 V. The calculated activation energy 91.66 KJ from CV data in these compounds are well in agreement with the values calculated from TGA data.

IP-16 : Synthesis, Spectral, Thermal and Antimicrobial Studies of Transition Metal Complexes of 14-membered Tetraaza [N_4] Macrocyclic Ligand

Sunil G. Shankarwar*

**Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University,*
Aurangabad-431004, Maharashtra
E-mail : shankarwar_chem@yahoo.com

A series of metal complexes of Mn(II), Fe(III), Co(II), Ni(II), Cu(II), have been synthesized with newly synthesized biologically active macrocyclic ligand. The ligand was synthesized by condensation of β-diketone 1-(2-hydroxyphenyl)-3-(4-methoxyphenyl)

propane-1,3-dione and o-phenylene diamine. All the complexes were characterized by elemental analysis, molar conductivity, magnetic susceptibility, thermal analysis, X-ray diffraction, FT-IR, ^{1}H-NMR, UV-Vis spectroscopy and mass spectroscopy. From the analytical data, stoichiometry of the complexes was found to be 1:2 (metal: ligand). Thermal behavior (TG/DTA) and kinetic parameters suggest more ordered activated state in complex formation. The antibacterial and antifungal activities of the ligand and its metal complexes, has been screened in vitro against Staphylococcus aureus, Escherichia coli and Aspergillus niger, Trichoderma respectively.

IP-17 : Thermal Studies on Binary Complexes of Some Lanthanide (III) Ions

Bhawna Varshney, Babita Agrawal and K.C. Gupta

Dept. of Chemistry, B.S.A. College, Mathura-281004
E-mail : kc.gupta78@gmail.com

The binary solid complexes of La(III) with Quinaldic acid and of Sm (III) with L-serine were isolated from the mixture of equimolar solutions of metal nitrates and ligands and pH was adjusted to 7.0. The mixture was refluxed in ethanol for 3-4 hours on water bath. The solid mass obtained on cooling was filtered, washed, recrystallised and dried at 60-70 C. The complexes were subjected to elemental analysis and the metal contents were estimated by conventional standard methods.

The kinetic parameters activation energy, order of reactions, frequency factor and activation entropy were calculated by applying zsako and coats and Redfern methods.

IP-18 : Analytical, Spectral and Structural Elucidation of The Complexes of Co(II), Ni(II), Cu(II) and Zn(II) with Furil-bis-(2-Aminothiophenol)

Anita Kumari[1] and K. Yadav[2]

[1]Research Scholar, University Deptt. of Chemistry, LNMU-DBG
[2]P.G. Deptt. of Chemistry, Samastipur College, Samastipur, LNMU-DBG
E-mail : yadav.kusheshwar@yahoo.com, yadavkspj@gmail.com

Binuclear complexes of Co(II), Ni(II), Cu(II) and Zn(II) with bis-biacetyl-2-aminothiophenol (Schiff base) ligand have been synthesized and characterized on the basis of molar mass, elemental analysis, IR and electronic spectral studies, molar conductance and magnetic susceptibility measurement. On the basis of above physicochemical and spectrometric measurements it is proposed that the compounds act in a bi-dentate manner. Such complexes have varieties of useful pharmaceutical activities and many of

them gained wide acceptance in clinical practice. The resulting complexes have been tested for their antifungal activity against various organisms. Complexes, excepting that of Zn(II), are colored. Electronic spectra and magnetic susceptibility study proposes octahedral geometry of the complexes.

IP-19 : Synthesis and Characterization of Some Trasition Metal Complexes Using Bis-(a-benzil)-2-Aminothiophenol

Anita Kumari[1] and K. Yadav[2]*

[1]Research Scholar, L. N. Mithila University, Darbhanga
[2]P.G. Department of Chemistry, Samastipur College, Samastipur, LNMU-DBG
E-mail : yadav.kusheshwar@yahoo.com, yadavkspj@gmail.com

Binuclear complexes of Co(II), Ni(II), Cu(II) and Zn(II) with bis-(a-benzil)-2-aminothiophenol, Schiff base ligand, have been synthesized and characterized on the basis of molar mass, elemental analysis, IR and electronic spectral studies, molar conductance and magnetic susceptibility measurement. On the basis of above physicochemical and spectrometric measurements it is proposed that the compounds act in a bi-dentate manner. Such complexes have varieties of useful pharmaceutical activities and many of them gained wide acceptance in clinical practice. The resulting complexes have been tested for their antifungal activity against various organisms. Complexes, excepting that of Zn(II), are colored. Electronic spectra and magnetic susceptibility study proposes octahedral geometry of the complexes.

IP-20 : Cu(II) Complexes with 4-Amino-3,5-Dimethyl Isoxazole and Substituted Aromatic Aldehyde Schiff Bases : Synthesis, Crystal Structure, Antimicrobial Activity, DNA Binding and Cleavage Studies

Marri Pradeep Kumar and Shivaraj*

Department of Chemistry, Osmania University, Hyderabad-500007, Telangana
E-mail : shivaraj_sunny@yahoo.co.in

Three novel isoxazole Schiff bases 2-((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-6-methoxyphenol (L1), 2-((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-4,6-diiodophenol (L2), 2-((E)-(3,5-dimethylisoxazol-4-ylimino)methyl)-6-bromo-4-chlorophenol (L3) and their Cu(II) complexes [Cu(L1)2] (1), [Cu(L2)2] (2), [Cu(L3)2] (3) were synthesized. All the complexes have been characterized by elemental analysis, FT-IR, ESI mass, UV-Visible, ESR, TGA, magnetic moments and single crystal X-ray diffraction analysis. Based onanalytical data, a square planar geometry assigned to all Cu(II) complexes

with N2O2 donor atoms from the Schiff base ligands. The single crystal X-ray diffraction measurements of complexes 1 and 2 are confirmed the square planar geometry. DNA binding studies from electronic absorption titrations, viscosity measurements and fluorescence quenching studies indicated an intercalation mode of binding of Cu(II) complexes with CT-DNA. DNA cleavage experiments of Cu(II) complexes with supercoiled plasmid pBR322 DNA have also been investigated by agarose gel electrophoresis in the presence of H_2O_2 (Oxidative Cleavage) and UV light (Photolytic cleavage). All the synthesized compounds were screened for antibacterial (Escherichia coli, Pseudomonas putida, Klebsiella pneumoniae, Bacillus subtillis and Staphylococcus aureus) and antifungal (Candida albicans and Aspergillus niger) activity by paper disc method. It is found that all Cu(II) complexes showed better activity than corresponding Schiff bases.

IP-21 : Synthesis, Characterization, Biological Activity, DNA Binding and Cleavage Studies of Metal(II) Complexes of 6-Amino Benzothiazole Schiff Bases

Sreenu Daravath and Shivaraj

Department of Chemistry, Osmania University, Hyderabad, Telangana-500007
E-mail : shivaraj_sunny@yahoo.co.in

A series of two novel Schiff bases, L^1 = (2-((E)-benzo[d]thiazol-6-ylimino)methyl)-4,6-dichlorophenol, $C_{14}H_8Cl_2N_2OS$), L^2 = (1-((E)-benzo[d]thiazol-6-ylimino)methyl)-6-bromo-4-chlorophenol, $C_{14}H_8BrClN_2OS$), and their bivalent transition metal complexes $M[L^1]_2$ and $M[L^2]_2$(where M = Cu(II), Co(II) and Ni(II)) have been synthesized and fully characterized by elemental analysis, FT-IR, ESR, TGA, UV–Visible, SEM, EDX, ESI mass, ^{1}H NMR, ^{13}C NMR, powder XRD and magnetic susceptibility measurements. Based on experimental data all the metal(II) (1a-2c) complexes exhibited square planar geometry around the metal ion. The binding interactions of the complexes (UV absorption, fluorescence and viscosity titrations) studied with double stranded calf thymus DNA (CT-DNA). It is observed that all the metal complexes strongly bound to CT-DNA by an intercalation mode. DNA cleavage (oxidative and photo cleavage) is also investigated against supercoiled pBR322 DNA in presence of oxidant H_2O_2 and UV light (long UV-365 nm), and it is found that all the complexes cleaved DNA effectively. Moreover, the ligands and their metal complexes have been screened for biological activity by paper disc method against bacterialspecies Escherichia coli (E. coli),Bacillus amyloliquefaciens

(B. amyloliquefaciens) and fungal speciesagainst Sclerotiumrolfsii (S. rolfsii) and Macrophominaphaseolina (M. Phaseolina). It is observed that all the metal complexes were more potent in biological activity than their free ligands.

IP-22 : Synthesis, Structural Characterization and Antimicrobial Studies of Mixed O and N Donor Ligand Compounds of Mn(II), Co(II) and Ni(II)

Vinod Kumar

Department of Chemistry, Agra College, Agra
E-mail : vinodkchem@gmail.com

This paper reports the synthesis of mixed ligand complexes of type $[ML_1L_2]Cl_2$ where L_1 = 2-N-(metaphenoxybenzylidene) furfurylamine, L_2 =4-N-(metaphenoxybenzylidene)aminoantipyrine. The resulting complexes have been characterized on the basis of elemental analysis, magnetic measurements, IR, electronic spectral studies, thermal analysis and conductivity measurements. The metal complexes show ratio 1:1:1 with metal, ligand L_1 and ligand L_2. The ligands are bonded through oxygen and nitrogen to metal ion. Biological studies have been carried out on E. coli and S. aureus. Antimicrobial study was seen quite enhanced in metal complexes.

IP-23 : Design, Spectroscopic Studies and Molecular Modelling of Macrocyclic Metal Complexes of Isatin

Monika Kamboj[1*], Kiran Jain[2] and D.P. Singh[3]

[1]Department of Chemistry, Amity School of Applied Sciences, Amity University, Lucknow (U.P)
[2]Department of Chemistry, M.L.N College, Yamuna Nagar (Haryana)
[3]Department of Chemistry, National Institute of Technology, Kurukshetra(Haryana)
[*]E-mail : mkamboj@lko.amity.edu; dpsinghchem@yahoo.co.in

Metal-containing macrocyclic complexes are enthralling the attention of chemists. Macrocyclic chemistry specially highlighting the metal complexation has remarkable applications in medicinal realm. This has led to the synthesis of large number of well-designed and complex functional cyclized structures. There is a growing interest in the application of synthetic macrocycles to chemical biology, potentially leading to drug discovery. In order to further assess the properties of these complexes, synthesis, spectroscopic characterization and molecular modelling of the trivalent chromium and iron complexes derived from carbohydrazide and isatin have been presented in this paper. Template methodology was adopted for the condensation of carbohydrazide and isatin in the presence of trivalent metal ions in methanolic medium, that

had resulted in the formation of the macrocyclic complexes of type: [M ($C_{18}H_{14}N_{10}O_2$) X] X_2, where M = Cr (III) and Fe (III); X = Cl^-, NO_3^-, CH_3COO^-. The synthesized complexes have been characterized with the help of various physico-chemical techniques.

IP-24 : Physicochemical Studies on Schiff Bases Derived from Substituted Coumarins with Substituted Diamines in Aqueous-Alcohol Medium

Uma Desai, Vindhya R. and Suresh*

Department of Chemistry, Ballari institute of Technology & Management, Ballari - 583 104, Karnataka
E-mail : umadesai6@gmail.com

Schiff bases derived from substituted coumarines with substituted diamines were synthesized by cyclo-condensation. Proton-ligand ionization constants and metal-ligand stabilty constants at constant ionic strength in aqueous-alcohol medium (50/50% V/V) were evaluated using Irving-Rossotti method. The ligands exhibit pKa values around 11.5 due to the phenolic –OH group. The metal ligand stability constants with Cu(II), Co(II), Ni(II), Zn(II), Cd(II) and Hg(II) were also determined. The effects of substitutions on the stability constants were studied.

IP-25 : Spectroscopic and Antimicrobial Studies of some Novel Complexes of Mn(II) and Cu(II)

Jwalant J. Vora[1], Hardikkumar D. Chaudhary[1] and Jabali J. Vora[2]

[1]Department of Chemistry, M.G. Science Institute, Navrangpura, Ahmedabad-380009, Gujarat
[2]Department of Chemistry, Hemchandracharya North Gujarat University, Patan - 384 265, Gujarat
E-mail : jwalantvora@gmail.com

In this study, complexes were synthesized in marginal yields via the coordination of metal perchlorates with the ligand. Kynurenic acid (KYNA) ligand reacts with solution of Mn(II) and Cu(II) perchlorates and solid kynurenic acid – metal complexes are synthesized. The ligand and its complexes have been investigated with IR, UV-VIS, mass spectrometry, elemental analysis, TGA – DSC technique etc. These compounds were subjected to their biocidal efficacy against Escherichia coli , Bacillus, Staphylococcus aureus and Salmonellatyphii A and also results have been compared with standard drugs streptomycin and ampicilin.

IP-26 : Synthesis, Characterization and Biological Activity of Cu(II), Ni(II), Co(II) and Zn(II) Complexes of New Thiosemicarbazone Derivative

Javed G. Mahetar, Devang N. Mokariya and Manish K. Shah*

Inorganic Section, Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : javed.mehtar@yahoo.com, drmks2000@hotmail.com

Synthesis was carried out for the new Copper(II), Nickel(II), Cobalt(II) and Zinc(II) complexes of thiosemicarbazone moiety. The characterization of the ligand and metal complexes were done by various Spectroscopic techniques like Mass, IR, ^{1}H & ^{13}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.

ORGANIC CHEMISTRY SECTION

Sectional President's Address

Total Synthesis of Hyrtiocarboline, Characterization and Anticancer Activity

Prof. Balakrishna Kalluraya

Department of Studies in Chemistry, Mangalore university, Mangalagangothri-574 199
**E-mail : bkalluraya@yahoo.com*

Alkaloids are the highly predominant and the most potent naturally occurring heterocyclic compounds. They are the products of the life process, and their diversity is similar to the diversity of life on earth. They are either identified in or isolated from terrestrial plants, terrestrial microorganisms, marine organisms, terrestrial vertebrates and invertebrates. They are a great source to derive many synthetic and semi synthetic drugs which are available in the market. In fact, more than half of all the anticancer drugs approved internationally were either natural products or their derivatives, and were developed on the basis of knowledge gained from small molecules or macromolecules that exist in nature.

In 2010, Inman et al reported the isolation of a new 1-imidazoyl-3-carboxy-6-hydroxy-?-carboline alkaloid, named Hyrtiocarboline, from a Papua New Guinea marine sponge, Hyrtios reticulatus. This compound exhibited selective antiproliferative activity against H522-T1 non-small cell lung, MDA-MB-435 melanoma, and U937 lymphoma cancer cell lines. Hence a total synthesis of the same was planned to further explore its anticancer activity.

The target molecule 'hyrtiocarboline' is composed of a β-carboline ring alongside an imidazole heterocycle. Accordingly, it was planned

to synthesize these two moieties and introduce the carbonyl group between these two heterocyclic rings. The total synthesis proceeded efficiently to synthesize β-carboline ring from the readily available 5-hydroxy-L-tryptophan via Pictet-Spengler cyclization. The retrosynthesis of the alkaloid includes a total of eleven steps, including Pictet-Spengler cyclization followed by aromatisation, Grignard reaction and hydrolysis to mention a few. During the synthesis every single intermediate was well characterized by ^{1}H-NMR and mass spectral analysis.

Antiproliferative / Cytotoxic effect of the test compounds on various cell lines like HGC-27, MCF-7, DU-145 and K-562 was assessed using the MTT assay in vitro as described by Mossman.

OIL-01 : Construction of Carbon-Carbon and Carbon-Heteroatom Bonds by Novel Aerobic Oxidative Coupling Approaches

Gopalaiah Kovuru

Department of Chemistry, University of Delhi, Delhi-110007

Oxidative coupling reactions are essential methods for material transformations. To realize sustainable society, it is important to develop coupling reactions using a highly atom-efficient oxidant and a readily available abundant transition metal catalyst. Hence, oxidative coupling reaction using ubiquitous molecular oxygen as the oxidant and non-toxic abundant iron or copper salts as the catalysts has attracted a growing interest.

In this context, we have recently investigated iron-catalyzed oxidative coupling reaction, and we could report the first example of iron-catalyzed oxidative coupling of benzylamines with 2-amino/ hydroxy/mercapto anilines using iron(II) bromide as the catalyst to synthesize 1,3-benazoles. Based on the mechanistic study of this coupling reaction, we could further discover highly efficient self- and cross-coupling of primary amines. We could also propose that these coupling reactions proceed via a benzylimine, followed by N-benzylbenzaldimine and N-arylbenzaldimine intermediates. Based on these investigations, we further envisaged that the N-benzylbenzaldimine serve as an electrophile to react with indole, and we could report a new approach for synthesis of bis(indolyl)methanes using iron(II) triflate as a catalyst for the first time. These reaction protocols could be applied for synthesis of various biologically potent 1,3-benzazoles and bis(indolyl)methanes.

OIL-02 : Current Status of Medicinal Plants Leading Toward the Discovery of Anticancer Agents

D. N. Singh

Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad- 224001

E-mail : dnsinghsaket@yahoo.com

Plants have been used for the treatments of various diseases for the thousands of years in the traditional system of medicines and remain an important source for the developments of new drugs, new drugs leads and new chemical entities. Cancer is the major public health problems in the world and it is an abnormal growth of the cell in the body that can lead to death. Cancer cells usually invade and destroy normal cells. There are several chemotherapeutic agents currently in the market to treat the

various type of cancer but none of them found to be fully effective and they cause severe toxicity that prevent their uses. Plant derived compounds have played significant role in pharmaceutical industry in the development of several clinically useful anticancer agents. These include vinblatine, vincristine, camptothecin, topotecan, irinotecan, etoposide, alvocidib, combretastatin, homoharringtonone and taxol. Many plant derived compounds are in clinical development based on selective activity against cancer-related molecular targets including flavopiridol, roscovitine and combretastin A4 phosphate. The current status of plant-derived anticancer drugs and their clinical significance, The detailed mechanism of actions and bioactive lead molecules of other pharmacological activities isolated from medicinal plants in our laboratory will be presented in great detail.

OIL-03 : Multicomponent Reactions as a Green Approach Towards the Synthesis of Nonsteroidal Anti-Inflammatry Drugs (NSAD's)

G. M. Nazeruddin

Dept. of Chemistry (PG and Research Centre), AbedaInamdar Sr. College Camp, PUNE-411001
E-mail : gmnazeruddin@yahoo.co.in

Organic synthesis is one of the main driving force in the development of chemistry of various Drugs and makes a significant contribution addressing several of the scientific challenges currently faced by our society. Green chemistry is a philosophy of chemical engineering that encourages the design of products and processes that minimize the use of and generation of hazardous substances. In recent years, various multi-component like Biginelli reaction, Ugi reaction, Kabachnik field reaction, Hantzsch reaction, Mannich reaction etc.are exploited for the synthesis of new non-steroidal anti-inflammatory drugs (NSADs).

OIL-04 : Chemistry by Nature - Inspiration lessons

R. L. Jagadish

Dept. of Polymerscience, University of Mysore, Sir M. V P G Center, Tubinakere, Mandya - 571402

In a world where scientists are using nature,s best ideas and imitating natural designs and processes to solve the human problems has changed the quality of human life. The chemistry by the nature is outstanding and it is slow slower and slowest. The interest about natures chemical lab is not the recent one. Man was very curious about the natures healing powers. As we all aware recently an antibiotic Thixobactin was prepared from soil bacteria. The

investigation were limited to Medicine Initially. But the curious scientists started to look for more from nature. They started studying various techniques adopted by the living kingdom for their survival. They were successful in getting effective guidance for their material design. The best example is of the design of bullet train in Japan inspired by the bird Kingfisher .Japnese engineers modeled a bullet train after a kingfisher which is a bird found in many parts of the World. Kingfishers have large head and narrow long beak this is what the design of Japanese bullet train.

If you observe hippopotamus the sweat looks red colour. The zoo keepers in San Diego Zoo work on the concept of Biomimicry were interested in this and found that the red sweat protects the skin of The animal against sun light. Further they were able to found out the structure of the chemical present in the Sweat.

You can have number of examples about the intelligent chemistry by animals. Coming to the Bombardier Beetle's defense mechanism it produce a chemicals @ a temperature of 100°C and sprays against the attackers and make them to run away. The chemistry of this is very interesting to adopt in our laboratories. A new discipline using nature for sustainable solutions to Human Problems was named as Biomimicry.

We use adhesives in our day to day applications in numerous ways. The adhesive secreted by the Molluscs is really an extraordinary that it will stick to the slipperiest material Teflon too.

OIL-05 : Isolation of Bioactive Components from the Rhizomes of Curcuma Zedoaria

M. Himaja

Professor, Department of Chemistry, School of Advanced Sciences, VIT University, Vellore-632014 (TN)

Curcumazedoaria(Christm.)Roscoe is a member of Zingiberaceae family (Ginger family), which is widespread throughout the tropical and subtropical regions of the world. Species from this family have been used for centuries as food, spices, dyes, perfumes, and also used in traditional Chinese, Japanese, and Indian medicine (Endo, K. 1990). Curcuma zedoariais traditionally used for the treatment of carminative, digestive stimulant and microbial infection, especially skin infections which do not have allopathic medicines.

The crude extracts of the rhizome part of Curcuma zedoariaare reported to exhibit various biological activities like antimicrobial, antiulcer, antimutagenic, hepatoprotective and cytotoxic properties.

In addition to reported phytoconstituents, five more compounds have been isolated from the rhizome extracts and the structures were elucidated by spectral analysis. The extracts were evaluated for in vitro antioxidant, antidiabetic, anticancer and antibacterial activities. Potent activity was observed for antioxidant and anticancer but poor antidiabetic and antibacterial activities. Recently the aqueous extract, rich in flavonoids, exhibited in vitro potent inhibitory activity against struvite kidney stones and potent in vivo inhibitory activity against calcium oxalate kidney stones in Male Wistar rats. Thus C. zedoaria is found to be a rich source of alternative medicine to prevent kidney stones.

OIL-06 : Perspectives and New Protocols for the Synthesis of Selenium Containing Peptidomimetics

Vommina V. Sureshbabu

Room No. 109, Peptide Research Laboratory, Department of Chemistry, Central College Campus, Dr. B. R. Ambedkar Veedhi, Bangalore University, Bangalore-560 001
E-maiil : sureshbabuvommina@rediffmail.com; hariccb@gmail.com; hariccb@hotmail.com

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 chemistry rose to prominence with the identification of various selenoproteins where selenium is predominantly present as selenocysteine (Sec, U). Selenoamides have gained 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 PCl_5/ 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 N^{α}-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.

OO-CYSA-01 : Synthesis and Characterization of 1-Hepta-*O*-Benzoyl-β-D-Maltosyl-3-Substituted Benzothiazolyl Carbamides

Anuja M. Mopari* and Shirish P. Deshmukh

P. G. Department of Chemistry, Shri shivaji collage, Akola-444001, (M.S.)
E-mail : anu.mopari@gmail.com

Carbohydrates based drugs show low toxicity and immunogenicity and have much interest in synthetic and medicinal chemistry. Benzothiazoles are bicyclic ring system with multiple applications as muscle relaxants. Simple benzothiazole nucleus present in compound involved in research aimed at evaluating new product that possess interesting biological activity such as anti-tumor, antimicrobial, anticonvulsant and anti-inflammatory.

Carbamides and their derivative show strong antimicrobial activity and act as diuretic and bacteriostatic agents which are also used as antifungal, antitumor, antidiabetic agents.

In view of these applications, we report the synthesis of new series of 1-hepta-*O*-benzoyl-β-D-maltosyl-3-substituted benzothiazolyl carbamides by the interaction of 1-hepta-*O*-benzoyl-β-D-maltosyl isocyanates with various substituted benzothiazole. The identities of these newly synthesized compound have been established on the basis of elemental analysis of IR,NMR and Mass Spectral analysis.

OO-CYSA-02 : One Pot Click Chemistry Approach for the Synthesis of Coumarinyl-Benzimidazole Linked 1,2,3-triazole Hybrids and their Investigation as Anti-Tubercular Agents

Ashish Anand and Manohar V. Kulkarni*

Department of Chemistry, Karnatak University, Dharwad-580003
**E-mail : manohar274@gmail.com, ashishchem19@gmail.com*

Designing drugs for the treatment of tuberculosis has been a challenging area in medicinal chemistry in view of the multi-drug resistance and high mortality rate associated with this disease. Emergence of resistance against new TB drugs is an alarming issue demanding new drug profiles. Clinically accepted drugs in chemotherapy like Isoniazid, Rifampicin, Pyrazinamide and Delamanid possess a nitrogen heterocycle *viz* pyridine, piperazine, piperidine and pyrazine ring systems with azomethine and aryloxy moieties which constitute their core structural features.

In recent years, 1,2,3-triazoles generated using Click chemistry

have gained multidimensional importance in view of their binding ability with various enzymes through hydrogen bonding. Privileged structure of benzimidazole has been found to be promising in chemotherapy of tuberculosis. 2-mercaptobenzothiazole-triazole-conjugates have been reported to be bactericidal and inhibited the growth of H_{37}Rv strain at the concentration of 8µg/mL. Coumarin triazole hybrids with an aryloxy moiety have been reported from our laboratory as potential anti-tubercular agents.

2-propargylthiobenzimidazole, 4-bromomethyl coumarins/1-aza-coumarins and sodium azide have been reacted in one pot under Click chemistry conditions to give exclusively 1,4-disubstituted triazoles. Anti-tubercular assays against *M.tuberculosis* (H_{37}Rv) coupled with *in silico* molecular docking studies showed dimethyl substituents with promising activity with higher C-score values.

OO-CYSA-03 : Synthesis, Characterization and Biological Evaluation of Some Novel Chalcone-Based Sydnone and Pyrazole Derivatives

Asma and Balakrishna Kalluraya*

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka
E-mail : bkalluraya@gmail.com

Sydnones, which are representatives of mesoionic heterocyclic compounds, possess a broad spectrum of pharmacological activities *viz,* antimicrobial, antiviral, antitumor, analgesic, anti-inflammatory, anthelmintic, free radical scavenging, nitric oxide donor and anticancer. Whereas, due to the easy preparation and rich biological activity, pyrazole framework plays an essential role in biologically active compounds and therefore, represents an interesting template for medicinal chemistry. Indeed, pyrazole-based derivatives have shown several biological activities such as antibacterial, antifungal and pharmacological activities such as anti-inflammatory, antitubercular, anticancer, analgesic, antipyretic, anticonvulsant activities.

So prompted by these observations, we have synthesized a novel series of chalcone containing both sydnone and pyrazole moiety such as 1-(3-arylsydnon-4-yl)-3-(5-aryloxy-3-methyl-1-phenyl-1H-pyrazol) - 2-propen-1-one by the Claisen-Schimdt condensation of 4-acetyl-3-arylsydnone with 5-aryloxy-3-methyl-1-phenyl-1H-pyrazol-4-carbaldehyde in presence of base catalyst. The structure of these compounds was confirmed by NMR, XRD and Mass Spectral analysis. The compounds were also screened for their biological properties and result of such studies will be presented.

OO-CYSA-04 : Multicomponent Reaction for the Synthesis of Hexasubstituted Dihydropyridines Catalyzed by Zinc Oxide Nanoparticles

Gagandeep Kour Reen and Pratibha Sharma*

School of Chemical Sciences, Devi Ahilya Vishwavidyalaya, Khandwa Road, Indore (M.P.), 452001

**E-mail :drpratibhasharma@yahoo.com, reengagandeepkour@gmail.com*

Recently, extensive ability of zinc oxide nanoparticles (ZnO NPs) has been explored for various organic reactions. Our endeavor is to develop catalytic activity of synthesized ZnO NPs in the synthesis of hexasubstituted dihydropyridine scaffolds.

Present paper elicits for the first time, the use of zinc oxide nanoparticles (ZnO NPs) as heterogenous catalyst for the preparation of 1,4-diaryl dihydropyridines (1,4-DDHPs). Herein, zinc oxide nanoparticles manifested remarkable catalytic activity in generating the title compounds in 82-94% yields. The underlying protocol embraces the tenets of green chemistry viz., solvent free media, simple work-up procedure, cost efficient, short reaction times and reusability of the catalyst up to five synthetic cycles with no significant loss in the catalytic activity.

Zinc oxide nanoparticles were characterized by XRD, SEM, TEM, EDX, UV-visible and FTIR spectroscopy. A library of dihydropyridines has been constructed and structural elucidation was carried out by IR, 1H-NMR, 13C-NMR and Mass spectrometry.

OO-CYSA-05 : Synthesis and Biological Evaluation of New Coumarin Ethers

Geeta Pawashea[1] and M.V. Kulkarni[2]

[1]Dept. of Chemistry, Karnatak Science College, Dharwad-580001

[2]Dept. of Chemistry, Karnatak University, Dharwad-580003

Present work describes the synthesis of substituted 4-phenylphenols and 6-phenyl-4-bromomethylcoumarin by Pechmann cyclization. The synthesized compounds were further utilized for the preparation of various coumarin ethers. The compounds were tested for in vitro and in silico DNA interaction and biological studies. The combined activity studies along with density functional theory results were used to rationalize structure-activity relationship.

OO-CYSA-06 : Transition Metal Schiff Base Complexes Intercalated in Layered Double Hydroxide for Selective Oxidation of Ethylbenzene

Savita Khare[1], Jagat Singh Kirar[*], Swati Parashar and Priti Shrivastava

School of Chemical Sciences, Devi Ahilya University, Takshashila Campus, Khandwa Road, Indore (M. P.) - 452001
**E-mail : j.skirar007@gmail.com, kharesavita@rediffmail.com*

Transition metal Schiff base complexes intercalated in layered double hydroxide were prepared using Cu(II) and Co(II), abbreviated as LDH-NAPABA-Cu(II) and LDH-NAPABA-Co(II) respectively and characterized by XRD, SEM, EDX, AAS, FT-IR, TGA and BET surface area analysis. The catalytic activity of these catalysts has been studied for the oxidation of ethylbenzene using *tert*-butyl hydroperoxide under solvent free condition. In both the cases ethylbenzene was oxidized to acetophenone and benzaldehyde. A maximum, 89.18 and 57.37% conversion of ethylbenzene with 99.25 and 99.57% selectivity of acetophenone was obtained with LDH-NAPABA-Cu(II) and LDH-NAPABA-Co(II) respectively at 120 ºC after 7 hours. Acetophenone was the major product and it is used widely in perfumes and pharmaceuticals. The catalyst, LDH-NAPABA-Cu(II) was reused three times without significant loss of catalytic activity.

OO-CYSA-07 : Oxadiazole and Pyrimidine Fused Derivatives of 1,4-benzodiazepine Analogues Through Oxyphenyl Spacer

Navjeet Kaur and D. Kishore

Department of Chemistry, Banasthali University, Banasthali (RAJ. 304022)
E-mail : nvjithaans@gmail.com

The quest to develop effective therapies for the treatment of human immunodeficiency virus (HIV) infection has demonstrated that clinical benefits can be achieved with the combination of anti-retroviral drugs-'the HAART' (viz; Highly active Anti Retroviral therapy). But the therapeutic effectiveness of 'HAART' is limited as the load of drug is often not well tolerated by patient due to their adverse toxic effects and by rapid emergence of the multi-drug resistant mutants of the virus. So the development of novel, selective, potent and safe anti-HIV agents effective against HIV mutant strains to counter their resistance remains in a high priority, in medicinal chemistry research.

Inspired by the promising anti-HIV activity shown by the 1,4-

benzodiazepine, pyrimidine and oxadiazole nuclei based anti-HIV agents (such as TIBO and FDA approved Nevirapine and Etravirine respectively). We decided to proceed with our investigation in the direction of transforming the above hypothesis into a reality, by using the inherent potentialities of these nuclei in this endeavour.

An examination of the structure of 1,4-benzodiazepin-2-one-5-methylcarboxylate **(3)** (which was obtained readily from the ring expansion of 1-chloroacetylisatin **(2)** under the influence of methanolic solution of hexamine) revealed that C_5 methyl of carboxylate and C_2 carbonyl function (which existed as a part of NH-C=O group) in the molecule were the only two sites in its seven membered ring which provided scope for its further funtionalization and elaboration to produce the structural analogues of medicinal utility. It consisted of the conversion of the methylcarboxylate derivative **(3)** to its amide by its reaction with N-methylpiperazine. Subsequently, the C_2 (NH-C=O) group was converted to its 2-chloro analogue on treatment with $POCl_3$ and DMA. The 2-Cl atom (an imino chloride/ imidoyl chloride) is a highly reactive species known to be activated for nucleophillic attack. Its nucleophillic displacement with p-hydroxybenzonitrile **(6)** yielded **7.** The key intermediate (**8)** formed from the reacton of **(7)** with H_2N-OH.HCl + KOH (in MeOH) following the procedure reported in the literature for such reactions on other substrates containing the nitrile group. Established protocols on amidine derivative **(8)** was applied, employing the reagents **(9)** and **(10)** to form the compounds **(11)** (oxadiazole bearing) and (**12)** (pyrimidine bearing) benzodiazepine nucleus respectively. The structures of the compounds were established on the basis of their spectral data. Exploration of the chemistry and biological activity of all the compounds are under study.

OO-CYSA-08 : Synthesis, Biological Evaluation and Docking Study of 1,4-disubstituted 1,2,3-triazoles

Nitin Dubey, Pratibha Sharma and Ashok Kumar*

School of Chemical Sciences, Devi Ahilya University, Khandwa Road, Indore-452 001 (M.P.)

**E-mail : drashoksharma2001@yahoo.com, ni3svpc@gmail.com*

Copper-catalyzed azide-alkyne cycloaddition (CuAAC), a prototype of “click reaction,” has become one of the most important reactions for the preparation of 1,2,3-triazoles. This important reaction is widely applicable in organic synthesis, biochemistry, medicinal chemistry, and material science. In continuation of our research in field of click chemistry, herein, we report synthesis of

a small library of novel amalgamated pyrazole-triazole derivatives. Structures of all the synthesized compounds were confirmed by ESI-MS, FT-IR and NMR (^{1}H, ^{13}C) spectra as well as elemental analyses data. The synthesized compounds were screened for their *in vitro* antibacterial activities against a representative panel of Gram-positive (*Staphylococcus aureus* and *Bacillus cereus)* and Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*). Bio-evaluation studies revealed that, most of the compounds exhibited promising inhibition towards Gram-positive pathogenic strains, while mild inhibitory effects were observed towards Gram-negative bacterial strains. Furthermore, the docking studies for all synthesized compounds against E. coli FabH have also been carried out.

OO-CYSA-09 : Evaluation of Free Radical Scavenging Activity of N-Aryl Hydroxamic Acids

Rainy Agrawal, Shakuntala Raj and Rama Pande*

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur-492010, Chhattisgarh
E-mail : rainyagrawal14@gmail.com

Free radicals are ground laying to any biochemical process and represent an important part of aerobic life and metabolism. Even though free radicals like Reactive Oxygen Species (ROS) and Reactive Nitrogen Species (RNS) which are products of normal cellular metabolism leads to oxidative stress. Antioxidants offer resistance against oxidative stress by scavenging the free radicals, inhibiting the lipid peroxidation and by many other mechanisms and thus prevent the disease sequence. The present study represents the antioxidant activity of N-phenyl-2-4-dichlorobenzo, N-p-chlorophenyl-2-chlorobenzo, N-p-Tolyl-2-chlorobenzo and N-p-chlorophenyl-4-methoxy benzohydroxamic acids. These compounds were assessed for their antioxidant activity by the DPPH (1,1-diphenyl-2-picryl-hydrazyl) free radical scavenging assay, β-carotene linoleate method and DNA cleavage protection method. All four hydroxamic acids exhibited strong antioxidant activity, with varying IC_{50} values ranging between 310.72-389.55 mM concentration against DPPH. The rate of degradation of β-carotene and percentage inhibition of lipid peroxidation varying between 41.85-42.87 % shows free radical scavenging activity of hydroxamic acids. Gel electrophoresis analysis indicates that all the four compounds show DNA cleavage protection activity against H_2O_2 mediated damage.

OO-CYSA-10 : Synthesis and Docking Studies of 3-[(benzyl/benzylthio-2H-tetrazol-2-yl) Methyl-2-chloro-6-substituted Quinolines as Anti-Proliferative Agents

Saba Kauser J. Shaikh and Ravindra R. Kamble*

Department of Studies in Chemistry, Karnatak University, Pavate Nagar, Dharwad-580003

**E-mail : kamchem9@gmail.com, saba9805@gmail.com*

A new series of 2,5 and 1,5-regioisomers viz., 3-[(5-benzyl/ benzylthio-2H-tetrazol-2-yl) methyl]-2-chloro-6-substituted quinoline (6h-q) and 3-[(5-benzyl/benzylthio-1H-tetrazol-1-yl) methyl]-2-chloro-6-substituted quinolines (7h-q) were synthesized and characterized by IR, ^{1}H NMR, ^{13}C NMR, Mass spectroscopy and single crystal X-ray crystal studies. Docked into DNA as target using enzyme 1AU5 and 453D revealed that the compounds 6h and 6i act as covalent cross linker on the DNA helix of the former and as an intercalator with higher C score values. The compounds were screened for anti-proliferative activity (primary cytotoxicity) against NCI-60 Human tumor cell line at a single high dose (10^{-5} M) concentration assay. Tested compounds, 6h has shown GI of 99.28 % against Melanoma (SK-MEL-5) and 6i has shown GI about 97.56 % against Breast Cancer cell line (T-47D) and have been found to be potent anti-proliferative agents.

OO-CYSA-11 : Synthesis, Structure, Biological Screening and Special Prominence on DNA Binding / Cleavage Study of Quinoline-2H-1,2,4-triazol-3(4H)-One

Shilpa M. Somagond and Ravindra R. Kamble*

Department of Studies in Chemistry, Karnatak University, Pavate Magar, Dharwad 580003

**E-mail : kamchem9@gmail.com, shilpasomagond@gmail.com*

Abstract 1,2,4-Triazoles appended to Quinoline viz., 7h-q and 11h-q have been synthesized. Interaction of compounds 7n, 11k and 11p with calf thymus DNA (CT-DNA) was explored. The interaction of these newly synthesized molecules viz., 7n, 11k and 11p with DNA was investigated at physiological pH. UV/Visible absorption revealed that interactions between these molecules and DNA base pairs along with phosphate–sugar backbone due to its non-covalent mode of binding as evidenced by hypochromism. Hyperchromism due to displacement of the ethidium bromide probe by synthesized molecules was observed in the emission spectroscopy, which also confirmed the strong

interaction between DNA and the reported molecules. CD studies indicated the decrease percentages in maximal DNA positive and negative absorption, which is in agreement with an intercalative binding mode of interaction. Further, molecular modeling showed the intercalative binding mode at binding sites such as oxygen of phosphate backbone and pyrimidine nitrogen of guanine thus corroborating the experimental findings. Also, the nucleolytic cleavage activities against CT-DNA, anti-proliferative, and anti-TB properties have been investigated. Notably, compound 11k and 11p exhibited potent anti-proliferative activity against HeLa cancer cell line where as the compounds 7h, 7n, 7p, 11h, 11k and 11p exhibited compelling anti-TB properties.

OO-CYSA-12 : Design, Synthesis and Bioevaluation of Novel 2-(6-Chloro-9-((2-Oxo-2H-chromen-4-yl)Methyl)-9H-carbazol-2-yl)Propanoic Acid as a Potent Anti-inflammatory and Anti-Cancer Agents

Shivarudrappa H. P. and K. M. Hosamani*

**P. G. Department of Studies in Chemistry, Karnatak University, Dharwad-580003*
E-mail : dr_hosamani@yahoo.com, shivarudrappa.h.p@gmail.com

Carprofen and coumarins are promising biologically potent heterocyclic compounds, both have shown very good biological activities, since carprofen is a potent non-steroidal anti-inflammatory drug. In the modern days, the pathogens are getting immune to older drug, so it is very much necessary to develop a new potent drug which would lead us to synthesize novel 2-(6-chloro-9-((2-oxo-*2H*-chromen-4-yl)methyl)-*9H*-carbazol-2-yl)propanoic acid. This is a carprofen condensed coumarin new derivative. All the synthesized compounds are characterized by elemental analysis and spectroscopic techniques. The titled compounds (1a-1i) are evaluated for their *in-vitro* anti-inflammatory activity by using protein denaturation bioassay, anti-cancer and antibacterial studies. The tested compounds have shown most potent anti-inflammatory activity amongst compound (1a) showed very potent anti-inflammatory activity. Other tested compounds (1b), (1d) and (1f) showed good activity. Among all the titled compounds (1a), (1b) and (1d) compounds have been selected to NCI-60 for the further study of anticancer activity on 60 human cancer cell lines One dose screening. The suggested compounds containing $-CH_3$,$-OCH_3$ and halogenated groups are promising lead compounds for the next investigation in the development of new drug formulation against inflammation and cancer.

OO-CYSA-13 : Synthesis and Biological Screening of Some Glycosylated-1,2,4-thiadiazolidines

Sneha U. Jadhao* and Shirish P. Deshmukh

P. G. Department of Chemistry, Shri Shivaji College, Akola-444003, (M.S.)
E-mail : jadhaosneha2@gmail.com

The heterocyclic derivatives of sugar possess antibacterial and antitumor activities. With this point of view 1,2,4 thiadiazoles are an important class of heterocycles. The 1,2,4 thiadiazoles exhibit broad spectrum of biological activities, possible due to the presence of toxphoric N-C-S moity. 1,2,4 thiadiazoles have been the subject of great interest because of their biological activity. The drugs having 1,2,4 thiadiazole nucleus enhance pharmaceutical, medicinal, agricultural and industrial applications. The drugs showed a diverse range of physiological activities, plant growth promoting activity, antitumor, herbicidal, antibacterial, amoebicidal and antidibetic. So, we report the synthesis of title compounds 2-o--tolyl-3-glycosylimino-4-glycosyl-5-o--tolylimino-1,2,4-thiadiazolidines by oxidation of various 1-β-D-glycosyl-3-o--tolyl thiocarbamides using hydrogen peroxide in ethanolic medium. The identities of these newly synthesized compounds have been established on the basis of usual chemical transformation and IR, ^{1}H NMR and Mass spectral studies. The polarimetric studies of these title compounds have also been carried out. The synthesized compounds were assayed for their antimicrobial and antifungal activity.

OO-CYSA-14 : Design, Synthesis, Biological Evaluation and Molecular Modelling of α, β-Unsaturated Group as Potential COX-2 Inhibitors

K. Srinivas

Department of Chemistry, GITAM School of Technology, GITAM University, Hyderabad Technological Park campus, Rudraram, Sanga Reddy Dist (Telangana) – 502 329
E-mail : drksrinivas@gitam.in, kummarisrinivas@gmail.com

Non-steroidal anti-inflammatory drugs (NSAIDs) such as aspirin exhibit their anti-inflammatory effects by inhibiting cyclo oxygenase (COX) which catalyzes the bioconversion of arachidonic acid to prostaglandins.Selective inhibition of COX-2 over COX-1 is useful for the treatment of inflammation and inflammation-associated disorders with reduced gastrointestinal toxicities when comparedwith NSAIDs.

In the present work, Initially *o*-Nitroaniline is reacted with cyano acetic acid in propionic anhydride resulting in the formation of 2-cyano-N-(2-nitrophenyl)acetamide, the latter compound is

reacted with benzaldehyde in ethanol as solvent and piperidine as base resulting in the formation of (E)-2-cyano-N-(2-nitrophenyl)-3-phenylacrylamide. This reaction was found to be general and extended with other derivatives of nitroaniline & benzaldehyde. In continuation of the work, we have prepared series of library compounds having α, β-unsaturated group followed by molecular modeling studies and screened for their biological activity towards the inhibition of COX-2 enzyme.

OO-CYSA-15 : Design and Synthesis of Biomolecule-based *O*-ethyl S-(6-methyl-2-oxo-2H-chromen-4-yl)Methyl Carbonodithioate Hybrids as Potent Anti-Cancer Agents, their Anti-Oxidant and Anti-Inflammatory Studies : A Microwave Synthetic Approach

Suresh S. Kumbar and Kallappa M. Hosamani*

P. G. Department of Studies in Chemistry, Karnatak University, Dharwad-580003
**E-mail : dr_hosamani@yahoo.com, gsureshkumbar88@gmail.com*

In modern days, an easy and rapid protocol for the synthesis of *O*-ethyl S-(6-methyl-2-oxo-2H-chromen-4-yl) methyl carbonodithioate hybrids **(1a-1j)** under microwave-irradiation and also conventional method has been described. Further, efforts underwent towards the development of microwave assisted synthetic protocols, through which the yields of the compounds were improved drastically in very short time as compared to conventional method. The chemical structures of newly synthesized compounds were characterized on the basis of elemental analyses and spectroscopic techniques. All the newly synthesized compounds were screened for their *in-vitro* antioxidant and anti-inflammatory activities. Amongst the titled compounds (**1a)**, (**1c)**, (**1d)**, (**1f)**, (**1h)** and (**1j)** have been selected for NCI-60 Human Cancer Cell Lines One-Dose screening. Therefore, we designed the compounds and analyzed for their physicochemical properties set by Lipinski rule and found that, none of the compounds violated the rule and they fall well in the range of Rule of five [**RO5**].

OO-CYSA-16 : NBS/Oxone Catalyzed One Pot Synthesis of 2-Substituted Benzimidazoles

Ujla Daswani, Pratibha Sharma and Ashok Kumar*

School of Chemical Sciences, Devi Ahilya University, Takshashila Campus, Indore-452001, M. P.
**E-mail : drashoksharma2001@yahoo.com, ujladaswani@yahoo.com*

Benzazoles represents a noteworthy class of fused heterocycles

with widespread pharmacological properties. Especially 2-substituted benzimidazoles are found to display properties such as analgesic, anticonvulsant, antimicrobial, antiviral, anticancer and antioxidant. Of all the known 2-substituted derivatives, 2-aminobenzimidazoles (2-ABI) has been considered as target molecule for the synthesis.

Herein, we present an efficient transition metal-free strategy for the synthesis of 2-aminobenzimidazoles using cyclohexanone and guanidine as model reactants. Initially, this environmentally, benign method uses a stoichiometric combination of NBS/oxone in acidic conditions to get α-halogenated cyclohexanone. Later on, guanidine and its derivatives are made to react with this *in situ* generated α-bromocyclohexanone to yield a series of 2-aminobenzimidazoles. Screenings of solvent system have also proved beneficial in terms of productivity. The structures of synthesized compounds have been confirmed by FT-IR, ^{1}H-NMR mass spectrometry and elemental analyses data. This facile protocol provided greater selectivity and cost-efficiency along with environmental compatibility. Additionally, absence of chromatographic purification, clean reaction profiles, simple work-up procedure and high yields are among the other added advantages that make this approach an attractive alternative for the synthesis of target heterocycles.

OO-CYSA-17 : Synthesis and Characterization of 4-Aryl-3, 5-di-(*o*-Tolylimino)-1, 2, 4-Dithiazolidines (Hydrochloride) as Potential Antimicrobial Agent

Varsha S. Zade

P. G. Department of Chemistry, Shri Shivaji College, Akola-444 003 (Maharashtra)
E-mail : 29varshazade@gmail.com

Today heterocyclic compounds have gained immense importance in human life. The structural diversity and biological importance of nitrogen-sulphur heteroatom containing compounds have made heterocyclic compounds attractive synthetic targets over many years. They are found in bioorganic and medicinal chemistry with applications in drug discovery. Most of the modern drug contain heterocyclic pharmacophore shows diverse pharmacological activities like antimicrobial, cardiovascular, and anesthetic agents and also in agricultural as herbicides, insecticides, pesticides, and fungicides.

In view of these observations, some efforts have been developed for the synthesis of novel 4-aryl-3, 5-di-(*o*-tolylimino)-1, 2, 4-dithiazolidines (Hydrochloride) by the interaction of 1-*o*-tolyl-3-aryl thiocarbamides with *N*-phenyl-*S*-chloro-isothiocarbamoyl chloride.

Initially 1-*o*-tolyl-3-aryl thiocarbamides were prepared by the interaction of *o*-tolyl isothiocyanate with different aryl amine in benzene medium. The structures of newly synthesized 1, 2, 4-dithiazolidines (Hydrochloride) have been established on the basis of chemical transformation, elemental analysis, and IR, ^{1}H NMR, and Mass spectral studies. The title compounds have been assayed for their biological activity against gram-positive as well as gram-negative microorganisms namely *Escherichia coli, Staphylococcus aureus, Penicillum notatum* and *Aspergillus niger*. The title compounds showed most significant activity against the microbial strains used.

OO-CYSA-18 : 1,3-Dipolar Cycloaddition Reaction of Azomethine Ylides to 5–Substituted Furfuryl/Thienyl Chalcones : Study of the Effect of Substituents on the Regioselectivity

Anish Kumar K. and Balakrishna Kalluraya

Department of studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka.
E-mail : bkalluraya@gmail.com

The history of 1,3-dipolar cycloaddition reaction starts with Curtius, who discovered a dipole diazoacetic ester in 1883. Later a huge amount of works was done on this field and in 1960's, Huisgen established the general concept and the synthetic scope of 1,3-dipolar cycloaddition by publishing a large number of research articles. He classified 1,3-dipolar cycloaddition reactions and formulated the basic definitions. Gradually 1,3-dipolar cycloaddition reaction became one of the important method for the preparation of five membered heterocycles.

Usually in 1,3-dipolar cycloaddition reaction, a dipole reacts with dipolarophile in the presence of suitable catalyst and give possible regioisomers. Hence we were interested in the study of effect of substituents on the regioselectivity of the reaction. For that purpose azometine ylide was taken as dipole. It was generated *in-situ* by the reaction of ninhydrine with sarcosine. This *in-situ* generated azomethine ylide was reacted with different 5-substituted furfuryl/thienyl chalcones and the regiochemistry of the resulted spiropyrrolidines was studied by spectral and analytical techniques. It was found that simple furfuryl/thienyl chalcones when reacted with azomethine ylides resulted in pair of regioisomers. When the 5-nitro furfuryl/thienyl chalcones were used, only one among the two possible regioisomer was formed. Dramatic change in the regiochemistry of products during cycloaddition was found, pointing

the importance of the electronegative nitrofuran or nitrothienyl moiety in the vicinity of the C=C double bond of chalcone. In the presence of electron withdrawing group, chalcone position â becomes electron rich due to the presence of electron withdrawing nitro group attached to furan or thiophene ring which resulted in the regioselectivity of the resulting spiropyrrolidies. Same result was obtained even when the 5-nitro furfuryl/thienyl goup of chalcone is replaced with 5-aryl furfuryl/thienyl group in which the aryl group has an electron withdrawing group.

OO-CYSA-19 : Microwave Induced Synthesis, Characterization and Biological Screening of Triazine Substituted Thiadiazolidine and Dithiadiazine Heterocyclic Compounds

Roshani S. Mulani* **and Pradip P. Deohate**

Department of Chemistry, Shri Radhakisan Laxminarayan Toshniwal College of Science, Akola

E-mail : roshanimulani05081992@gmail.com, pradip222091@yahoo.co.in

Triazine as a heterocyclic compound is an excellent core structure with diversified therapeutic applications. It's fascinating use as a medicinally important compound is evidential from its varied biological properties. Thiadiazolidine and dithiadiazine also shows remarkably unique antimicrobial properties. Triazine substituted thiadiazolidine and dithiadiazine heterocyclic compounds prove to be excellent biological compounds.

The microwave assisted synthesis of substituted 1-(5-arylimino-2-phenylimino-[1,3,4]-thiadiazolidin-3-yl)-2-(4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-ethanones and 1-(6-arylimino-3-phenylimino-[1,2,4,5]-dithiadiazin-4-yl)-2-(4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-ethanones have been achieved by the cyclisation of (4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-acetic acid N-(N'-aryl-thioamido)-hydrazides with N-phenyl isocyanodichloride and N-phenyl-S-chloro isocyanodichloride respectively at 800 W. The required hydrazides were synthesized by the condensation of ethyl (4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-acetate with hydrazine hydrate followed by the interaction with N-aryl isothiocyanates under microwave irradiation. The required acetate was prepared by conventional heating of 2,4-diamino-6-methyl-[1,3,5]-triazine with benzaldehyde followed by interaction with ethyl chloroacetate using microwave. The formation all synthesized compounds was confirmed by TLC and their structures were established on the basis of chemical transformation, elemental analysis, equivalent weight determination and IR, ^{1}H-

NMR, mass spectral studies. The title compounds have been screened for their biological activity against gram-positive as well as gram-negative microorganisms.

OO-CYSA-20 : Synthesis, Characterization and Catalytic Properties of Titanium Doped Zinc Oxide Nano-Particles by Co-precipitation Method

Niraj Jadhav and Ramdas Pawar

Department of Chemistry, PDEA's Baburaoji Gholap College, Sangavi, Pune– 411027
E-mail : rapawar@hotmail.com, rapawar9@gmail.com

Titanium Doped Zinc oxide Nano-particles, Ti_xZnO_{1-x} (where x = 0.025, 0.05, 0.75, and 0.1) have been synthesized by tartarate co-precipitation method, which allowed control of their composition and morphology. The preparation processes were monitored by FTIR and thermal studies (TG-DTA). The obtained catalysts were characterized by FTIR, XRD, SEM, EDS, BET and Particulate properties measurement. The phase identification of the materials by X-ray diffraction reveals the single-phase nature of the materials. This reagent can be used as an efficient, recyclable, Heterogeneous catalyst for the synthesis of Fluorescein in solvent-free conditions. The presented method is mild, environment friendly, inexpensive, short reaction time and highly effective to give the products in good to excellent yield compared to conventional method. Characterization and structural elucidation of the products have been done on the basis of chemical, analytical and spectral analysis. In addition, in this article some novel Fluorescein derivatives were synthesized effectively.

OO-01 : Thiamine Hydrochloride (VB_1) as an Efficient Catalyst for the Synthesis of 4H-Pyrimido [2,1-b] Benzothiazole Derivatives

Sayujiata R. Vaidya[1] and Jaishri J. Chamergore[2]

[1]Department of Chemistry, Vivekanand Arts, Sardar Dalipsingh Commerce and Science college, Aurangabad -431001, Maharashtra
[2]Department of Chemistry, Vasantrao Naik College, Aurangabad - 431001, Maharashtra
E-mail : srvaidyachem007@gmail.com

Heterocyclic compounds are highly important due to broad spectrum of their pharmacological properties which includes broad application in medicinal chemistry. In recent years much attentions has been paid to wards synthesis of 4H-pyrimido [2,1-b] benzothiazole derivatives due to their high affinity central benzodiazepine receptor ligands.

An efficient and convenient synthesis of 4H-pyrimido [2,1-b] benzothiazole derivatives have been achieved via one pot cyclocondensation of aromatic aldehydes, 2-aminobenzthiazole and ethyl acetoacetate using thiamine hydrochloride in water under reflux condition. The thiamine hydrochloride (VB1) 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-02 : Synthesis of Novel Tetrazole Fused with Isatin Nucleus and its Biological Activity

Jaishree Badiger[1] and K. Manjulatha[2]

[1]Smt. V.G. Degree College for Women, Kalaburagi, Karnataka State-585 102
[2]Department of Biochemistry, School of life Sciences, University of Hyderabad
[*]E-mail : jaya.b27@gmail.com

The synthetic versatility of isatin has stemmed from the interest in the biological and pharmacological properties has led to the extensive use of this compound in organic synthesis. In view of these importance of Isatin derivatives containing tetrazole moiety were prepared in the current study. The 5-substituted 2-chloro isatin was prepared from corresponding isatin by reported method, then it is made to react with NaN_3 in presence of acetonitrile as solvent it undergoes cyclisation to afford tetrazole derivatives. The newly synthesized tetrazole compounds were screened for their antibacterial activity and antioxidant activity. The compounds were confirmed by IR, ^{1}HNMR and LCMS spectral data.

OO-03 : Design, Synthesis of Novel Indolyl Oxadiazole Analogues as Potent Antioxidant and Antimicrobial Agents

R. Parveen[1,2*], S. Rahber[a] and J. S. Biradar[1]

[1]Central Research Lab, Department of Chemistry, Gulbarga University, Gulbarga-585 106, Karnataka State, India.
[2]Smt. V. G. Degree College for Women, Gulbarga-585 102,Karnataka State, India.
[*]E-mail : parveenr.2008@rediffmail.com

A novel and efficient method is developed for the synthesis of 2,5-bis(3,5-disubstituted-1H-indol-2-yl)-1,3,4-oxadiazole by reacting 3,5-disubstituted-indole-2-caboxyhydrazide with 3,5-disubstituted indol-2-carboxylic acids. The newly synthesized compounds were confirmed by IR, ^{1}HNMR, ^{13}CNMR, mass spectral and analytical data. The novel compounds were screened for their antioxidant and antimicrobial activities. Most of the compounds have shown potent activity when compared to the standard.

OO-04 : Conventional and Microwave Synthesis of Highly Functionalized 4-Nitro-Indazolo-1,3-Thiazolidinone-1,2,4-Triazoles and their Anti-microbial Activity

Srivastava S. K.* **and Srivastava S. D.**

Department of Chemistry, Synthetic Organic Chemistry Laboratory
Dr. H. S. Gour Vishwavidyalaya (A Central University) Sagar (MP)-470003
E-mail : professorsks@rediffmail.com

Several azoles scaffold have been described in literature including indazole derivatives are important nitrogen containing nine membered bicyclic heterocyclic compounds with application as several biological activities and agrochemicals besides possessing important pharmacological significance such as antimicrobial, protein kinase inhibitors, antiproliferative and antiprotozoal activity. Despite the many useful applications of indazole derivatives, indazole chemistry remains less studied as compared to other heteroaromatic compounds such as indole or benzimidazole. Indazole resembles both pyridine and pyrrole and its reactivity reflects this dual behaviour. Thiazolidine ring system derives special importance from the fact that it plays an very active role in medicinal chemistry. As a part of our continuing efforts to develop novel heterocyclic compounds with potential bioactive molecules starting from 4-nitroindazole, we have synthesized several new compounds by conventional as well as microwave technology viz. ethylethanoate-(4-nitroindazole);hydrazinoacetyl-(4-nitroindazole);3- (4 - nitroindazole)-methyl – 4 - amino-5-mercapto-1,2,4-triazoles;3- (4-nitroindazole)-methy l- 4- arylidenes – 5 -mercapto-1,2,4-triazoles; 3-(4-nitroindazole)-methyl-4-(4-oxo-2-substituted aryl-1,3-thiazolidines)- 5-mercapto-1,2,4-triazoles and 3-(4-nitroindazole)-methyl-4-(5-substituted arylidenes-2-substituted aryl-4-oxo—1,3-thiazolidines)- 5-mercapto-1,2,4-triazoles respectively. Some of the compounds displayed antibacterial activity against E. coli and S. aureus and antifungal activity against C. albicans and A. niger.

OO-05 : Novel Series of Thiazole-Based Chalcones : Synthesis, Characterization and Antioxidant Property

Jean Baptiste Nkurunziza and BalakrishnaKalluraya

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199 Karnataka, India.
E-mail : bkalluraya@gmail.com; kurujean@yahoo

Thiazolederivatives constitute a class of heterocyclic compounds with good pharmaceutical profile. They are found in many biologically

active drugs such as niridazole, sulfathiazole, combendazole and nitazoxanide.They were also reported to play the key role in drug development for the treatment of hypertension, inflammation, diabetes, cancer, oxidative stress, fungal and bacterial infections. Furan and thiophene derivatives represent an essential group with broad spectrum of biological activities such as antitumor, antifungal, antibacterial, antiviral, analgesic, anticonvulsant. In addition, chalcone functionalityhas attracted significant attention because of its wide biological activities.

Keeping in view of the above observations, the present work focused on the synthesis, characterization and antioxidant study of novel series of thiazole based chalconesincorporating substituted thiophene/furan moieties.

The title compounds were synthesized by acid/base catalyzed ClaisenSchimidt condensation reaction between 1,3-thiazole-5-carbaldehyde with various substituted acetylfuran or acetylthiophene. The structures of these newly synthesized compounds were confirmed by their ^{1}H-NMR, IR, Mass spectroscopy and elemental analysis. All the new compounds were screened for their antioxidant activity.

OO-06 : Design, Synthesis and Biological Evaluation of Isoniazid Derivatives Actingas Potent Antimicrobial and Antioxidant Agents via Betti's Reaction

J. S. Biradar*, A. S. Rathod and S. S. Godipurge

Central Research Lab, Department of Chemistry, Gulbarga University, Gulbarga-585 106 Karnataka State
**E-mail : jsbiradar@rediffmail.com*

A novel synthesis of isoniazid derivatives achieved by the condensation of aldehydes, isoniazid, and phenols via Betti reaction has been described. The reactions were carried out at room temperature using fluorite as catalyst. The catalyst is efficient, benign, reusable, cost effective, and ecofriendly. The synthesized moieties were characterized on the basis of IR, ^{1}H-NMR and mass spectrometry and elemental analysis. The objective of this study was to evaluate the biological activity of various hydrazides derivatives of Indole, Phenols and Isoniazid via Betti's reaction. The title compounds (3a-d), (4a-d) and (5a-d) were investigated for their in vitro antimicrobial activity against (E.coli, Enterococcus fecalis, Shegella and Salmonella typhi) by cup plate method. The synthesized compounds exhibited MIC ranging from 0.05 and 0.1µg/ml. Among the series of compounds tested (4b) and (5d) were found

to be most active with E.coli, (3c),(4a) with Enterococcus fecalis (3a),(3b) and(4a) Salmonella typhi at 0.05 and 0.1µg/ml. and antioxidant activity by DPPH radical scavenging method, compounds (3a),(3d)and(5a) exhibited good radical scavenging activities.

OO-07 : Synthesis Antimicrobial and Molecular Docking Studies of Novel Indole Substitutedimidazo-Pyridines

J. S. Biradar[*], S. Rahber, S. S. Godipurge[1] and B. S. Naraboli[1]

Central Research Lab, Department of Chemistry, Gulbarga University, Gulbarga-585 106 Karnataka State
[*]E-mail : drbiradar@gmail.com.

A series of novel indole substituted imidazo-pyridines(4a-h) have been synthesized from 2,5-disubstitutedindole-3-carboxaldehyde, triethylorthoformate and 2-aminopridines. The structures of the newly synthesized compounds were determined by using IR, ^{1}HNMR, Mass Spectral and analytical data. All the compounds were evaluated for their in vitro antibacterial and antifungal activities against a panel of pathogenicstrains of bacteria and fungi respectively by broth dilution MIC (Minimum Inhibitory Concentration) method. Some of them exhibited excellent activity when compared with the standard drugs. Further, in silico molecular docking study indicates that the synthesized compounds are novel inhibitors of the enzyme Glucosamine-6-phosphate synthase.

OO-08 : Biginelli Reaction Used for Synthesis of 2-Benzyl thio-1,4-dihydropyrimidine Derivatives as Non-Steroidal Anti-inflammatory Drugs

G. M. Nazeruddin[1*], Y. I. Shaikh[2] and S. S. Mulani[2]

[1]Dept. of Chemistry (PG and Research Centre), AbedaInamdar College,Pune-411001
[2]Dept.of Chemistry (PG and Research Centre) Poona College, Pune-411001
E-mail : gmnazeruddin@yahoo.co.in

Multicomponent reactions (MCRs) are chemical reactions in which three or more compounds react to form a single product. The reaction gives highly selective products that retains majority of atoms present in the starting material. MCRs provide great possibility for getting molecular diversity and complexity in few steps within less time. Biginelli reaction was accomplished just by grinding equimolar quantities of ethyl acetoacetate, thiourea and aryl aldehyde with few drops of water for 10 to 15 minutes without any solvent and catalyst. The crude product was recrystallized by ethanol followed by alkylation with benzyl bromide in presence of pyridine using methanol as a solvent at 40 to 50° C to furnish 2-benzyl thio-1,4-dihydropyrimidine derivatives. These compounds may have required anti-inflammatory activity.

OO-09 : Facile Synthesis of Novel 2-(4-halostyryl)-1,6-dialkyl-9-oxo-6,9-dihydro-1H-imidazo[4,5-f] quinoline-8-Carboxylicacid Derivatives as Potential Anti-Tuberculosis Agents

A. Mohana Rao, B. Mahesh Goud, T. Ashok Kumar and B. Rama Devi*

Department of Chemistry, Jawaharlal Nehru Technological University Hyderabad, College of Engineering, Kukatpally, Hyderabad (T.S.) – 500085
E-mail : mohanorganic@gmail.com

Tuberculosis is one of the oldest documented infectious disease and threat to worldwide public health, mainly caused by Mycobacterium tuberculosis (M.tb.) bacteria species. It is the only disease that does not require any vector for transformation from one person to another. Various 5-bromo-2-styrylbenzimidazoles and Fluoroquinolones were showed significant activity against M.Tuberculosis bacteria which include both replicating and non-replicating types. Quinolone antibiotics constructed of quinoline ring system which can be considered as a privileged structure and is the most spectacular example of the potential efficiency in medicinal chemistry. By observing the anti-tubercular activities of both 2-styrylbenzimidazoles and fluoroquinolones and from the QSAR approach, the synthesis of novel 2-(4-halostyryl)-1,6-dialkyl-9-oxo-6,9-dihydro-1H-imidazo[4,5-f]quinoline-8-carboxylicacid derivatives have been proposed.

OO-10 : Development of Qsar Models for Predicting Mutagenicity of A Series of Chemical Mutagens

Navneeta Upadhyay[1] and Apoorva Upadhyay[2]

[1]Department of Chemistry, Chameli Devi Group of Institutions, Indore-452020
[2]Department of Chemistry, Dr. H. S. Gour University, Sagar-470003

Quantitative Structure Activity Relationship analysis has been carried out on a series of aromatic and hetero aromatic amines which correlate the mutagenic activity and molecular structure of compounds by using structural and sterimol parameters. From a larger pool of structural and sterimol parameters we selected a smaller set consisting of three parameters. Selection is done by using NCSS software in that successive regressions were attempted using maximum R^2 method. The best QSAR model was selected; having the Regression coefficient (R^2= 0.9300) and Standard error of estimation (SE= 0.201).Predictive power of proposed model was confirmed by significant statistical tools.

OO-11 : One Pot Synthesis of 2-((4-Methylpiperazin-1-yl (Phenyl) Methyl) Benzene-1,3-Diol and its Derivatives

Nikita Umrigar*, Ketan C. Parmar and J. J. Vora

**Department of Chemistry, Sir P. T. Sarvajanik College of Science, Surat-395007, Gujarat*
Department of Chemistry, Hemchandrachraya North Gujarat University, Patan, Gujarat
**E-mail : nikitaumrigar@gmail.com*

The one pot reaction between 2-naphthol, aryl aldehydes and ammonia or amines yields aminobenzylnaphthols in process known as Betti reaction. This procedure can be interpreted as extension of the Mannich condensation with formaldehyde replaced by aromatic aldehydes, secondary amine by ammonia and the C – H acid by an electron-rich aromatic compound such as 2-naphthol.Betti base derivatives of 2-((4-methylpiperazin-1-yl(phenyl)methyl)benzene-1,3-diol were prepared through reactions of resorcinol, aromatic aldehydes and amines in ratio 1:2:1 in presence of CaF_2 at room temperature. The structures of the all synthesized compounds were confirmed by IR, ^{1}H-NMR, and Mass spectral studies.

OO-12 : Calcium Oxide Catalyzed Synthesis of Chalcone Under Microwave Condition

Pramod Kulkarni

Department of Chemistry, Hutatma Rajguru Mahavidyalaya, Rajgurunagar, 410505 (MS)
E-mail : pramodskulkarni3@gamil.com

Calcium oxide was found to be an efficient solid base catalyst for synthesis of chalcone under microwave condition. We employed this method for the synthesis of various chalcone from various substituted ketone and aldehyde including o-hydroxy ketone and o-amino ketone. The merits of this method are inexpensive and easily available solid base catalyst, shorter reaction time, high yield compared to other reported methods, avoid use of toxic reagents and solvent free condition, and they are applicable to base sensitive functional groups.

OO-13 : Smith Degradation Studies of Periodate Oxidised Seeds Polysaccharide from Cassia Alata Linn. Plant

R. B. Singh

Department of Zoology, School of Life Sciences, Dr. B. R. Ambedkar University, Khandari Campus, Agra-282 002 (U.P.)
E-mail : rbsinghugc@gmail.com

Cassia alata Linn. plant belongs to family- Caesalpiniaceae and

occurs in Northern India. Seeds yielded a water soluble polysaccharide as D-galactose and D-mannose in 2:3 molar ratio by column and paper chromatographic analysis. Present investigation mainly deals with the polyalcohols by Smith degradation studies of periodate oxidised seeds polysaccharide. Periodate oxidised polysaccharide on reduction with sodium borohydride and hydrolysis with sulphuric acid and obtained hydrolysate on paper chromatographic analysis to revealed 2 spots corresponding to glycerol and erythritol in 0.81:2.56 molar ratio. Derivative of glycerol was prepared with pyridine and p-nitrobenzoyl chloride after recrystallisation with acetone as : glycerol-tri-O-p-nitrobenzoate, had m.p. & mixed m.p. 187-189^{0}C while erythritol as : tetra-O-tosyl-erythritol had m.p. & mixed m.p. 164-166^{0}C. Absorbance and colour intensity were recorded at 530 mμ photoelectrocolorimeter. Large amount of erythritol released with acid hydrolysis of polyalcohols produced by sodium borohydride serves as evidence that the main polymer chain linkages are of (1→4)-β-type and (1→6)-α-type linkages at non-reducing end. Ratio of erythritol to the amount of glycerol indicated that the branching point on the average of 4th unit in the backbone of the polysaccharide structure of Cassia alata Linn. plant.

OO-14 : Synthesis and Characterization of α-zirconium Phosphate Intercalated Metal-Salen Complexes and their Catalytic Applications

Savita Khare[1], Priti Shrivastava[*], Jagat Singh Kirar and Swati Parashar

School of Chemical Sciences, Takshashila Campus, Khandwa Road
Devi Ahilya University, Indore-452 001 (M P)
*E-mail : [1]kharesavita@rediffmail.com, *pritis026@gmail.com*

Metal-Salen intercalated a-zirconium phosphate, abbreviated as {a-ZrP.M(Salen), where M = Fe(III) and Mn(II)} was synthesized insitu by the flexible ligand method. The structure of resulting compounds was characterized by BET surface area, powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), X-ray photoelectron spectroscopy (XPS), Thermogravimetric analysis (TGA) and UV-visible spectroscopy. The catalytic activity of α-ZrP.M(Salen) was tested for the oxidation of cyclohexane using dry tert-butylhydroperoxide as an oxidant. In the oxidation reaction, cyclohexane was oxidized to cyclohexanol (A), cyclohexanone (K) and some unidentified products. It was found that the reactivity of α-ZrP.Fe(Salen) is greater than α-

ZrP.Mn(Salen) in the oxidation reaction. Influence of various reaction parameters viz. reaction temperature, catalyst concentration, substrate to oxidant molar ratio was studied using α-ZrP.Fe (Salen) catalyst to obtain maximum conversion (29.30%) of cyclohexane. The catalyst was reused for five cycles.

OO-15 : An Efficient Synthesis of Quinoline-3-N-Phenylpyrazoles and Quinalone-3-Cyclohexadienone Derivatives

K. Shiva Kumar[1,2], A. Naidu[1] and P. K. Dubey[1]

[1]Department of Chemistry, Jawaharlal Nehru Technological University Hyderabad College of Engineering, Kukatpally, Hyderabad (A.P)-500 085.
[2]Department of Chemistry, Osmania University, Hyderabad-500 007
E-mail : shivakumarkota@yahoomail.com

Quinalones, because of their numerous pharmacological properties are often considered as widely used N-heterocycls in both academia and pharmaceutical industries.[1,2] Here we are presenting an efficient synthesis of quinalone-3-(N-phenylpyrazoles) and quinalone-3-(cyclohexadienone) derivatives is described. 2-Chloroquinoline-3-carboxaldehyde, on reaction with 4N HCl gives 3-formyl-2(1H)-quinalone. The latter is reacted with acetophenone in the presence of NaOH as base to yield the corresponding quinalone-3-chalcone which on treatment with phenyl hydrazine gives 3-(dihydropyrazolo)quinolone. Dehydrogenation of with chloranil yields the corresponding quinalone-3-(N-phenylpyrazoles). Quinalone-3-chalcone on bromination yields the dibromo derivative which on treatment with phenyl hydrazine yields directly quinalone-3-(N-phenylpyrazoles). On the other hand, quinalone-3-chalcone on treatment with acetoacetanilide in methanol using acetic acid as a catalyst afforded the corresponding quinalone-3-(cyclohexenone) derivatives which on dehydrogenation with chloranil, afforded the corresponding quinalone-3-(cyclohexadienone) derivatives in excellent yields. The products are obtained in good yields and in a state of high purity. The structures of the synthesized compounds have been established on the basis of spectral and analytical data.

OO-16 : Synthesis and Characterization of Anti Microbial N-substituted Gamma Pipradols

B. Sri Ramudu[1], Sd. Khasim Sharif, A. Venkateswara Rao, B. Satyanarayana, S. Venkat Rao[3] and D. Rama Chandran[2]

Acharya Nagarjuna University, Nagarjuna Nagar Guntur -522510
E-mail : sriram.elm.chem@gmail.com, dittakavirc@gmail.com

Synthesis of Anti microbial N-substituted gamma pipradol derivatives by using conventional chemical reactions to produces a

feasible and entirely new chemical entities (NCE'S) which are having a great potential microbial activity equivalent to fexofenidine used as a biological standard. This invention may help full for derive more potential pipradol molecules with (-HN-C=0) peptide bond formation.

OO-17 : Synthesis of the Molecules Containing Azetidinone Moiety by Conventional and Microwave Technology, their Comparative Studies, Antibacterial and Antifungal Activity

Srivastava, S. D.[*] and Srivastava, S. K.

Department of Chemistry, Synthetic Organic Chemistry Laboratory, Dr. H. S. Gour Vishwavidyalaya (A Central University) Sagar(MP)-470003
E-mail : drsavitri@rediffmail.com

The 2-oxo-azetidine skeleton has been recognized as a useful building block in the synthesis of biologically important compounds. This is mainly due to the strain energy associated with the four membered azetidine ring, which makes it susceptible for nucleophilic ring cleavage. This factor is also responsible for their application of azetidines as synthones for various stereoselective synthesis of biologically active heterocyclic compounds. 2-chloro 10H-phenothiazine is also of pharmaceutical importance because of different biological activities as reported in the literature. Chemically, 2-chloro-10H-phenothiazine has active site at N(10). We report on substitution at N(10) of 2-chloro-10H-phenothiazine and the combination with the 2-oxo-azetidine ring in a single molecule through propane bridge. We have synthesized some new compounds such as N10-(3-chlorophenyl)- 2-chloro-phenothiazine; N10-(2-amino)-2-chloro-phenothiazino-propyl)-hydrazine;N-10-(2-amino)-2-chloro-phenothiazino-propyl)-N-(substituted phenyl)-methylidene]-hydrazines and N10-(2-amino)-2-chloro-phenothiazino-propyl)-N-[(substituted phenyl)-3-chloro-2-oxo-1-iminoazetidines. A comparative studies in terms of time and yield have also been done using both the synthetic procedures. The final compounds were found to exhibit antibacterial activity against S. paratyphae and V. cholerae and antifungal activity against F. heterosporum and A. fumigatus respectively.

OO-18 : Quaternary Ammonium Tribromides as Green Reagents for Organic Transformations

Upasana Bora Sinha

Department of Chemistry, Nagaland University, Lumami-798627, Nagaland
E-mail : upasanaborasinha@gmail.com

Reagents involving bromine or bromine equivalents continue to

remain very important for organic synthesis. However, with environmental protection laws becoming more stringent, time and again concerns have been raised over the use of bromine (Br_2). Therefore there has been a necessity for development of alternative reagents which are environmentally benign. Quaternary ammonium tribromides (QATBs) are recognized as greener alternatives to elemental bromine. Quite a number of methods are available for QATB synthesis, but one of the most environmentally benign methods is from the reaction of the corresponding bromide with activated hydrogen peroxide.

QATB reagents have shown wide versatility and can be used in a variety of organic transformations[2] with activated aromatic compounds, multiple bonded compounds, polycyclic hydrocarbons, allyl alcohols, enones, etc, in different reaction conditions. This paper describes the details regarding methods of preparation of quaternary ammonium tribromides (QATBs) and presents an account of their versatility as reagents.

OP-CYSA-01 : Microwave Mediated Synthesis of Some Novel Pyrazole Carrying Cyclohexanone Derivative

Manju N.[1] and Balakrishna Kalluraya[2*]

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka
E-mail : bkalluraya@gmail.com

Pyrazoles are among the important scaffolds possessing various biological activities. Pyrazole and its derivatives are gaining importance in medicinal and organic chemistry. They have displayed broad spectrum of pharmacological and biological activities such as anti-bacterial, anti-depressant, and anti-hypoglycemic. The bioactivity of functionalized N-arylpyrazole was extensively studied and are also exploited in the design of pharmaceuticals and agrochemicals. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as cannabinoid hCB1 and hCB2 receptor, anti-inflammatory, inhibitors of p^{38} kinase, CB_1 receptor antagonists, antimicrobial activity. Extensive studies have been devoted to arylpyrazole derivatives such as Celecoxib, a well-known cyclooxygenase-2 inhibitor. As a consequence, much attention has been paid to the design and synthesis of pyrazole derivatives.

Keeping in view of these observations we synthesized a new series of 1-(furan/thiophene-2-yl)-3-(-3-methyl-5-phenoxy/alkoxy-1-phenyl-1H-pyrazole-4-yl)prop-2-en-1-one on reaction with ethylacetoacetate in anhydrous potassium carbonate gave the title pyrazole carrying cyclohexanone moiety. The structure of the newly

synthesized compounds was established by analytical and spectral data. The new compounds were also screened for their biological properties. The result of such studies will be presented.

OP-CYSA-02 : Design, Docking Studies and Molecular Iodine Catalyzed Synthesis of Benzo [a] Xanthen-one Derivatives as Hyaluronidase Inhibitors

Mahadev N. Kumbar and Ravindra R. Kamble*

Department of Studies in Chemistry, Karnatak University, Pavate nagar, Dharwad-580003

**E-mail : kamchem9@gmail.com, mahadevnkumbar@gmail.com*

A series of novel benzo[a]xanthen-11(12H)-one derivatives 4a-m were designed and thoroughly characterised by IR, NMR and GC-MS spectral studies. The title compounds were synthesized from 3-aryl-4-formylsydnones 1a-m, β-naphthol and dimedone in presence of molecular iodine as a catalyst. Docking studies were carried out on all the derivatives into the active site of hyaluronidase and evaluated for their in vitro inhibitory effects on the hyaluronidase.

OP-01 : Isolation and Structural Elucidation of New Flavonoid Glycosides from Aerial Parts of *Rivea Hypocrateriformis* and their Anti-Inflammatory Activity

J. S. Biradar[1]*, S. S. Godipurge[1], S. Rahber[1], B. S. Naraboli[1], A. S. Rathod[1], Pushpa H.[1] and N. Mahurakar[2]

[1]Central Research Laboratory, Department of P. G. Studies and Research in Chemistry, Gulbarga University,Kalaburagi-585 106, Karnataka State

[2]Department of Pharmacology, HKES Matoshree Taradevi Rampure Institute of Pharmaceutical Science, Gulbarga-585105 Karnataka State

**E-mail : jsbiradar55@gmail.com*

The present study was designed to isolate and characterize the anti-inflammatory compound of *Rivea hypocrateriformis*. The ethanolic extract from the aerial parts of *Rivea hypocrateriformis* was separated by chromatography and the structure of new compound was elucidated based on spectral analysis. Anti-inflammatory activity of the isolated compound was assessed in rats with carrageenan induced paw edema assay. The new flavonoid glycosides, named as hypocroside(compound **1**) was isolated from the ethanolic crude extract of the aerial parts of*Rivea hypocrateriformis*. They showed significant anti-inflammatory activity. In conclusion, compound **1**is new natural product, which showed significant anti-inflammatory activity in a dose dependent manner.

OP-02 : Synthesis and Antileishmanial Activity of Some Novel Series of π-Electron Deficient Heteroannulated Thiouracil Derivatives

N. Verma and D. N. Singh*

Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad- 224001

**E-mail: dnsinghsaket@yahoo.com, nvermasaket@yahoo.co.in*

Drug discovery leading to robust and viable lead candidates remains a challenging task, which is the transition from a screening hit to a drug candidate, requires expertise and experience. Nitrogen heterocycles possess a wide range of pharmacological activities and play a significant role in medicinal chemistry. Drugs currently in the market against leishmaniasis are sodium stibogluconate (Pentostam) and meglumine antimoniate (Glucantime) despite of their renal and cardiac toxicity. Amphotericin B and its liposomal form are effective but highly expensive and other newly introduced drugs, miltefosine and phosphocholine analogue are quite effective but instigate severe gastrointestinal problems and teretogenic effects and can not be used for pregnant women. Keeping in view importance of the search of the new safer and most effective drugs for the treatment of leishmaniasis, we envisioned our approach toward the synthesis of some novel series of ð-electron deficient heteroannulated thiouracil derivatives for their antileishmanial activity. In this presentation, the detailed synthetic procedure, mechanisms of the reactions, characterizations by their spectral data analysis and antileishmanial activity profiles of the synthesized compounds will be discussed.

OP-03 : Recent Advances in Synthesis of Biodiesel from Semecarous Anacardium Oil

Vustelamuri Padmavathi and Bhattiprolu Kesava Rao*

[1]Chairman-BOS, Department of Chemistry, University College of Sciences, Acharya Nagarjuna University, Nagarjunanagar – 522 510,Guntur District, Andhra Pradesh

**E-mail : krbhattiprolu@gmail.com, padma1202@gmail.com*

As petrol is a fast depleting natural resource, it became a tremendous need for the scientists to search for an alternative renewable resource to petrol, is a deemed necessity. Now serious efforts are being made on the production and utilization of biodiesel in India and other parts of the world. As an alternative invention of synthesis of biodiesel from naturally occurring herbal plants became the target. In this study, *Semecarpus Anacardium L.f.,*which grows naturally without any cost and care by the time, is analyzed

and investigated as a proper feedstock in producing biodiesel for the first time. In order to prove its suitability, its seed and oil were experimented first in our laboratory. The tree is widely distributed through the hotter part of India. It is frequent in dry deciduous forests of Central India and common in dry deciduous forests of Maharashtra spreading over Khandesi, Marathwada and East Maharashtra, in India. In the present study, biodiesel has been synthesized from *Semecarpus Anacardium L.f.* oil. The acid value of this oil was found to be as 0.5, which leads us to convert it to biodiesel by the esterification followed by trans-esterification process. The methyl esters produced by these methods were analyzed and found that some of them are suitable as biodiesel fuel to ascertain their suitability as diesel fuels.

OP-04 : Synthesis of Triazine Linked Dithiadiazines by Microwave Irradiation Technique, Comparison with Conventional Method of Heating and Antimicrobial Evaluation

Pradip P. Deohate* **and Roshani S. Mulani**

Department of Chemistry, Shri Radhakisan Laxminarayan Toshniwal College of Science, Akola
E-mail : pradip222091@yahoo.co.in, roshanimulani05081992@gmail.com

The heterocyclic compounds especially with distinguished pharmacological activities have proved to be excellent and versatile drugs in the field of medicinal chemistry. Triazine linked dithiadiazines have diversified therapeutic applications.

In present study synthesis of 1-(6-arylimino-3-phenylimino-[1,2,4,5]-dithiadiazin-4-yl)-2-(4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-ethanones have been carried out by interaction of (4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-acetic acid N-(N'-aryl-thioamido)-hydrazides with N-phenyl-S-chloro isocyanodichloride by microwave irradiation technique as well as conventional method of heating. The required hydrazides have been synthesized by the condensation of ethyl (4-benzylideneamino-6-methyl-[1,3,5]-triazin-2-yl-amino)-acetate with hydrazine hydrate followed by the interaction with N-aryl isothiocyanates by both methods. The substituted ethyl acetate was prepared by conventional method of heating of 2,4-diamino-6-methyl-[1,3,5]-triazine with benzaldehyde followed by interaction with ethyl chloroacetate using both methods. Structures of the compounds were established on the basis of IR, ^{1}H-NMR, mass spectral studies and their physico-chemical properties. The synthesis of title compounds by microwave irradiation technique and its comparison with conventional method

of heating was studied and confirmed by TLC. The title compounds have been evaluated for their antimicrobial study.

OP-05 : Synthesis and Characterization of Biologically Important (4*Z*)-4-[(2-Chloroquinolin-3-yl)Methylidene]-5-Methyl-2,4-Dihydro-3*H*-Pyrazol-3-One

Vineetha Telma D'Souza[1] and Janardhana Nayak[2]

[1]Deparment of Chemistry, M.I.T.E., Moodabidri-574 225
[2]Deparment of Chemistry, N.M.A.M. I.T, Nitte-574 110
E-mail : tel_mod@yahoo.com, jnayak@nitte.edu.in

There has been considerable interest in the development of novel compounds of quinoline derivatives with anticonvulsant, antidepressant, analgesic, anti-inflammatory, antiplatelet, antimalarial, antimicrobial, antitumoral and antiviral activities. Therefore, many researchers have synthesized these compounds as target structures and evaluated their biological activities. These observations have been guiding for the development of new quinoline derivatives such as (4*Z*)-4-[(2-chloroquinolin-3-yl)methylidene]-5-methyl-2,4-dihydro-3*H*-pyrazol-3-one, that possess varied biological activities. The synthesized compounds will be characterized FTIR, Mass Spectroscopy and NMR spectral data.

OP-06 : Conventional and Green Synthesis of Mercapto Triazoles Coupled with Azlactones, Characterization and Evaluation of Anti-Microbial Studies

Aliya Begum, Mamtha Padithem, Ameena Husain, S. Shahjahan and Sarala Devi*

Department of Chemistry, University College for Women, Koti, Hyderabad-095, Telangana
Department of Chemistry, University College of Science, Osmania University, Hyderabad-07, Telangana
E-mail : dr_saraladevi@yahoo.com

Green chemistry emphasizes the development of environmentally benign chemical processes and technologies. The reactions involving principles of green chemistry are effective in building highly functionalized organic molecules with diverse anti-microbial profile from readily available starting materials with inherent flexibility and feasibility coupled with minimization of time, labour, cost and waste production. In continuation of our search for new synthetic methodologies, we herewith report the conventional and green synthesis of mercapto triazoles coupled with azlactones of various

aromatic aldehydes, their characterization and anti-microbial studies. The reactions has been conducted by employing green methods which afforded the corresponding mercapto triazole derivatives in excellent yields. The reactions proceeded instantaneously and pure product was obtained without using any chromatographic techniques. The reaction protocol developed in the present study offers fast and eco-friendly methods for the synthesis of compounds possessing a broad spectrum of biological activity.

OP-07 : Synthesis and Biological Evaluation of Novel Indole Analogues Incorporated with Imidazolone, Thiosemicarbazone and Thiazolidinone Moieties

Saundane Anand R.* **and Annapurna Halu**

Department of Post-Graduate Studies and Research in Chemistry,
Gulbarga University, Gulbarga -585 106, Karnataka
E-mail : arsaundane@rediffmail.com

Schiff bases are well known for their pharmacological properties as anti-bacterial, antifungal, anti-cancer and anti-viral agents. The occurrence of indole ring system in numerous biologically active molecules has been recognized which plays an important role in animal and plant kingdom. Different indole bearing compounds possess activities such as antibacterial, antifungal, antiviral, antimalarial, and anti-HIV.

In the present study series of new Schiff bases containing indole moiety such as,(E)-2-{1-[4-((Z)-4-[(5-substituted-2-phenyl-1*H*-indol-3-yl)methylene]-5-oxo-2-phenyl-4,5-dihydro-1*H*-imidazol-1-yl)phenyl]ethylidene}hydrazinecarbothioamide (**5a-c)** and their cyclocondensation products (Z)-2-{(E)-{1-[4-((Z)-4-[(5-substituted-2-phenyl-1*H*-indol-3-yl)methylene]-5-oxo-2-phenyl-4,5-dihydro-1*H*-imidazol-1-yl)phenyl]ethylidene}hydrazono} thiazolidin-4-one (**6a-c)**, were prepared.

The structure of the newly synthesized compounds have been confirmed on the basis of their elemental analyses, IR, ^{1}H &^{13}C NMR and mass spectral studies. These compounds were screened for their antioxidant and antimicrobial activities.The RSA results revealed that the compound **6a** showed excellent activity of 80.53, 83.33, 84.75 and 85.13% at concentrations 25, 50, 75 and 100 µg/mL respectively. Whereas compound **4a** exhibited good activity of 78.84 % at 100 µg/mL concentration.Differences in standard deviation. Compound **6a** showed excellent activity against *S. Aureus*, *E. Coli* and *P. Aeruginosa* and rest of the compounds showed moderate activity against tested bacteria.

OP-08 : Microwave Assisted Synthesis of Sydnone Containing 2,5-Disubstituted-1,3,4-Thiadiazines Under Solvent Free Condition

Aparna K. and Balakrishna Kalluraya*

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka
E-mail : bkalluraya@gmail.com

1,3,4-thiadiazines are an important class of six-membered heterocycles with a broad spectrum of biological activities. They demonstrated excellent cardiotonic, spasmolytic and hypertensive activities. Additionally, compounds of this class are used in the treatment of anaemia, asthma and allergies. Some 1,3,4-thiadiazines are also applied in agriculture as herbicides, fungicides, insecticides and they displays wide range of therapeutic activities like antibacterial, cardiovascular, antiHIV, antidiabetic, antidepressant.

The most common route for the synthesis of 1,3,4-thiadiazine derivatives is via the condensation of semithiocarbazides and α-haloketones. Literature survey revealed that neither solvent free nor the microwave irradiation was used for the synthesis of this class of compounds. In addition,use of MW energy in sydnone chemistry is yet to begin due to their unique properties. Contemplated by the above observations, novel series of sydnone containing 1,3,4-thiadiazine derivatives were synthesized using microwave and solvent free methods, as faster and efficient methods for their synthesis. The structure of the newly synthesized compounds was established by analytical and spectral data.

OP-09 : Synthesis of Novel N-Substituted Tetrazolonaphthalenes

K. Venkatanarsimha Rao[1] and Bethanamudi Prasanna[1,2*]

[1]Research & Development Center, Bharathiar University, Coimbatore, Tamilnadu, India & Rakshit Pharmaceuticals Ltd, Plot No 68/A, Parawada, 531021, Vishakhapatnam, (AP)
[1,2]Research Center, Chaitanya Post Graduate College (Autonomous), Hanamkonda, Warangal, Telangana State- 506 001.*
E-mail : prasschem@gmail.com

Agomelatin, a naphthalene derivative which is combination of both agonist of human cloned melatonergic MT1 and MT2 receptors. Agomelatine may represent the prototype of a new drug which is the first antidepressant and it does not block the re up take of monoamines, It is also a 5-HT_2C selective antagonist which was revealed to potent in resynchronization of circadian rhythms.

Novel analogues of Agomelatine were synthesized from 2-(7-methoxynaphth-1-yl)acetonitrile. From last twenty years, Agomelatine, a melatonin-like antidepressant drug which is based on a naphthalene moiety has received a huge attention. This drug molecule gets short plasma half-life as a result of undergoing very important liver first pass effect. So in order to overcome this drawback, we have come up with an approach which is based on the use of substituted aryl derivatives of tetrazole scaffold to replacement of the *N*-acetyl side chain. We successfully designed aryl substituted tetrazolo naphthalene scaffolds, a much centered template which can be elaborated further into agomelatine compounds. Along with this work, further important works are under progress.

OP-10 : Synthesis and Biological Activity Substituted of 2-((1H-benzo[d]imidazol-2-yl) thio)-N-(4-(4-(1H-indol-3-yl)-1H-Benzo[b][1,4]Diazepin-2-yl)Phenyl) Acetamide and their Derivatives

Basavaraj S. N., Shaik Rahber, Shivakumar G., Anil R., Pushpa H. and J. S. Biradar*

Department of Studies and Research in Chemistry
Gulbarga University, Kalaburagi – 585106
Karnataka.

A new series of novel Benzodiazepine derivatives bearing a Benzimidazole and Indole moieties are reported. Claisen–Schmidt condensation of 2-(1H-benzo[d]imidazol-2-ylthio)-N-(4-acetylphenyl) acetamide and 2,5-disubstituted indole-3-carboxaldehydes will give (E)-2-((1H-benzo[d]imidazol-2-yl)thio)-N-(4-(3-(1H-indol-3-yl)acryloyl)phenyl)acetamides. The acid catalysed cyclo condensation of synthesised chalcones with substituted ortho-phenylenediamine has produced the titled compounds in good yields. All the newly synthesized compounds are characterised by IR, ^{1}H NMR, Mass spectral and analytical data. Compounds prepared have been subjected to antimicrobial and antioxidant evaluations.

OP-11 : Bismuth Chloride Mediated Prenylation of Carbonyl Compounds in Aqueous Media : An Issue of Regio and Stereo Selectivity

B. Jadhav and S. K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
**E-mail : skpar@chem.unipune.ac.in*

The bismuth chloride mediated, aluminum promoted aqueous

Barbier type coupling of prenyl unit with carbonyl compounds which gives the corresponding homoallyl alcohol is studied. The method provides a convenient route for the direct γ-prenylation of carbonyl compounds in a highly regioselective manner using inexpensive and convenient catalytic system. By simply altering the reaction solvent and temperature, the method allows the achievement of a highly notable reverse regio-control, affording the desired α-regiochemical product. The results show that the most reactive intermediate species mediates prenylation of electronically divergent aldehydes and ketones with excellent yields in aqueous medium.In addition the role of solvent, temperature and additives on the formation of prenyl alcohol is also elaborated.

OP-12 : In Water-Ultrasound Promoted Synthesis of Teraketones and 2-Substituted-1H-Benzimidazoles Catalyzed by BiOCl Nanoparticles

Bharatkumar M. Sapkal and Prakash K. Labhane

Post Graduate and Research Recognized Department of Chemistry, M.G.S.M'S Arts, Science and Commerce College Chopda, Dist.: Jalgaon. (M.S.)

Highly efficient, green procedure has been developed for the synthesis of various structurally diverse teraketones and 2-substituted-1H-benzimidazoles derivatives. The reaction was performed in water under ultrasound irradiation, using BiOCl nanoparticle catalysts. The nano-catalyst was found to be re-usable for seven subsequent reactions without much loss in the activity. Simple methodology with short reaction times, mild reaction conditions with easy work-up procedure is the salient feature of this method.

OP-13 : Synthesis of Novel N, N-dialkyl-(1H-indol-3-yl)Methylarylamidesand their Biological Evaluation

J. S. Biradar[1*],Pushpa H.[1], S. S. Godipurge[1] and A. S. Rathod[1]

[1]Central Research Laboratory, Department of P. G. Studies and Research in Chemistry, Gulbarga University,Kalaburagi-585 106, Karnataka State
[*]E-mail : jsbiradar@rediffmail.com

N-alkylation of indole-3-carboxaldehyde (I) was carried out with distinct alkyl halides using K_2CO_3as a base resulted N-alkyl indole -3- carboxaldehydes (II). Reaction of compounds IIwith primary aminesusing p-TSA resulted in an imine and subsequent reduction using $NaBH_4$ resulted the corresponding secondary amines (III). Secondary amines (III) were reacted with t aryl acid chlorides to form corresponding tertiary amides (IV). All the final compounds were existing as rotamers and the structures were confirmed by

spectral data (^{1}H NMR, mass, & IR). All these novel compounds were submitted for distinct biological activities.

OP-14 : Synthesis of Substituted 1,3-thiazines and their Nanoparticles on Phytotic Growth of Some Vegetable Crops

Chhaya D. Badnakhe[1] and P. R. Rajput[2]

[1]Department of Chemistry, Dr.Manorama and Prof.H.S.Pundkar, Arts, Commerce and Science College, Balapur, Dist. Akola.
[2]Department of Chemistry,Vidyabharti Mahavidyalaya, Amravati-444604
E-mail : chhayadeotalu@rediffmail.com, prsrajput@rediffmail.com

The synthesis, spectral analysis and biological activities of 4-phenyl-2-hydroxychlorosubstituted-2-imino-1,3 thiazines have been carried out. In this case 4-(2'-hydroxy-3',5'-dichlorophenyl)-6-(4"-nitrophenyl)-2-imino-3,6-dihydro-1,3- thiazine (A), 4-(2'-hydroxy-3',5'-dichlorophenyl)-6-(4"-nitrophenyl)-2- iminophenyl-3,6-dihydro-1,3-thiazine(B), and 4-(2'-hydroxy-3',5'-dichlorophenyl)-6-(4"-nitrophenyl)-2-iminophenyl-6H-3Nphenyl-1,3-thiazine (C) have been screened. The compounds A,B and C were synthesized from 2'-hydroxy-3,5-dichlorophenyl-4-(4”-nitrophenyl) chalcone (a) by the action of thiourea, phenylthiourea, diphenylthiourea. The compound (a) was synthesized from 2’-hydroxy-3’,5’-dichloroacetophenone by the action of p-nitrobenzaldehyde in ethanol and 40% NaOH. The nanoparticles of the compounds A, B and C have been prepared by using ultrasonic technique. The titled compounds and their nanoparticles were screened for their growth promoting activity on some vegetable crop plants viz.. *Momordica Charantia-L-Bitter* guard (Karela), Lagneria siceraria-snake guard (Lavki), Luffa cylindrica L-sponge guard (Gilke) and Benincasa hispida-Pumpkin (Kohle).

OP-15 : Synthesis and Characterization of Some Primidine-2-Thiols as Potential Antibacterial Agents

Dayanada P[1*] and Janardhana Nayak[2]

[1]Department of Chemistry, Excellent Science and Commerce PU College Moodibidri, Mangalore.
[2]Department of Chemistry, NMAM Institute of Technology, Nitte-574 110, Karkalla Taluk, Udupi District
E-mail : pdayanada@gmail.com, jnayak@nitte.edu.in

Pyrimidine derivatives exhibit a variety of biological activities like antimalarial, anti-inflammatory, antimicriobial, anticonvulsant, antipyretic etc. Keeping in view of these observations, we planned to synthesize some substituted 1,4,5,6-tetrahydropyrimidine-2-thiol. So in the present investigation 1-[5-(4-substituted phenyl)-1,3,4-thiadiazol-2-yl]thioureas were made to react with substituted

chalcones. During this reaction we ended with a new series of substituted -1,4,5,6-tetrahydropyrimidine-2-thiol. The structures of the new compounds were characterized by spectral and analytical data. The new compounds were also subjected to antibacterial activity studies.

OP-16 : Synthesis of Oxadiazole Clubbed Thiadiazole as Antimicrobial Agents

Alpa Dave[*1], Piyush Vyas[2], Vipul Prajapati[2], Kalpesh Parikh[2] and Deepkumar Joshi[2]

[1]Dept. of Chemistry, HNGU, Patan-384265
[2]Chemistry dept., Sheth M. N. Science College, Patan-384265
[*]E-mail : alpadave450@gmail.com

A series of heterocyclic derivatives bearing oxadiazole and thiadiazole rings were synthesized using multi step reactions. The titled derivatives were screened for their structural characterization using FT-IR, ^{1}H NMR and Mass spectra and were found to be correct. These compounds were tested for their antimicrobial activity against various strains of gram positive bacteria, gram negative bacteria and fungi.

OP-17 : Synthesis and Pharmacological Studies of Novel Triazole-Linked Pyrazoline Hybride Compounds

Desta Gebretekle and Balakrishna Kalluraya

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka

E-mail : bkalluraya@gmail.com, destish2002@gmail.com

Pyrazoline and its derivatives have vast value in synthetic medicinal chemistry as they display a broad spectrum of pharmacological and biological activities. Research survey reveals that introduction of acetyl group at 1st position of pyrazoline ring enhances the biological activity and stability of pyrazolines. Chalcones are convenient precursors for the synthesis of pyrazolines. Although a large number of pyrazoline derivatives were reported, there are only few reports involving the synthesis of aryl furfuryl-[1, 2, 3]-triazolo-pyrazolyl hybrids.

With a view to further contribute in the development of chemistry and to assess the microbial profile of this class of compounds, it has been thought valuable to synthesize some pyrazolines carrying biologically active [1,2,3]-triazolyl and furfuryl moieties in single molecular frame work. The novel series of

biologically active pyrazolines were synthesized from the reaction of triazole linked chalcones with hydrazine hydrate in glacial acetic acid. Chalcones were obtained by condensation of triazole containing ketone with aryl furfuraldehydes. Furthermore, triazole containing ketones were synthesized by 1, 3-dipolar cycloaddition of p-azido acetophenone with acetyl acetone as dipolarophiles. The structural elucidations of newly synthesized products were done by elemental analysis and spectral data. All the synthesized compounds were also screened for in vitro antibacterial and antifungal activities.

OP-18 : A Green Synthesis of 3-Cinnamoyltropolones using Grinding Technique Under Solvent Free Conditions

Dinesh Kumar Sharma[1*] and Surender Kumar[2]

[1]Department of Chemistry, Kishan Lal Public College, Rewari, 123401
[2]Department of Chemistry, The Technological Institute of Textile & Sciences, Bhiwani-127021
[*]E-mail : dksharma_84@rediffmail.com

A simple, efficient and eco-friendly procedure for the synthesis of 3-cinnamoyltropolones via Claisen-Schmidt condensation involving grinding of 3-acetyltropolone and substituted benzaldehydes with pulverized potassium hydroxide at room temperature under solvent free conditions has been described. The protocol is much more efficient as the reactions are carried out at room temperature and yields are also quite high and also avoids the use of hazardous chemicals and organic solvents at any stage of the reaction.

OP-19 : Antimicrobial Activity of 1,1 Bis- {2- Hydroxy-3-(1´- Chloro Phenyl -5´-Aryl-pyrazoline 3´-yl) – 5 Methyl Phenyl} Methanes

R. P. Ganorkar[1] and R. E. Bhadange[2]

[1]Department of Chemistry, Mahatma Fule Arts, Commerce & Sitaramji Chaudhari Science Mahavidyalaya, Warud Dist. Amravati - 444 906
[2]Department of Chemistry, ShriShivaji College, Akola - 444 101
E-mail : rajesh.ganorkar@rediff.com

The present investigation was focused on the Antimicrobial Studies of newly synthesized compounds 1,1 Bis- {2- Hydroxy-3-(1´-Chloro Phenyl -5´-Aryl-Pyrazoline 3´-Yl) – 5 Methyl Phenyl} Methanes have been evaluated for their in vitro growth of inhibitory activity against one Gram-positive strain Staphylococcus aureus and three Gram-negative strains like Escherichia coli, E. aerogens and Salmonella typhi using paper disc-method at concentration of 50ìg/ml using DMF as solvent. The culture medium was nutrient agar medium After 24± 2 hours of incubation at 37 ± 2 ^{0}C. It has

been observed that newly synthesized compounds were found more or less effective against, Staphylococcus Aureus, Escherichia Coli, E. Aerogenus and Salmonella Typhi.

OP-20 : Solvent Free and Catalyst Free Synthesis of Biscoumarin Derivatives Just by Grinding Under Ambient Condition A Green Chemistry Approach

G. M. Nazeruddin*, Khurshid Ahmed, Ruqia Shailkh and Shifa Khan

Dept. of Chemistry (PG and Research Centre), AbedaInamdar College,Pune-411001
E-mail : gmnazeruddin@yahoo.co.in

Solvent free and catalyst free synthesis of Biscoumarin derivatives through condensation reaction of aromatic aldehydes and 4-hydroxy coumarin with few drops of water is accomplished just by grinding under ambient condition with excellent yield is described.

OP-21 : Synthesis and Characterization of Bifunctional Reactive Dyes and their Application on Various Fibres

Jigna A. Patel[1], Paresh S. Patel[1] and Keshav C. Patel[2]

[1]Narmada College of Science and Commerce, Zadeshwar, Bharuch-392011,Gujarat
[2]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007.
E-mail : ncscpsp@gmail.com

A series of bifunctional reactive dyes has been synthesized by coupling of diazotized 2-amino-5-(3-carboxy-4-(2-methyl-4-oxoquinolin-3(4H)-yl)benzyl) benzoic acid with various 2-(4-amino-3-methoxy phenyl sulphonyl) ethyl hydrogen sulphato cyanurated components such as H-acid, Gamma acid, J-acid, N-Methyl J-acid, N-Phenyl J-acid, Chicago acid, S-acid, K-acid, Bronner acid, Peri acid, Laurent acid and Koch acid. They were characterized by nitrogen elemental analysis, IR and ^{1}H-NMR spectra. The dyeing performance of all these dyes on wool, silk and cotton fibres gave fair to good light fastness, good to excellent fastness to wash and rubbing fastness.

OP-22 : Synthesis of Novel Azetidinone and Thiazolidinones Derivatives and Evaluation of Their Antimicrobial Activity

D. M. Vashi* and K. B. Kurmi

Department of Chemistry, Narmada College of Science & Commerce, Bharuch, Gujarat
E-mail : kurmi7sinh@gmail.com,

4[(2E)2-benzylidenehydrazinyl]6-tert-butyl-3-(methylsulfanyl)-

1,2,4-triazin-5(4H)-one was prepared from 4-amino-6-tert-butyl-3-(methylsulfanyl)-1,2,4-triazin-5(4H)-one. This amine on facile condensation with aromatic aldehydes afford Schiff Base. These anils on cyclocondensation reaction with chloro acetyl chloride and thio glycolic acid (i.e. mercapto acetic acid) yields 2-azetidinones and 4-thiazolidinones respectively. The structure of the 2-azetidinones and 4-thiazolidinones were confirmed by elemental analysis (C. H. N.) and FT-IR, ^{1}H-NMR spectroscopy. The prepared compounds have been screened on some stains of bacteria.

OP-23 : Microwave Assisted Synthesis, Chareacterisaion and Biological Activity of 4-(2-(Substituted Aryl) Hydrazono)- 1-(*p*- Tolyloxyacetyl)-3- Mehyl-1H-Pyrazol-5-One

Kaushik B. R. and Balakrishna Kalluraya

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574199, Karnataka
E-mail : bkalluraya@gmail.com

Pyrazole and its derivatives are important in synthetic medicinal chemistry as they display a broad spectrum of pharmacological activities such as anti-microbial, anti- oxidant, and anti-inflammatory. Pyrazole with various substituent moieties were reported to be selective inhibitors of cyclooxygenase, and also exhibit anti diabetic, herbicidal properties. Therefore synthesis of pyrazole has immense importance in the field of medicinal chemistry.

Prompted by the above observations, we synthesized a novel series of pyrazolones derivatives from *p*- tolyloxyacethydrazide and ethyl-2-arylhydrazono-3-oxobutyrate by employing microwave irradiation in glacial acetic acid. The ethyl-2-arylhydrazono-3-oxobutyrate were in turn prepared starting from different substituted anilines. The substituted anilines were converted into diazonium salt and this was treated with ethylacetoacetate in presence of sodium acetate to get corresponding oxobutyrates. The reaction of *p*- cresol with ethylchloroaceteate affords ethyl-*p*-tolyloxyacetates in excellent yield which on treatment with hydrazine hydrate yield *p*- tolyloxyacethydrazides. The newly synthesized compounds were characterized by spectral and analytical data and tested for antibacterial, antifungal and antioxidant activities.

OP-24 : A Versatile Synthesis and Antimicrobial Activity of 5-tetra-*o*-benzoyl-β-d-glucopyrano sylimino-3-oxo-2-aryl-4-aryl -1, 2, 4,-thidiazolidines

Kishor N. Puri* **and Gajanan. V. Korpe**

P.G. Department of Chemistry, Shri Shivaji College, Akola- 444003 (M.S.)
E-mail : knpuri@rediffmail.com

5-Tetra-*O*-benzoyl-β-D-glucopyranosylimino-3-oxo-2-aryl-4-*m*-tolyl-1, 2, 4 thidiazolidines have been prepared by the interaction of Tetra-*O*-benzoyl-β-D-glucopyranosyl-*S*-chloro-isothiocarbamoyl chloride and 1-aryl-3-*m*-tolyl carbamides. This converted high isolated yields which find applications in the area of medicinal chemistry. The identities of these newly synthesized compounds are established on the basis of elemental analysis IR, ^{1}HNMR, ^{13}C NMR, and Mass spectral analysis. These compounds were assayed for their antibacterial and antifungal activity against some selected pathogenic organisms like *E. Coli, P. Vulgaris, S. Aureus, Ps. Aeruginosa, B. Cereus and A. Niger, C. Albicans* to get potent bioactive molecule.

OP-25 : Synthesis, Characterization and Spectrophotometric Studies of Charge Transfer Interaction Between Donor Imidazole and π-Acceptor 2,4-Dinitro-1-Naphthol In Various Polar Solvents

Lal Miyan and Afaq Ahmad*

Department of Chemistry, Faculty of Science, Aligarh Muslim University, Aligarh-202002 (UP)
E-mail : lalmiyankhanalig@gmail.com

A novel charge transfer complex has been obtained between good donor imidazole (IZ) and π acceptor 2,4-dinitro-1-naphthol (DNN) in various polar solvents such as chloroform, ethanol, acetonitrile and DMF at room temperature. The molecular composition of the formed CT complex was recognized in 1:1 with the maximum absorption band. The high value of the formation constant confirmed the stability of the CT complex, which was estimated using Benesi-Hildebrand equation. The solid complex was synthesized and characterized using FTIR, TGA-DTA, powder XRD, ^{1}H NMR, UV-visible and ESI-mass spectra. Various important parameters such as formation constant (K_{CT}), molar extinction coefficient (ε_{CT}), and Standard Gibbs free energy (ΔG°), oscillator strength (f), transition dipole moment (μ_{EN}), resonance energy (R_N) and ionization potential (I_D) were calculated using Benesi-Hildebrand equation in different polar solvents. CT complex was formed by

proton transfer from DNN to IZ showing N^{+}—H---O^{-} bonding. Understanding the interaction between donor and acceptor able to interpret the donor–acceptor interaction and acting mechanism between these compounds. The formation constants of the CT complex were determined in different polar solvents from which ΔG° formation of the complexes was estimated

OP-26 : The Synthesis, Characterization and Application of Reactive Dyes Based on 4,4'-Methylene Bis-Orthonilic Acid on Various Fibres

Lina A. Patel[1] and Keshav C. Patel[2*]

[1]Department of Chemistry, C. U. Shah Science College, Near Income Tax, Ahmedabad-380 014 (Gujarat)
[2]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007 (Gujarat)*
E-mail : patlina@rediffmail.com

Ten hot brand bisazo reactive dyes have been synthesized by coupling tetrazotized 4,4'-methylene bis-orthonilic acid with various cyanurated coupling components and their dyeing performance on silk, wool and cotton has been assessed. The purity of dyes was checked by thin layer chromatography. The IR spectra showed all characteristic band and PMR spectra of representative dye showed all the signals. The percentage dye bath exhaustion on different fibres was reasonably good and acceptable. The dyed fibres showed moderate to very good fastness to light, washing and rubbing.

OP-27 : Synthesis, Characterization and Dyeing Performance Studies of Monoazo Pyrazolone Dyes based on 1,3,4-Thiadiazol Moiety

Malik G. M.[*] and Mitchla S. M.

[*]Department of Chemistry, Navyug Science College, Surat.
[*]E-mail : gmmalik2010@gmail.com, simiroserose@yahoo.com

Here in this paper we report a new series of 1,3,4-thiadiazol based heterocyclic monoazo dyes which have been derived by the diazotization of N^{4}-(5-benzyl-1,3,4-thiadiazol-2-yl)-1,3-thiazole-2,4-diamine with various phenyl pyrazolone as coupling components. The structure of the synthesized dyes was characterized by elemental analysis and IR, ^{1}H-NMR, UV spectroscopy. All the synthesized compounds were studied and their dyeing performance was evaluated. The fastness properties were measured. The synthesized disperse dyes were found to possess very good dyeing properties.

OP-28 : O-Acylation of Alcohols and Phenols Under Solvent Free Conditions Using Ionic Liquids as Efficient, Mild and Environmentally Benign Catalyst

Manoj A. Pande[1*] and K. Gajanan Sharma[2]

[1] Manoj A. Pande, Dept. of Chemistry, Tai Golwalkar Mahavidyalaya, Ramtek, Dist.: Nagpur
[2]K. Gajanan Sharma, Dept. of Applied Chemistry, KITs Ramtek, Dist.: Nagpur;
E-mail : pandemanoj82@gmail.com, gajanan_2k@yahoo.com

O-Acylation of Alcohols and Phenols was carried out using ionic liquid as catalyst under solvent free condition with acetic anhydride as acylating agent in high yields and short reaction time. The use of safe, mild, relatively non toxic catalyst making reaction condition environmentally benign.

OP-29 : Synthesis and Spectral Evaluation of the Imidazole Based 5-Substituted-Ene-3-(3-Imidazole-1-yl-Propyl)-2-Phenyl-3,5-Dihydro-Imidazole-4-ones

Jaydeep A. Patel and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : drnavinbpatel@gmail.com, jaydeep073@gmail.com

Spectral studies of imidazole containing 5-substituted-ene-3-(3-imidazole-1-yl-propyl)-2-phenyl-3,5-dihydro-imidazole-4-one molecule. This prepared from reaction between hipuric acid and substituted aldehyde, which gives 2-phenyl-4-substituted-ene-4H-oxazol-5-one as intermediate to react with 1-(3-aminopropyl) imidazole to give the final derivatives. Synthesized compounds were characterized by IR, ^{1}H NMR, ^{13}C NMR and Mass spectral data.

OP-30 : Newer Analogous of N-(Substituted-Benzothiazol-2-yl)-3-(2, 2 Dicholroethyl)-2 2-di Methyl Cyclopropane Carboxamide by Using Cypermethric Acid Chloride

Chetan Bulsara and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : drnavinbpatel@gmail.com, chetankumar.bulsara@bayer.com

Synthesis of newer compound N-(substituted- benzothiazol-2-yl)-3-(2,2-dicholroethyl)-2,2-di methyl cyclopropane carboxamide were achieved by condensation of substituted benzothiazole with 3-(2,2-dichlorovinyl)-2,2-dimethyl cyclopropane-1-carboxylic acid chloride. 3-(2,2- dichlorovinyl)-2,2-dimethyl cyclopropane-1-

carboxylic acid chloride were prepared via neat reaction using thionyl chloride. All the synthesized compound were characterized by IR, NMR, Mass Spectral analysis.

OP-31 : Synthesis, Characterization and Dyeing Assessment of New Acid Azo Dyes Based on 4,4'-Sulfonylbis (4,1-Phenylene) Bis (3-Amino Benzene-Sulfonate) on Wool, Silk and Nylon Fibers

Snehal N. Patel, Hiren S. Patel and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007, Gujarat
E-mail : drnavinbpatel@gmail.com, snehalpatel164@gmail.com

New tetra azo acid dyes were synthesized by the coupling of diazonium salt solution of 4,4'-Sulfonylbis(4,1-phenylene)bis(3-aminobenzenesulfonate) with different aromatic amine based acid. The resulting dyes were characterized by spectroscopic techniques, i.e., IR, ^{1}H-NMR and UV–visible spectroscopy. The dyeing performance of all the dyes was evaluated on wool, silk and nylon fabrics. Dyeing of wool, silk and nylon fabrics resulted in pink, orange and red shades with very good depth and levelness. The dye on fabrics showed moderate to very good light, washing, perspiration, and rubbing fastness. Some of the dye showed very good exhaustion and fixation properties on fiber.

OP-32 : Synthesis and Characterization of Monoazo Reactive Dyes and their Application on Various Fibres

Paresh S. Pate1[1], Dharmishtha H. Pate1[1], Rajesh B. Patel[2] and Keshav C. Patel[2]

Narmada College of Science and Commerce, Zadeshwar, Bharuch-392011, Gujarat
[1]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
[2]B.P.Baria Science Institute, Sayaji Road, Near fuvara, Navsari, Gujarat
E-mail : ncscpsp@gmail.com

A series of monoazo reactive dyes has been synthesized by coupling of diazotized aniline with various 4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amino cyanurated coupling components such as H-acid, Gamma acid, J-acid, S-acid, Koch acid, Bronner acid, Tobias acid, Cleve acid, Peri acid and Laurant acid. They were characterized by nitrogen elemental analysis, IR and ^{1}HNMR spectra. The dyeing performance of all these dyes on wool, silk and cotton fibres gave fair to good light fastness, good to excellent fastness to wash and rubbing fastness.

OP-33 : Synthesis of Monoazo Reactive Dyes and their Application on Silk, Wool and Cotton Fibres

Paresh S. Patel[1], Rajesh B. Patel[2] and Keshav C. Patel[3]

[1]Narmada College of Science and Commerce, Zadeshwar, Bharuch-392011, Gujarat
[2]B.P.Baria Science Institute, Sayaji Road, Near fuvara, Navsari, Gujarat
[3]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : ncscpsp@gmail.com

Various monoazo reactive dyes have been synthesized by coupling of diazotized o-anisidine with various 4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amino cyanurated coupling components such as H-acid, Gamma acid, J-acid, S-acid, Koch acid, Bronner acid, Tobias acid, Cleve acid, Peri acid and Laurant acid. They were characterized by nitrogen elemental analysis, IR and ^{1}HNMR spectra. The dyeing performance of all these dyes on wool, silk and cotton has also been assessed.

OP-34 : Acid Functionalized □-Fe_2O_3: An Efficient Protocol towards Multi component Synthesis of 2,4,5-tri substituted imidazole derivatives

Manisha Bora[1,2], Prakash K. Chhattise[1], Pravin Adhav[1], Sunita Salunkhe[3] and Vasant V. Chabukswar[1*]

[1]Department of Chemistry, N. Wadia College , 19, Bund Garden Road, V. K. Joag Path, Pune- 411001 (MS)
[2]Department of Chemistry, BhartiyajainSanghtana's ASC College, Wagholi, Pune
[3]Departmrnt of Chemistry, Savitribai Phule Pune University, Pune
E-mail : vvchabukswar@gmail.com

An efficient, eco-friendly and cost effective protocol for the synthesis of 2,4,5-tri substituted imidazole derivatives was developed using acid functionalized and magnetically separable □-Fe_2O_3nano catalyst. The synthesis of 2,4,5- tri substituted imidazole derivatives involves one pot condensation of benzil, aryl aldehydes and ammonium acetate in ethanol at 60-80^{0}C.The tartaric acid functionalized maghematite (□-Fe_2O_3) nanoparticles were prepared by simple and facile in situ co precipitation method by using Fe^{2+}:Fe^{3+} ions (1:2 molar ratio) and ammonia in aqueous solution of tartaric acid.The magnetic nanoparticles were characterized by FTIR, XRD, and SEM techniques. The synthesized derivatives of imidazole were characterized by FTIR, NMR spectroscopy techniques.

Multi-substituted imidazole derivatives are an important class of pharmaceutically significant compounds.Organic molecules containing imidazole moiety have numerous pharmacological properties and play important roles in biochemical processes.2,4,5

tri aryl 1-H imidazole derivatives have gained remarkable importance because of their wide spread biological activity.

OP-35 : Synergistic Study of Tetra Butyl Ammonium Salts in Polymerization of Vinyl Monomers to Form Polyvinyl Chloride and Polyvinyl Alcohol

P. A. Tomar, S. M. Yadav and A. A. Jahagirdar

Rajarshi Shahu College of Engineering, Tathawade, Pune
E-mail : preetitomar @gmail.com

Chemical engineering involves new technologies employing highly novel materials whose unusual response at the molecular level endows them with unique properties. In recent years, polymer science seizes an attention of scientific community. Polymeric materials like Poly-vinyl chloride (PVC) and Poly-vinyl alcohol (PVA) are widely exploited for wide range of applications in academics as well as in industries due to their structure related properties. Both Poly-vinyl chloride (PVC) and Poly-vinyl alcohol (PVA) are thermally unstable and requires thermal stabilizers during processing. Nowadays, the thermal stabilizers used for the processing of PVC and PVA are based on heavy metals those are toxic in nature and causes adverse effect on environment. In view of this, attempt being made to study thermal degradation of these polymers in presence of tetra-butyl-ammonium salts (Tetra butyl ammonium Chloride TBAC and Tetra butyl ammonium bromide TBAB), which proved to be compatible and environmental beginnen thermal stabilizers.

OP-36 : Microwave Assisted One-Pot Synthesis and Biological Evaluation of Imidazol-Pyrimidin Hybrids as Anticancer Agents

D. Ashok[1*], M. Sarasija[2] and K. Padmavati[1]

[1]Green and Medicinal Chemistry Laboratory, Department of Chemistry
Osmania University, Hyderabad-500007
[2]Department of Chemistry, Satavahana University, Karimnagar
E-mail : ashokdou@gmail.com

Application of multi component reactions (MCRs) to the construction of natural product-based libraries would be most beneficial for the synthesis of new heterocyclic molecules. Such processes in which three or more reactants are combined together in a single reaction flask to produce a product incorporating most of the atoms contained in the starting materials have the advantages of the intrinsic atom economy, simple procedures and equipment, time and energy savings, as well as environmental friendliness.

Despite the extensive use of MCR approaches for the preparation of medicinal libraries, their use in natural product chemistry is rare. The elegant application of the four-component reaction to the one-step synthesis of cytotoxic as pergillamides and their analogues by Domling and co-workers is one of the few examples, and it serves as a good illustration of how streamlined the preparation of natural product-based libraries can be made with the use of MCRs. Heterocyclic molecules are of biological interest due to their potential physical and chemical properties. Nitrogen containing heterocyclic ring such as pyrimidine is a promising structural moiety for drug design. Imidazole scaffolds are a vital class of heterocycles because of their abundance in natural products, and broad use in the field of medicinal chemistry. The traditional anticancer drugs are the basis for the new drug development for cancer in which imidazole is an important moiety. The incorporation of imidazole nucleus, a biologically accepted pharmacophore in medicinal compounds, has made it versatile heterocyclic nucleus possessing wide spectrum of biological activities such as anticancer, anti-Parkinson, anti-inflammatory, anti-convulsant, analgesic, anti-tubercular, and antimicrobial activities.

Motivated by the environmentally benign synthesis and potential bioactivity of imidazole and pyrimidine moieties and also in contribution to our work on green synthesis of biologically important heterocycles herein we wish to report the synthesis of some new imidazole-pyrimidine derivatives under microwave-assisted, one-pot multi component method. All the synthesized compounds were evaluated for their anticancer activity on human cancer cell lines.

OP-37 : Synthesis of Oxepin, Oxocin and Oxonin-Annulated Coumarins by Ring-Closing Metathesis

D. Ashok*, B. Vijaya Lakshmi and M. Sarasija

[1]Green and Medicinal Chemistry laboratory, Department of Chemistry Osmania University, Hyderabad-500 007, Telangana
[2]Department of Chemistry, Sathavahana University, Karimnagar-5050 001, Telangana, E-mail : ashokdou@gmail.com

Coumarins fused with other heterocycles are known to have interesting biological and photodynamic properties which, in turn, have encouraged research with regard to procedures for the preparation of families of these compounds. Thus a number of methodologies have been reported for the synthesis of various 3,4-, 6,7- and 7,8-fused furoand pyranocoumarins. Some members belonging to these two families have shown useful levels of biological activities. On the other hand, very little information is known about medium ring oxacycle fused coumarins which may, in part,

be due to lack of general methods for the synthesis of such ring systems. In recent years, ring-closing metathesis (RCM) has emerged as a valuable tool for the construction of various carbocyclic and heterocyclic ring systems especially for medium to large rings. Olefin metathesis is a unique carbon skeleton redistribution in which unsaturated carbon- carbon bonds are rearranged in the presence of metal carbene complexes. With the advent of efficient catalysts, this reaction has emerged as a powerful tool for the formation of C-C bonds in synthetic organic chemistry. Although alkene metathesis constitutes, for example, the most widely utilized type of metathesis reaction, recent years have witnessed the discovery and development of a number of related processes employing a broader range of substrates. Prominent amongst these are the enyne metathesis, which involves the union of an alkyne with an alkene to form 1,3-diene system. Enyne metatheses are wholly atom economical and therefore, driven by enthalpic rather than entropic factors.

In present work, we have demonstrated that the combined Claisen rearrangement and ring-closing metathesis (RCM) reactions is a viable strategy for the synthesis of some potentially bio-active oxepin, oxocin and oxonin -annulated coumarins and synthesized some new coumarin based macrocyclic compounds using Grubb's-II catalyst.

OP-38 : Confirmation of Gum Polysaccharide from Moringa Oleifera Lam. Plant by Periodate Oxidation Studies

R. B. Singh and Ravi Prakash*

Department of Zoology, School of Life Sciences, Dr. B. R. Ambedkar University, Khandari Campus, Agra-282 002, U.P.
**Department of Chemistry, B.S.A. College, Mathura-281 004, U.P.*
E-mail : rbsinghugc@gmail.com

Moringa Oleifera Lam. plant belongs to family- Moringaceae and called as Sainjna upto 10m in height. Plants are occurs in all over India, Thailand, Pakistan, Sri Lanka, Africa, Nepal, Mexico, Philippines and America. It is used in Ayurvedic and indigenous system of medicine for cardiovascular and gastro-intestinal diseases. Plant gums are used for the treatment of dental infection, astringent and blood pressure. Gum yielded a water soluble polysaccharide as : L-arabinose and D-galactose in 1:4 molar ratio with traces of L-fucose by GLC, Column and Paper chromatographic analysis. Periodate oxidation studies of gum polysaccharide is one of the most important chemical reaction in the structural determination

of gum polysaccharide. Gum polysaccharide was oxidised with sodium metaperiodate by Fluery & Lange's method for more extensive use of periodic acid for oxidation of glycol. It liberated 1.264 moles of formic acid per equivalent of gum polysaccharide with simultaneous consumption of 6.024 moles of periodate ions. Presence of (1→6)-β-type, (1→3)-β-type and (1→5)-α-type linkages are also confirmed by periodate oxidation results. Glycol groups undergoes cyclic ester formation with oxidant and reaction is considered to be dialdehyde type of oxidation. Gum polysaccharide structure of Moringa Oleifera Lam. were obtained from methylation results was confirmed by periodate oxidation studies.

OP-39 : Synthesis, Characterization and Biological Evaluation of Novel 1, 2, 3 Triazole Based Pyrimidine 2-Ones and Pyrimidine 2-Thiones

A. Pavithra, S. Sathiya, B. Divya, A. Keerthika and R. Ravikumar*

Department of Chemistry, Vivekananda College of Arts and Sciences for Women (Autonomous) Tiruchengodu-637205, Tamilnadu
E-mail : drravikumarsastra@gmail.com

Opportunistic fungal and bacterial infections increase rapidly due to resistance acquired by the organisms towards the current antifungal and antibacterial compounds. Obviously there is a need to focus on developing structural variations in the existing compounds or to develop a new class of compounds to overcome the prevailing situation. The 1,2,3- and 1,2,4- triazole based derivatives have received their attention due to wide coverage of biological properties. Huisgen cycloaddition reaction of azide with alkynes is a popular method for the construction for the 1,2,3-triazole with few limitations such as requirement of a electron withdrawing group either on azide or alkynes, high temperature and prolong period of time required for the isolation of 1,4 and 1,5-disubstituted region isomers (Huisgen1967)and influence of electronic effect of the substituent on the phenyl ring. Modification on the hetero cyclic ring through acylation is a tedious one due to chelating properties of nitrogen with metal catalyst used in the Friedal Craft's reaction. Recently a new method has been established (Kamalraj et al.,2008) to synthesis 4-acetyl-5-methyl-1,2,3-triazole from organoazide and acetylacetone pave a way to come out with acylated 1,2,3-triazole. In the present study a series of novel 1,2,3 triazole based Pyrimidine 2-ones and pyrimidine 2-thiones have been synthesized under green aqueous conditions and characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and Mass spectral analysis. All the compounds were evaluated for their in vitro anti bacterial and antifungal activity.

OP-40 : Synthesis of Some Novel Bioactive Pyrazoles, Isoxazoles and their Anti Oxidant and Antibacterial Property

Ramesh M. Chimbalkar

Department of Chemistry, Bhandarkars' Arts and Science College, Kundapura, Udupi District, Karnataka

A series of novel substituted isoxazoles and pyrazoles were prepared from 1,3-disubstituted propenones.Substituted propenones were inturn prepared by the Claisen Schmidt reaction of suitably substituted acetophenone with appropriate aldehyde. These newly synthesized chalcones were made to react with hydroxylamine/ hydrazinehydrateto give substituted isoxazoles or substituted pyrazoles. The newly synthesised compounds were screened for antibacterial and antioxidant activity. Both Pyrazoles and Isoxazoles having methoxy and hydroxy substituents showed excellent antioxidant activity.

OP-41 : Synthesis and Charectorision of 3–Halo Flavone

Ranjeet E. Bhadange[1] and Rajesh P. Ganorkar[2]

[1]Shri Shivaji College of Arts, Commerce & Science, Akola (M.S.)
[2]Mahatma Fule Arts, Commerce and Sitaramji Chaudhari Science Mahavidyalaya,Warud, Dist – Amravati (M.S.)
E-mail : ranjeet.bhadange@gmail.com

Nitro Substituted acetophenone was reacted with Substituted benzoic acid in pyridine medium as a base in presence of phosphoryl chloride ($POCl_3$) for 5 hrs. and the thick mass was decomposed by 1:1 HCl to get Substituted benzoyloxy Nitro acetophenone. This product was further subjected to BVT reaction to get Substituted benzoylmethane further treated with pure Bromine / ICl / SO_2Cl_2 in DMF gives 3- halo Flavone . These synthesised compounds were Screened for their invitro growth of antimicrobial activity against the following organisms E. Coli, S. Aureus and P. Mirabilis,

OP-42 : Graphene and Graphene Oxide : Applications and Future Aspects

Ranjita Das

E-mail : ranjitadasvnit@gmail.com

Graphene is one of the most promising nano-materials because of its unique combination of excellent properties, which opens a way for its exploitation in a wide spectrum of applications in the fields of physics, chemistry, biotechnology, material science as well as medical science. Graphene is the mother element of graphite,

fullerenes and carbon nanotubes. Graphene oxide (GO) is the functionalized form of Graphene with oxygen-containing chemical groups. Graphene and GO exhibits a wide range of unique physico-chemical properties such as good electrical and thermal conductivity, mechanical flexibility, low thermal expansion coefficient and optical transparency. These versatile features have added a revolutionary discovery in the field of both academics and industries. These materials show a wide range of applications in energy production and storage, nanocarrier in drug delivery, wastewater treatment, and adsorptive remediation for emerging pollutants and also used in electronics, sensors and bio devices. This paper reviews the recent advances of Graphene based nano-composites, its synthetic aspects and its applications in the field of environmental science. These materials will be helpful in removing the environmental pollutants which is an emerging key issue in wastewater treatment. This review also analyzes the recent trends in Graphene research and its applications and attempts to identify future directions in which the field is likely to develop.

OP-43 : Micellar Catalysis in Reaction of Cationic Mono-2-Mehoxy Phenyl Phosphoramide with Hydroxide Ions

Ravi Prakash, Seema Kumari* and Neelesh Kumar Pandey

Deptt. of Chemistry, B.S.A. College, Mathura – 281004
**Deptt. of Chemistry, Agra College, Agra - 282002*
E-mail : drravichem@gmail.com

Identification of micellar catalysis in reactions of mono-2-methoxy phenyl phosphoramide (2-MPPA) with hydroxide ions have been carried out at 40±0.5°C in presence or absence of detergent (10^{-2} – 10^{-4} mol dm^{-3}) at pH (8.0 – 10.0) using borate buffers. Effect of cationic cetyltrimethyl ammonium bromide (CTABr) detergent on the rate of hydrolysis of 2-MPPA in presence of hydroxide ions has been measured spectrophotometrically by the rate of appearance of inorganic phosphate. Micellar effect upon reactions of hydroxide ion with chemically similar substrate of different hydrophobicity would occur either largely in aqueous pseudophase or with a more hydrophobic substrate large in aqueous pseudophases. If the pseudophase ion exchange model the ratio of the counter ions to the ionic head groups in the micelle and K^{OH}_{Br} the ion exchange constant should be applicable to the reactions of structurally similar substrate occurring in either micellar or aqueous pseudophases kinetic study of micellar catalysis of the reactions of mono-2-methoxy phenyl phosphoramide with (OH^-).

OP-44 : Seeking Towards Novel Method for the Synthesis of Heterocycles using Easy Available Nitro-Compounds

Richa Gupta, Nagaraju Vodnala, Dhananjaya Kaldhi, R. K. Linthoinganbi, S. C. Pinky Promily and Chandi C. Malakar*

Department of Chemistry, National Institute of Technology Manipur, Imphal - 795004, Manipur
E-mail : chdeepm@gmail.com

Owing to their enormous medicinal profiles, the synthesis of novel heterocyclic scaffolds is one of the frontier areas of research. It is envisaged that nitro compounds are the potential precursor and offers new vistas for construction of variety of biologically active heterocyclic architectures. In this context, novel methodology has been developed for the synthesis of N-heterocyclic compounds via exploration of reductive cyclization of nitro aromatics. The present protocol offers several advantages like operational simplicity, high atom economy, appreciable structural diversity and easy purification procedure.

OP-45 : Synthesis of Quinolines from Drug Amines by using Inorganic Composites of Transition Metals as a Catalyst

S. A. Dhanmane, S. S. Pawar, B. T. Hake, S. M. Vhankate and V. B. Tadke*

Department of Chemistry, Fergusson College, Pune
E-mail : sushorganic@gmail.com, vijaytadke@gmail.com

Quinolines from drug amines and ethyl acetoacetate were synthesized using various inorganic transition metal composites as a catalyst. The yield of the quinolines obtained using this novel protocol are significantly higher than those utilizing the conventional method.

OP-46 : Synthesis and Characterisation of Glycosyl Bis-Thiocarbamides

Samidha S. Kadu

P. G. Department of Chemistry, Shri.Shivaji College, Akola (MS)
E-mail : samidhakadu@gmail.com

The chemistry of thiourea and their derivatives of saccharides are extensively elaborated and documented for their biological properties. Literature survey reveals that urea and thiourea derivatives showed a broad spectrum of biological activities. In view of the advantage conferred by glycosylthiourea, it was interesting to carry out synthesis of various per-O-acetyl and per-

O-benzoyl glycosylthiocarbamides by the interaction of per-O-acetyl and per-O-benzoyl glycosylisothiocyanate witho-phenylenediamine in 2:1 ratio. The identities of these newly synthesized compounds were established on the basis of usual chemical transformations, IR, ^{1}H NMR, and Mass Spectral studies. All the synthesized compounds have been evaluated for their antibacterial and antifungal activity against different bacteria and fungi by agar diffusion method.

OP-47 : Preparation, Characterization and Therapeutic Study of Some Novel Schiff-Base Derived from Pyrimidine

S. P. Vyas

Organic Chemistry Research Lab., Chemistry Division
The H.N.S.B. Ltd. Science College, Himatnagar -383 001, Gujarat
E-mail : vyas_sandip2005@yahoo.co.in

In this present study, 6-chloro 2,4-diamino pyrimidine condensed with various aromatic aldehyde. Final moieties have been characterized by conventional and instrument methods. Their structures were determined by FT-IR, ^{1}H NMR and Mass Spectra and important therapeutic properties were studied.

OP-48 : Novel Synthesis of Pyrimidin-2-yl-Cyanamide and Their Derivatives by Nucleophilic Substitution

Santosh G. Badne* and Gajanan W. Belsare

P. G.Department of Chemistry, Shri Shivaji College of Arts, Commerce and Science, Akola (MS)
E-mail : santoshbadne@gmail.com

Recently some fused heterocyclic compound containing nitrogen atom show wide range of pharmacological. Fused pyrimidines continue to attract considerable attention because of their great practical usefulness, primarily due to very wide spectrum of biological activities. This is evident in particular from publications of regular reviews on the chemistry of systems where the pyrimidine ring is fused to various heterocycles such as purines, quinazolines, pyridopyrimidines, triazolopyrimidines, pyrazolopyrimidines, pyrimidoazepines, furopyrimidines and pyralopyrimidines. A large number of pyrimidine derivatives are reported to exhibit antimycobacterial, antitumor, antiviral, anticancer, antiinflammatory and antimicrobial activities. In addition pyrimidine also posses antibacterial, antifungal, antileishnent, anti-inflammatory, analgesic, antihypersensitive, antiviral, antidiabetic, antiallergic, antioxidant. In the same pyrimido also have good biological important it also act a good pharmacophore.

The parent compound which will show the substitution reaction at 4-position consist of replicable Methylthio group at 4-position, the derivative was prepared from 5-Cyano-6-imino-4-methylsulfanyl-1, 6-dihydro-pyrimidin-2-yl-cyanamide and p- substitutedAnilines / p-substitutedPhenol in presence of solvent DMF and catalyst anhydrous K_2CO_3 reflux for 4hrs cool at room temperature and pour it in ice cold water solid separates out filter and dry it.

OP-49 : Synthesis, Characterization and Dyeing Performance of Novel Azo Disperse Dyes Derived from Substituted Phenyl Thiazole Derivatives

Patel Sejal S. and Malik G. M.*

Department of Chemistry, Navyug Science College, Surat
E-mail : sejalpatel444@yahoo.com

A new series of azo disperse dyes (D_1-D_{10}) were synthesized by diazotization of different substituted primary amines and coupled with N-(4-(4-chlorophenyl)-thiazol-2-yl)-2-((4-nitrophenyl)-amino)-acetamide in acidic media. Coupling component was derived from 2-amino 4-(4'-chlorophenyl) 1, 3-thiazole reacted with chloro acetyl chloride gave acetamide derivative having free –Cl group; which on further reaction with p-nitro aniline in suitable solvent; yielded component used as coupler for utilizing a new series of dyes. These synthesized dyes (D_1-D_{10}) were characterized by elemental analysis, UV, IR, ^{1}H NMR spectra. These dyes (D_1-D_{10}) were applied on polyester fabric and their dyeing performance as well as fastness properties were evaluated.

OP-50 : Synthetic Studies on 1,2,4-Triazoles Derivatives and Biological Evaluation as Antifungal and Antibacterial Agents

Sujatha K.[2], A. M. A. Khader[1] and Balakrishna Kalluraya[1]

[1]Department of studies in Chemistry, Mangalore University, Mangalagangotri-574199, Karnataka
[2]Department of Studies in Chemistry, Karnatak University, Dharwad-580003 Karnataka

Several five membered ring systems, e.g., triazole, oxadiazole dithiazole and thiadiazole with three heteroatoms at symmetrical or asymmetrical positions have been studied because of their interesting pharmacological properties. In this article our emphasis is on synthetic development and pharmacological activity of the triazole moiety which exhibit a broad spectrum of pharmacological actiivty

A series of 4H-1,2,4-triazoles was synthesized by using phenol precursors via conversion to corresponding hydrazides, then thiosemicarbazides and finally to 1,2, 4-triazole derivatives. The synthesized compounds were characterized through various instrumental techniques viz., FTIR, FT-NMR, and MS. All the compounds were tested against different strains of bacteria and two different strains of fungi. Few Compounds showed remarkable activities against the test microorganisms. The MICs of the compounds were also determined and reported.

OP-51 : Sm_2O_3/Fluoroapatite as a Reusable Catalyst for the Facile, Green, One-pot Synthesis of Triazolidine-3-thione Derivatives Under Aqueous Conditions

Surya Narayana Maddila*, Suresh Maddila, Kranthi Kumar Gangu, Werner E. van Zyl and Sreekantha B Jonnalagadda

**School of Chemistry & Physics, University of KwaZulu-Natal, Westville Campus, Chiltern Hills, Durban-4000, South Africa.*
**E-mail: suryamaddila@gmail.com*

A new series of fourteen triazolidine-3-thione derivatives (11 compounds) were synthesized via the reaction of aromatic aldehydes with thiosemicarbazide with samaria loaded fluorapatite, (Sm_2O_3/ FAp) as catalyst in aqueous media. Fluoroapatite proved superior as support relative to hydroxyapatite in terms of improved yield and reduced reaction time. The new catalyst, Sm/FAp was characterized by various instrumental techniques including XRD, SEM, TEM and BET. Catalyst was easily separable and reusable for seven runs without any apparent loss of activity. The reported strategy has many benefits such as ease of preparation, green solvent, reduced reaction times, excellent product yields (92-97%) and operational simplicity.

OP-52 : Synthesis of Quinolines from Drug Amines by using Inorganic Composites of Transition Metals as a Catalyst

S. A. Dhanmane, S. S. Pawar, B. T. Hake, S. M. Vhankate and V. B. Tadke*

Department of Chemistry, Fergusson College, Pune
E-mail : sushorganic@gmail.com, vijaytadke@gmail.com

Quinolines from drug amines and ethyl acetoacetate were synthesized using various inorganic transition metal composites as a catalyst. The yield of the quinolines obtained using this novel protocol are significantly higher than those utilizing the conventional method.

OP-53 : Layered Double Hydroxide Immobilised Substituted Cu(II) Schiff Base Complexes : Synthesis, Characterization and Catalytic Activity

Savita Khare[1], Swati Parashar[*], Jagat Singh Kirar and Priti Shrivastava

School of Chemical Sciences, Devi Ahilya University,
Takshashila Campus, Khandwa Road, Indore (M. P.) - 452001
E-mail: kharesavita@rediffmail.com[1], swatiparashar1990@gmail.com[*]

Heterogeneous catalyst, copper schiff base complex intercalated in layered double hydroxide, abbreviated as LDH-SALABA-Cu(II) was synthesized using salicylaldehyde and 4-amino benzoic acid. Then to examine the effect of substitution on styrene oxidation, various forms of salicylaldehyde like 5-chloro-salicylaldehyde, 5-bromo-salicylaldehyde, 4-hydroxy-salicylaldehyde and 3, 5-di-tert-butyl salicylaldehyde were used to synthesize four different schiff base complexes named as LDH-{Cl-SALABA-Cu(II)}, LDH-{Br-SALABA-Cu(II)}, LDH-{OH-SALABA-Cu(II)}, LDH-{DTB-SALABA-Cu(II)} respectively. These catalysts were characterized by XRD, FT-IR, SEM, EDAX, ICP-AES, TGA and BET surface area analysis. All the catalysts exhibit wonderful activity in oxidation of styrene with tert-butyl-hydroperoxide. The catalytic efficacy towards olefin oxidation has been widely studied by varying solvent, oxidants, substrate to oxidant molar ratio, catalyst concentration, temperature etc and the obtained results beautifully support the statement that free radical reactions can be enhanced by both electron releasing as well as electron withdrawing substituents.

OP-54 : Isolation of Anew Flavanone from Tephrosia Spinosa

Namratha Vaddhiraju*

Department of Chemistry, Satavahana University, Karimnagar-505001, Telangana

The genus Teproshia belongs to the family fabaceae, consisting of 300 species. A large number of flavonoids including chalcone, flavones and flavonones with unusual structures has been identified in tephrosia species. Flavonoids are known to possess wide range of pharmacological activities such as Cardiotonic avtivity, antioxidant activity, hepatoprotective activity and anti microbioal activity.The immense range of structures is due to variation in the position of hydroxyl substituents or isoprenyl substituents. Earlier phytochemical investigation on tephrosia spinosa resulted in the isolation of new flavonones and chalcone derivatives. A new di isopropenylated chalcone was also isolated from the roots of tephrosia spinosa.

OP-55 : Kinetic and Thermodynamic Studies of the Oxidation of Aromatic Primary Alcohols using Polymer Supported Oxidizing Agent

Vilas Y. Sonawane

Department of Chemistry, B.Raghunath Arts, Commerce and Science College, Parbhani, 431401, Maharshtra
E-mail : sonawane_vy@rediffmail.com

Oxidation is one of the most important industrial reactions as it yields useful products. Literature survey indicates the use of a variety of organic oxidants for the oxidation of alcohols to the corresponding carbonyl compounds but inorganic oxidants have rarely been used. The quantitative conversions of alcohols to aldehydes / ketones have been reported by several workers but there are relatively few reports about the kinetic and thermodynamic investigators of the oxidation of alcohols. I report herein the kinetics of controlled oxidation of aromatic primary alcohols like Benzyl alcohol and its P-substituted derivatives using potassium permanganate (KIO4) in 1:4 dioxane. The oxidation was carried out under Zero order kinetic conditions with respective to the inorganic oxidant. The progress of the reaction was monitored by spectrophotometrically of the oxidant at regular time intervals during the course of the reaction. For all the aromatic primary alcohols studied, it was found that, the oxidation rate increased with increase in alcohol concentration, solvent, oxidizing agent and temperatures.

OP-56 : Comparitive Study and Amp; Antimicrobial Activity of Hepta-o-Benzoyl-β-d- Lactosyl Isothio-cyanate and Their Nanoparticals

Poonam T. Agrawal

P.G. Department of Chemistry, Shri R.L.T. College of Science, Akola-444001 (M.S.)
E-mail : poonamagrawal2575@rediffmail.com

Nanoparticles exhibit new physical-chemical properties which are not observed either in individual molecules or in bulk In recent years nanoparticles have been the subject of focused researchers due to their unique properties that are significantly different from their bulk materials. Chemistry of lactosyl isothiocyanate with special reference to their utility as starting material in the synthesis of nitrogen and sulphure containing open chain and cyclic compound has been investigated by earlier workers. It appeared quite interesting to prepared Nanoparticals of the lactosyl isothiocyaate to investigate the chemistry of these new compound with reference to their synthetic application.

OP-57 : Synthesis and Dyeing Performance of Some New Disperse Dyes Based on Coumarin Moiety

D. M. Vashi[*1], Anant Desai[2], Sonam Singh[1], Krushna Kurmi[1]

[1]Department of Chemistry, Narmada College of Science and Commerce, Zadeshwar Affiliated to Veer Narmad South Gujarat University, Surat
[2]Department of Dyes & Pigments, Shroff S.R. Rotary Institute of Chemical Technology Valia Road, Ankleshwar
E-mail : singhsonam884@gmail.com

Synthesis of disperse dyes derived from diazotization of 3-(2-amino-thiazol-4-yl) coumarin and coupled with various tertiary aromatic amines as coupling components. Their dyeing performance as disperse dyes has been assessed on polyester fabric. These dyes were characterized by IR spectra, ^{1}H-NMR spectra and elemental analysis. The dyed fibre showed good to excellent washing and perspiration fastness. The dye bath exhaustion and fixation on different fibres were found to be very good.

PHARMACEUTICAL CHEMISTRY SECTION

Sectional President's Address

Synthesis and Antiplasmodial Studies of Adamantane-Based Aminophenols

Kulathu Iyer Sathiyanarayanan

Chemistry Division, School of Advanced Sciences, VIT University, Vellore 632014,

Adamantane based aminophenol derivatives were synthesized and tested for their antiplasmodial activity in vitro against Plasmodium falciparum (Pf_NF54) and resistant strain (Pf_K1).The compounds are exhibiting excellent activity against these two strains. In addition to this activity they also showed excellent selectivity index against THP1cell line. This work demonstrates that we have developed a low molecular weight lead series that shows druggability potential as a novel antiplasmodial agents. Representative compounds were profiled for various in vitro DMPK properties and selectivity against the hERG channel. The compounds from this series showed desirable physiochemical properties, moderate to excellent solubilities, moderate human plasma protein binding (PPB), moderate to high clearance in rat hepatocytes, low to moderate clearance in human microsomes and low hERG inhibition.

PCIL-01 : Synthesis And Biological Evaluation of Diverse Heterocyclic Library Consisting of Macrocycles and Bis-Heterocycles

D. Ashok

Green and Medicinal Chemistry Laboratory, Department of Chemistry
Osmania University, Hyderabad-500 007, Telangana State
E-mail : ashokdou@gmail.com

Heterocycles are among the most frequently encountered scaffolds in pharmaceutically relevant substances and are essential for the human well being. The remarkable ability of heterocyclic nuclei to serve both as biomimetics and reactive pharmacophores has largely contributed to their unique value as traditional key elements of numerous drugs. Certain possible modifications on the heterocyclic ring may lead to new products with better biological profiles. Macrocyclic rings are commonly found structural units within the frame work of a variety of natural products, which is the main reason for the growing importance of such class of compounds. Moreover for an equal number of atoms, cyclic analogues inherently possess a lower number of rotatable bonds than their acyclic analogues. As a result cyclic counterparts are more conformationally restricted than their acyclic analogues, which potentially can impart higher target binding, selectivity and improved oral bioavailability. The relevance of compounds composed from two or more heterocyclic rings for drug discovery, irrespective of the target, bis-heterocyclic compounds are identified as the most potent ones. Among the top 50 prescription drugs there are twelve bis-heterocycles. As a part of our research program towards the green synthesis of bioactive molecules and above observations prompted us to take up the synthesis and biological evaluation of diverse heterocyclic library consisting of macrocycles and bis-heterocycles.

PCIL-02 : *In Vitro* and *In Vivo* Assessment of 1,3,4-Oxadiazole Bearing Biologically Active Scaffolds

N. B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007, Gujarat
E-mail : drnavinbpatel@gmail.com

In the present scenario of the Medicinal chemistry, there is a real need to discover new drug entities with high efficiency towards pathogens and less toxicity, which may be different from available resistant drugs. This provides a great opportunity to synthetic chemists for the synthesis of such new compounds having lower

cytotoxicity and better antimicrobial properties. Among heterocyclic compounds, 1,3,4-oxadiazole has become an important building block for the development of new drugs and more widely studied by researchers because of their many important chemical and biological properties. Compounds containing 1,3,4-oxadiazole cores have a broad spectrum of different biological activities. The ability of 1,3,4-oxadiazole heterocyclic compounds to undergo various chemical reactions has made them important for making building block and for molecule planning, such as, conversion into 1,2,4-triazole, one more important pharmacophore, using various amino benzimidazoles & benzothiazoles with enormous biological potential. On the basis of recent progress in understanding the pharmacological effects of 1,3,4-oxadiazole, new strategies are in development to better exploit the pharmacological potential of 1,3,4-oxadiazole & 1,2,4-triazole based newer biologically active candidates. With this concern we have developed 1,3,4-oxadiazole based analogues coupled with various heterocycles viz, benzothaiazole, 1,2,4-triazole, pyrimidines, etc. All the synthesized compounds were screened for their different biological potential such as antibacterial, antifungal, antiprotozoal, antitubercular, anti HIV-1, anti tumor, cytotoxicity etc. Moreover, short-term *in vivo* model on *Trypanosoma cruzi* has also been studied with one of the derivative containing 1,3,4-oxadiazole.

PCIL-03 : Myeloperoxidase Inhibitor : Cardiovascular Disease Perspective (*)

D. Rajagopal

Department of Chemistry, School of Advanced Sciences, VIT University, Vellore, 632014
E-mail : rajagopal.desikan@vit.ac.in

Myeloperoxidase (MPO), an enzyme is released during degranulation of neutrophils and monocytes, has been strongly linked to the pathogenesis of atherosclerosis and related risk factors. In view of this, the pathophysiologic role of MPO in cardiovascular disease has attracted considerable interest for development of MPO inhibitors. MPO is responsible for oxidation of several biomolecules, High Density Lipoprotein, Low Density Lipoprotein and DNA leading to impaired biological function. Many phenolic structures, particularly ferulic acid and its derivative structures are widely present in many biological sources. Recently we have developed MPO inhibitors based on ferulic acid moieties which may exert beneficial effects against biological oxidants and possesses anti-oxidant effects. With the application of docking module, potent FrA derivatives were synthesized as inhibitor of MPO and validated using several biochemical assays. We suggest

that identified lead FrA derivatives are potent MPO inhibitors which may exert specific effects on MPO mediated processes in the cardiovascular system. We believe that our work is of significant importance as it demonstrates comprehensive approach to design and validation of novel myeloperoxidase (MPO) inhibitors. We also believe these findings will be of great interest to broad audience generally, and particularly to researchers working on MPO.

PCIL-04 : Validated TLC Densitometric Method for Stress Degradation and Accelerated Stability Study of Asiaticoside from *Centella Asiatica*

Patel Samir G.

Pharmaceutical Chemistry and Analysis Department,
Ramanbhai Patel College of Pharmacy, Charotar University of Science and Technology, Changa, Anand-388 421, Gujarat
E-mail : samirpatel.ph@charusat.ac.in

Stress degradation and accelerated stabilty studies were carried out on Asiaticoside (triterpenoid component extracted form *Centellaasiatica*) following the conditions prescribed in the parent drug stability testing guideline (Q_1AR_2) issued by International Conference on Harmonization(ICH). The present study describes degradation of Asiaticoside under different ICH prescribed stress conditions (acid and base hydrolysis, oxidation, and photodegradation) as well accelerated stability study and establishment of a stability indicating HPTLC assay. The method employed TLC aluminium plates precoated with silica gel $60F_{254}$ as the stationary phase. The optimized solvent system consisted of toluene:ethylacetate:methanol:glacial acetic acid 2:7:3:1 (*v*/v/v/*v*). The derivatization was carried out with 10% methanolic sulphuric acid reagent. This system was found to give compact spots for asiaticoside (R_f value of 0.43). Densitometric analysis of Asiaticoside was carried out in the absorbance mode at 595 nm. The linear regression analysis data for the calibration plots showed good linear relationship with r^2 = 0.982 and in the concentration range 200–1800 ng/ spot. The method was validated for precision, recovery and robustness. The accuracy for the *centella asiatica* plant powder and it's formulation was found to be 97.72 – 104.54 % and 100.33 – 102.67 % respectively. The limits of detection and quantitation were 51.127 and 154.93 ng/spot, respectively. All the peaks of degraded products were resolved from the standard Asiaticoside with significantly different Rf values. As the method could effectively separate the drug from its degradation products, it can be employed as a stability indicating one.

PCIL-05 : Stability Indicating HPLC Methods for the Assay of Drug in Bulk and Drug Formulations

Hemant Kumar Jain

Sinhgad College of Pharmacy, Pune-411 041 (MS)
E-mail : hemantkjain2001@yahoo.co.in

A Stability Indicating Method (SIM) is defined as a validated analytical procedure that accurately and precisely measure active ingredients free from process impurities, excipients and degradation products. Following important steps are necessary for developing a SIM. Critical study of the drug structure provides information to assess the likely decomposition route(s). Similarly physicochemical properties i.e. pKa & Solubility data are also useful for pH selection of mobile phase & solvent selection, respectively. The wavelength maxima and extinction of the drug and known degradation products are required for UV detection. But when degradation pattern has not yet been established, photodiode array (PDA) detector should be used. Forced decomposition studies employ change in temperatures, humidity, hydrolysis, oxidation and photolysis. Preliminary separation studies on stressed samples can be start with a C_{18} column with water-methanol or water-acetonitrile as the mobile phase. Retention time (RT) and relative retention times (RRT) of all products can be considered in final method development. Method optimization involves selection of HPLC column, column temperature, mobile-phase, flow-rate, elution mode, detection, etc. Obtained PDA spectra are critically evaluated to ascertain whether the products are same or different. Identification and characterization of degradation products are required to establish specificity/selectivity of the method. Finally, method validation is performed as per ICH guidelines.

PCO-CYSA-01 : Binding Studies Of Hydroxamic Acid-Vanadium(V) Complexes with Ct-DNA

Mamta Tripathi and Rama Pande

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur-492010, Chhattisgarh
E-mail : mamtat320@gmail.com

A high-throughput screening is necessary to identify the lead compounds that bind to the target with high affinity, for developing new drugs that target the DNA. Metal complex that bind to DNA have been an active area of research since the discovery of cisplatin and the other platinum based anti-cancer drugs. Hydroxamic acids (HA) represent an important family of organic bio-ligands. These are drug like molecules, show both Hydrogen Bond Donor and

Hydrogen Bond Acceptor capability. These compounds exhibit prominent activities due to their chelating properties with metal ions, hence constituting a very important class of chelating agents. To this end, herein present an assay to elucidate the specificity of DNA binding efficacy with p-TBHA-V(V) and PBHA-V(V) complexes. Biophysical techniques such as absorption spectroscopy, fluorescence spectroscopy viscosity measurements and molecular docking were applied to study the interaction between ct-DNA and ligand. UV-Visible absorption and Fluorescence quenching spectra revealed strong binding of both the Vanadium (V) complexes to ct-DNA. EtBr displacement shows the decrease in emission intensity for both hydroxamic acid metal complexes. The relative viscosities of hydroxamic acid-ct-DNA complexes have increased value as compared to DNA alone. The smaller value of binding energy obtained in docked structure confirms strong binding interactions. All the experimental evidences indicate that p-TBHA-V(V) and PBHA-V(V) complexes are strongly bonded to DNA. The results further level up our study to design DNA binding metal anti-cancer agents.

PCO-CYSA-02 : Synthesis of Gibberellic Acid by *Stenotrophomonas Maltophilia* Isolated from *Musa Balbisiana* (Banana)

M. S. Ambawade[1*] and G.R. Pathade[2]

[1]Microbiology Department, Haribhai V. Desai College, Pune (MH)*
[2]The Principal, Haribhai V. Desai, College, Pune (MH)
E-mail : ambawade2014@gmail.com

Totally twenty two isolates were screened out for their Gibberellic acid (GA) synthesizing capacity on spectrophotometer which are isolated from the roots of *Musa balbisiana*(Banana). Out of these isolates BE-25 isolate showed high amount of Gibberellic acid (GA) synthesizing efficiencywith and without L-tryptophan in medium. Gibberellic acid (GA)synthesized by BE-25 was further estimatedon High-Performance Liquid Chromatography (200.15, 282.92ppm at 254 nm) with and without L-tryptophan in medium for more accuracy. Based on morphological, cultural, biochemical and 16s rRNA gene sequencing a newly isolated endophytic bacterium (BE 25) from the roots of *Musa balbisiana*(Banana) was identified as *Stenotrophomonas maltophilia*. This bacterium will further be useful for preparation of liquid bioinoculant to improve the banana production as well as for ecofriendly and sustainable agriculture.

PCO-01 : Anti-Inflammatory and Analgesic Activities of Benzofuropyridine Derivatives

Channamma. M,[1] Raga Basawaraj[2] and S. Appala Raju[3]

[1,3]Mathoshree Taradevi Rampure Institute of Pharmaceutical Sciences, Kalburagi-585105
[2]Karnataka College of Pharmacy, Manahalli Road, Bidar-585403
E-mail : c.majage@yahoo.in

The bio-significance of pyridine nucleus has led to the exploration of several polycyclic heterocycles such as benzofuropyridines. While the benzofuro[2,3-b]pyridine, benzofuro[2,3-c]pyridine and benzofuro[3,2-c]pyridine, have received considerable attention and are reported to possess high analgesic, analeptic, anti-inflammatory, antiviral, anti-bacterial and anti-fungal activities, the isomeric benzofuro[3,2-d]pyridine has been little investigated biologically. We are reporting now different synthetic routes for this heterocycles. A convenient route developed for the synthesis of benzofuro[3,2-d]pyridines. The intermediate compound 5-bromo-3-amino-2-acetyl benzofuran was obtained easily by reacting 5-bromosalicylonitrile with chloroacetone in the presence of anhydrous potassium carbonate in dry acetone. The compound 5-bromosalicylonitrile was obtained from 5-bromo salicylaldehyde, which was from salicylaldihyde. The targeted molecules 8-bromo-2-phenylbenzofuran [3,2-b]pyridine-4-one**.(4a-f)** were achieved by cyclizing the chalcones**(3a-f)** in the presence of orthophosphoric acid in acetic acid. Chalcones were prepared by reacting various aromatic aldehydes with 5-bromo-3-amino-2-acetyl benzofuran in presence of sodium hydroxide solution in ethanol.

The molecules were subjected to anti-inflammatory and analgesic activities. The activities of these compounds were compared with the standard drugs. All synthesized compounds **(3a-f)** and (**4a-f**) were checked for purity by using TLC with appropriate solvent system. The structure of all synthesized compounds were established on the basis of analytical and spectral studies such as IR, ^{1}HNMR and Mass Spectrum.

PCO-02 : Pharmacological Approach Leading to the Isolation of Active Constituents from Medicinal Plants

D. N. Singh* and N. Verma

Department of Chemistry, K.S. Saket PG College, Dr. RML Avadh University, Faizabad- 224001
E-mail : dnsinghsaket@yahoo.com

Plants have been recognized for many years as a source of new

therapeutic agents and of structural diversity. 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, drugs currently in the clinical use are not effective against drug resistant parasitic strain. Thus development of drug resistant parasitic strain has emerged as major challenge to the scientist to search new effective therapeutic agents for treatment of patient suffering from drug resistant parasites. Keeping in view importance of new therapeutic agents in parasitic area, recently, by pharmacological approach we have isolated novel antigiardial and antimicotic agents of great therapeutic values from terrestrial medicinal plants. The details isolation procedure, structural elucidation and pharmacological activity of the isolated active constituents will be discussed during presentation.

PCO-03 : Use of Indian Herbal Formulations for Antimicrobial and Plasmid Curing Ability Against Multidrug Resistant Pathogens Causing Infections in the Female Genital and Urinary Tract

Rajashree B. Patwardhan*

**Haribhai V. Desai college of Arts, Commerce and Science, Department of Microbiology 596, Budhwar Peth, Pune 411002, Maharashtra*
E-mail : dr.rbpatwardhan@gmail.com

Infections in the women genital and urinary tract are caused by bacteria like *E. coli, Proteus, Klebsiella, N. gonorrhoeae, C. trachomatis, Trichomonas vaginalis, Mycoplasma, Enterococci, Group B Streptococci, Pseudomonas, S. aureus,* etc. Due to the use of heavy load of antibiotics in hospitals for treating genital and urinary tract infections, the community has contributed to selection pressures that have encouraged emergence of antibiotic resistant bacterial strains. To fight against the spread of pathogenic multidrug resistant bacteria, novel plasmid eliminating and antimicrobial agents of plant origin can be used which may eliminate antibiotic resistance and are more effective and not toxic. In the present investigation, we have isolated and identified the multidrug resistant bacterial pathogens causing genital and UTIs. Indian herbal pharmaceutical formulations used in ayurvedic medical practice like *Trunapanchamula* (*Saccharum spontaneum, Saccharum officinarum, Eragrostis cinosuroides* and *Oryza sativa* have been tested for their antimicrobial and plasmid curing ability against the multidrug resistant pathogens. They were found to be very effective in elimination of plasmids and their

antimicrobial properties. Hence, these root extracts could be therapeutically significant if provided in combination with antibiotic treatment. The findings and outcomes of this research would be useful from point of view of women's health.

PCO-04 : Microwave Irradiated Synthesis, Molecular Docking Studies and Anti-Mycobacterial Evaluation of *N*-((2-(Pyridin-4-Yl)-1*h*-Benzo[*D*]Imidazol-1-Yl)Methyl)-Substituted-Aminopyridine

Vatsal M. Patel and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : drnavinbpatel@gmail.com, patelvatsal1904@gmail.com

The recent increase in cases of tuberculosis, there is a progressive increase in multidrug resistant (MDR) tuberculosis. Therefore, the increasing clinical importance of drug-resistant mycobacterial pathogens has lent additional urgency to microbiological research and new anti-mycobacterial compound development. For this purpose, newer Mannich base namely viz., *N* ((2-(Pyridin-4-yl)-1*H*-benzo[*d*]imidazol-1-yl)methyl)-substituted-aminopyridine acquired from 2-(pyridin-4-yl)-1*H*-benzo[*d*]imidazole and amino pyridines by microwave irradiation as well as conventional pattern. Microwave induced synthesis offers considerable saving in energy with better yield and simplicity in procedure that compare to conventional approach. All the newly synthesized compounds were characterized by spectral (IR, ^{1}H NMR, ^{13}C NMR & Mass) study. and were evaluated for antimicrobial activity against certain bacterial and fungal strain. Some of them are significantly active and the others exhibited moderately active compared to standard drugs. Computational studies were undertaken to test the inhibitory effect of the synthesized molecule on protein kinase from *M. tuberculosis*. The docking results of newer Manich base were explained on the basis of minimum binding energy and were screened for *in vitro* anti tubercular activity against *M. Tuberculosis H37Rv* employing MABA method. Four of them were found to be an active.

PCO-05 : Precision Enhancement in Kinetic Parameter Measurements

Smt. Pawar S.P.[1], Adhyapak M.S.[1], Lingampalle D.L.[1] and Ubale S.B.[2]

[1]Department of Chemistry, Vivekanand College, Aurangabad.
[2]Department of Chemistry, Deogiri College, Aurangabad.
E-mail : adhyapak@vivekanandcollege.edu.in

Kinetic study has been gaining importance due to its applicability

in getting higher efficiency in many commercial processes and in controlling of biochemical transformations, as far as medical point of view is considered. Accuracy in the measurement kinetic parameters of chemical processes is most important aspect for getting precise data; which depends upon many internal and external factors. This paper describes how precision in the kinetic parameter measurements can be enhanced by controlling thermal parameters, time of reactants contact, time of initiation, dilution, agitation, etc. For above study, kinetic parameters of reaction between 2-chloro-3-formylquinoline and ceric ammonium nitrate were determined by measuring UV-VIS absorbance of the product 2-chloroquinoline-3-carboxylic acid. This exercise would help in getting better precision level in desired chemical processes.

PCO-06 : Molecular Docking of Hydroxamic Acids with DNA

Rama Pande

UGC-BSR Fellow, School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh
E-mail : rama.pande@gmail.com

Prediction of the structure and binding free energy of a ligand-receptor complex from Structure of free ligand and receptor only is known as molecular docking. It is the computational simulation of a candidate ligand binding to a receptor. Receptor is the large sized receiving molecule, generally protein/DNA. Ligand is the synthesized molecule binding to the receptor due to structural complementarily. The 3D structure of a potential ligand superimposed on the receptor target site to predict the structure of the Inter-molecular complex, thus formed. The regions of the receptors involved in the complexation are known as binding sites. Binding may occur in various possible conformations known as binding modes. It also predicts the strength of binding and binding affinity between ligand and receptor using scoring functions.

N-Arylhydroxamic acids showed Anti-Tumor/Anti-Cancer activity as reported from this laboratory. The tumor/cancer cells were damaged due to interaction of these molecules with DNA. To know the mechanism of these interactions, the docking studies were performed using Argus Lab and Hex software. The results show, groove /intercalating mode of binding depending upon the structure of hydroxamic acid derivative.

PCO-07 : Docking Studies, Synthesis, and Antimicrobial Evolution of Some Novel Quinoline Derivatives

Gopi R. and Senthil. S.*

Department of Chemistry, Government Arts College, Salem -636007, Tamilnadu
E-mail : mrgopiranganathan@gmail.com; shendils@gmail.com

A series of 1,2,3-triazole appended quinoline derivatives were synthesized through pfitzinger reaction. All the synthesized compounds have been characterized by the usual spectral techniques.All the compounds subjected to in vitro studies such as antimicrobial activity against three gram positive and three gram negative bacteria and four fungi strains and in silico studies were performed against topoisomerase II DNA gyrase enzymes. All the compound shows moderate to good biological activity and good binding interaction against receptor.

PCO-08 : Microwave Assisted Synthesis, Characterization and Applications of 1,3,4 Thiadiazole Derivative of Guar

Sangeeta Loonker and Akanksha Maheshwari*

Department of Chemistry, Jai Narain Vyas University, Jodhpur 342005, Rajasthan
E-mail : sangeetag@hotmail.com, maheshwari.akanksha90@gmail.com

Guar is a biodegradable polysaccharide. It is derivatized with 2-mercapto-5-(4-aryl amino)-1,3,4 thiadiazole using microwave assisted synthesis. Microwave assisted synthesis is a methodology of green chemistry, that focus on less use of harsh chemicals, reduction of other wastes and shortening of reaction time. The novel derivative prepared is then characterised using H^1 NMR, FT-IR, DART-Mass analysis and nitrogen estimation using Khjeldahl method. Antibacterial and antifungal activities were studied on different strains using well diffusion method. Antioxidant activity of the novel derivative is studied by H_2O_2 scavenging assay.

PCO-09 : *In-vitro* Anticancer Activity of Pd(II) and Ni(II) Chiral Schiff Base Ligand Complexes

Baliram Y. Waghamare, Dnyaneshwar D. Kumbhar, Ayesha Khan and Satish K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
E-mail : skpar@chem.unipune.ac.in

Optically pure α-amino acids viz. D - phenyl glycine, L - phenyl glycine, D - phenyl alanine and L – valine are effectively reduced to α-amino alcohols by using $NaBH_4/I_2$ in dry THF and condensed

with various aromatic aldehydes to obtain bidentate and tridentate mixed donor (O and N) chiral Schiff base ligands (CSBLs). All the CSBLs synthesized are well characterized before coordinating with metal ions. These CSBLs are coordinated with divalent nickel and palladium metal ions to get chiral transition metal complexes. These chiral complexes are screened for their *in vitro* anticancer activity with human breast cancer cells (MCF-7 cell lines). The IC_{50} (µM) values were determined from dose-response curves by exponential decay fitting (r2>0.9). Palladium (II) complexes exhibited highest anticancer activity against the cancer cells compared to the standard anticancer Dox as compared to Nickel (II) complexes. Among the chiral palladium (II) complexes PdL3 showed excellent anticancer activity against human cancer cells.

PCO-10 : Effect of Substituents Towards *In-vitro* Antioxidant Activity of Dialkyl - 2, 6 – Dimethyl - 4 – Alkyl / Aryl -3, 5- Pyridine Dicarboxylates

D. D. Kumbhar, B. Y. Waghamare and S. K. Pardeshi*

Department of Chemistry, Savitribai Phule Pune University (formerly Pune University), Ganeshkhind, Pune - 411007
E-mail : skpar@chem.unipune.ac.in

A series of dialkyl - 1, 4 - dihydro - 2, 6 - dimethyl - 4 - alkyl/ aryl pyridine - 3, 5 -dicarboxylates were synthesized and subjected to their antioxidant activity. The antioxidant activity of these various 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 Fe^{3+} to 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 dialkyl - 1, 4 - dihydro - 2, 6 - dimethyl - 4 - alkyl/aryl pyridine - 3, 5 – dicarboxylates.

PCO-11 : Traditional Uses and Pharmacological Action of Ocimum Kilimandscharicum : An Overview

Roli Agrawal

Department of Chemistry, S.V. College, Aligarh-202001, Uttar Pradesh
E-mail : roliagrawal47@gmail.com

The natural products have played a vital role in curing health

related problems and in ailment of various diseases. Herbal drugs are easily available and have fewer side effects. So many people are attracted towards the herbal drugs. The aim of the present review is to understand the knowledge of plants used for Ayurvedic preparations in relation of their traditional uses as therapeutic agents and pharmacological properties.

Ocimum kilimandscharicum is also known as camphor basil. It is an economically important medicinal perennial herb that is widely distributed in East Africa, India and Thailand. It is extensively grown in the Tropics. *Ocimum Kilimandscharicum* is a useful tropical plant. It is widely used in the management of various ailments including colds, coughs, aldominal pains, measles, anti-ulcer, bronchitis, Anorexia, memory disorders and diorrhoea.

PCO-12 : Synthesis, Spectral and Antimicrobial Studies of Medicinally Important Mannich Bases

Sheela Joshi and Kapil Vyas*

School of Chemical Sciences, D.A.V.V., Indore
E-mail : kapilgyan@gmail.com

The present invention deals with the synthesis of Mannich bases of (RS)-4-amino-3-(4-chlorophenyl) butanoic acid (Baclofen). A series of Mannich bases of (RS)-4-amino-3-(4-chlorophenyl) butanoic acid (Baclofen) were synthesized via Mannich reaction of (RS)-4-amino-3-(4-chlorophenyl) butanoic acid with primary amines. The purity of synthesized compounds were checked via TLC and Melting points were determined by open tube capillary method and were uncorrected. Their chemical structures were established on the basis of UV, IR, ^{1}HNMR and ^{13}CNMR Spectral data. The novel compounds have been tested for their antimicrobial activity against a representative panel of bacteria i.e. *E-coli,* and *S.aureus*. Synthesized compounds were found to exhibit profound antibacterial activity.

PCO-13 : Chemical And Pharmaceutical Aspects of the Traditional Ayurvedic Drug *Samudraphane*

Meera Deshmukh[1] and Mrudula Wadekar[2]

[1]Tilak Maharashtra Vidyapeeth Pune
[2]Bharati Vidyapeeth University Y. M. College Pune
E-mail : deshmukhmeera410@gmail.com

Samudraphane is marine product originated from the cuttlefish bone. It is white grey coloured hard material floating on sea water. Actually it is the excretion of the sea animal *Sepia Officinalis* which

is produced in huge quantities through oceanic calcification process involving biomineralization.

The pharmaceutical potential and medicinal utility of *Samudraphane* has been recognized in ayurvedic medicinal system long ago. Till today, this biomaterial is remained as a purely traditional drug and its use is restricted to few *ayurvedic* practitioners from India. Literature survey shows that *Samudraphane* is likely to be interesting biomaterial of applied importance. Its use in various complaints related to ear is well known in *ayurvedic* pharmacy. Apart from this characteristic property, it is claimed to be useful in skin diseases and better alternative for calcium lactate. It is also found to be effective adsorbent for dyes and other colouring materials. It has potential ability to remove fluoride from effluent water.

Considering the merits and advantages of this cheaply available bio material, we have undertaken a systematic detail study of *Samudraphane*. In this communication we would like to present our recent work on the chemical and pharmaceutical aspects of *Samudraphane.*

PCO-14 : Synthesis And Screening of Some Novel Series of N^1-[3-(Substituted Phenylamino) Propanoyl]-4-(1*h*-Pyrrol-1-Yl)-Benzohydrazide Derivatives for their Analgesic and Anti-Inflammatory Activities in Rodents

M.R. Pradeep Kumar[*1] and S.D. Joshi[2]

[1]*Department of Pharmaceutical Chemistry, KLE University's College of Pharmacy, Vidyanagar, Hubli-580031, Karnataka.*
[2]*Department of Pharmaceutical Chemistry, SET's College of Pharmacy, S. R. Nagar, Dharwad-580002, Karnataka.*
E-mail : pradeepmrpk@yahoo.co.in

As pain and inflammation are associated with most of the ailments and also due to the side effects associated with the long term use of most of the currently available drugs to treat analgesia and inflammation, there is a great need to develop some potent, less side effect having analgesic and anti-inflammatory agents. Thus here we have reported some new N^1-[2-(substituted phenylamino) propanoyl]-4-(1*H*-pyrrol-1-yl)-benzohydrazide derivatives. Initially ethyl-4-pyrrole-1yl-benzoate (II) was synthesized by the reaction of benzocaine (I) with 2, 5-dimethoxy tetrahydrofuran in presence of glacial acetic acid. Compound (II) on treatment with hydrazine hydrate in presence of ethanol yielded 4-pyrrole-1-yl

benzoic acid hydrazide (III). Compound (III) on treatment with chloropropionyl chloride yielded *N*^{1}-(2-chloropropanoyl)-4-(1*H*-pyrrole-1-yl) benzohydrazide (IV), compound (IV) on reaction with different aromatic amines and triethylamine yielded *N*^{1}-[2-(substituted phenylamino) propanoyl]-4-(1*H*-pyrrole-1-yl)-benzohydrazide derivatives (V a-o). The structure of all newly synthesized compounds was confirmed by spectral study such as IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopy. All the synthesized compounds were screened for analgesic and anti-inflammatory activities by glacial acetic induced writhing in mice method using aspirin as the standard drug and carrageenan induced rat paw edema method using diclofenac as the standard drug respectively. Results showed that compounds V a, V d, V g, V h, V k, V m, V n and V o have showed significant analgesic activity. In the same series compounds V a, V d, V e, V g, V f, V i, V k, V l, IV m, IV n and IV o have showed significant anti-inflammatory activity.

PCO-15 : PAM_2CSK_4 Lead Optimization : Development of Highly Potent, Metabolically Stable and Water Soluble Monoacyl Lipopeptide

Deepak B. Salunke

Assistant Professor, Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh

Vaccination has made a massive impact on human health; even antibiotics have not had such a major effect on mortality reduction and population growth. Contrary to early vaccines, which used killed whole organisms, or attenuated live vaccines, modern vaccines increasingly rely on subunit vaccines which have the distinct advantages of ease of production, quality control, and safety. However, such subunit antigens which are largely soluble proteins are poorly immunogenic, and require “adjuvant” to induce strong and long lasting immune responses.

Several ligands for the pattern recognition receptors (PRR), are known to induce the innate immunity, predominantly targeting the APCs and consequently influencing the adaptive immune response. Therefore, the members of nearly all of the PRR families are potential targets for adjuvant development. These include Toll-like receptors (TLRs), NOD-like receptors (NLRs), RIG-I-like receptors (RLRs) and C-type lectin receptors (CLRs).

Toll-like receptor 2-agonistic lipopeptides typified by S-[2,3-bis(palmitoyloxy)-(2*RS*)-propyl]-*R*-cysteinyl-*S*-serine (PAM_2CS) compounds are potential vaccine adjuvants. We determined that at

least one acyl group of optimal length (C16) and an appropriately orientated ester carbonyl group is essential for TLR2-agonistic activity. We also found that these structurally simpler analogues display agonistic activities with human, but not murine, TLR2. A cysteine *N*-acetyl analogue (*N*-Ac PAMCS) was found to be the most potent (EC_{50}: 1 nM) analogue with its potency comparable to that of PAM_2CS. This SAR investigation led to the design of a highly potent lead but with negligible aqueous solubility, necessitating the reintroduction of aqueous solubility. We explored several strategies of introducing ionizable groups on the lipopeptide, as well as evaluated several chemically stable bioisosteres of the ester-linked palmitoylgroup. We have been fortunate in being able to successfully apply principles of classical medicinal chemistry and rational drug optimization to an unexpected problem of chemical stability leading to a fully optimized, chemically stable, and highly water-soluble human specific TLR2-agonist with excellent safety profile and prominent adjuvantic activity.

Based on this background and the current research work, I will briefly talk about the concept of vaccine adjuvant development and the role TLRs as bridge between innate and adaptive immunity. Our recent investigation on the development of TLR2-specific monoacyl lipopeptides and recent updates related to this work will be discussed in detail.

PCP-CYSA-01 : Synthesis and Characterization of Yashad (Zinc) Bhasma

Babita Kale and Nilima Rajurkar*

Department of Chemistry, Savitribai Phule Pune University, Pune
E-mail : rnilima@rediffmail.com

Bhasma is unique Ayurvedic herbo-metallic preparation useful in various ailments. To strengthen the quality of final product, standardization of bhasma is essential. The present study deals with the synthesis of Yashad bhasma by methods mentioned in the literature of Ayurveda. It is zinc based bhasma generally used in the treatment of diabetes and eye diseases. The synthesis of this bhasma includes Purification (Shodhan), Levigation (Bhavana) and Incineration (Maran) process. The prepared bhasma was analyzed as per ayurvedic guidelines as well as modern analytical techniques viz. XRD, TEM, EDAX, SEM, FTIR. XRD spectra show major peaks of Zn and ZnO in synthesized bhasma. TEM analysis indicated polycrystalline nature while SEM shows the smooth and granular morphology having particle size of bhasma below 100nm.

PCP-01 : Synthesis and Antimicrobial Evaluation of [*N*-(4-Substitutedphenyl-Thiazol-2-Yl)Aminooxy]-Acetic Acid 4-Methyl-3-Nitro-2-Oxo-2*h*-Chromen-7-Yl Ester

Nilesh B. Chauhan and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : drnavinbpatel@gmail.com, nb_chauhan@yahoo.com

Coumarin segment shows remarkable broad spectrum of different biological activities with that thiazole derivative enhance the pharmacological profile. In view that we have synthesized newer coumarin based thiazoles and screened for their antimicrobial activity. 4-Phenyl-thiazol-2-ylamine **(2a-j)** condensed with 4-methyl-3-nitro-2-oxo-2*H*-chromen-7-yl chloroacetate **(1)** to afford [*N*-(4-substitutedphenyl-thiazol-2-yl)aminooxy]-aceticacid 4-methyl-3-nitro-2-oxo-2*H*-chromen-7-yl ester **(3a-j)**. The newly synthesized compounds were established by IR, NMR and mass spectral studies and were screened for their antimicrobial, antitubercular and antioxidant activities. Compound **3e** shows good antibacterial activity against *S. pyogenus* and compound **3j** shows comparably good anti fungal activity against *C. albicans* compared to the standard drug.

PCP-02 : In *v*itro Anti-Arthritic and Anti-Inflammatory Activity of Edible Phlogacanthus Thyrsiformis (Hardow) Mabb. Flowers

Poppy Das and M. Himaja*

Department of Chemistry, School of Advanced Sciences, VIT University, Vellore-632014
E-mail : drmhimaja@gmail.com

Phlogacanthus thyrsiformis (Hardow) Mabb. is a seasonal plant growing in eastern and north eastern regions of India. The flowers of the plant are consumed in various traditional recipes. Different parts of the plant are also conventionally used for the treatment of fever, diabetes, inflammation, kidney disorders etc. The objective of the present study was to assess the anti-arthritic and anti-inflammatory activity of the plant at a scientific level. The edible flowers of P. thyrsiformis were extracted using three water, ethanol and ethyl acetate by hot extraction method. The extracts were screened qualitatively and the total phenol, flavonoid, terpenoid and sterol contents were also quantified. The extracts were subjected to gas chromatography mass spectrometry technique and eight molecules were identified from the ethyl acetate extract using NIST library. The in vitro anti-arthritic and anti-inflammatory activity were evaluated for each extract. The potency of ethyl

acetate extract was observed to be higher than the other extracts for both the activities. Correlation studies between the extracts and their activities revealed that the presence of phenol, flavonoid, terpenoid and β-sitosterol in the ethyl acetate extract played a crucial role in its impressive activity.

PCP-03 : Synthesis, Antimycobacterial and Antimicrobial Study of Biologically Active Schiff Base of Isoniazid Clubbed Pyrimidines

Hetal I. Soni, Rahul B. Parmar and Navin B. Patel*

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007
E-mail : drnavinbpatel@gmail.com, sonihetal@ymail.com, rbparmar1990@yahoo.com

Present work deals with well organized synthetic approach of newer biologically active analogous of 2-(2-(3-bromo benzylidene)-1-isonicotinoyl hydrazinyl)-N-(4-(substituted phenyl)-6-(substituted aryl) pyrimidin-2-yl)acetamide derived from isoniazid. The structures of new compounds were ascertained by spectral (IR, ^{1}H NMR, ^{13}C NMR& Mass) study and were evaluated for their potential in vitro antimycobacterial activity against M. Tuberculosis and antimicrobial study. Few compounds show good activity towards $H_{37}RV$ and some of them are active against certain bacterial and fungal strain.

PCP-04 : In *v*itro Growth Inhibition of Struvite Crystals (Kidney Stones) by Leaf Extract of Tragia involucrate

Vinodhini V. and Himaja M.*

Department of Chemistry, School of Advanced Sciences, VIT University, Vellore-632014
E-mail: drmhimaja@gmail.com

Tragia involucrata is a traditional medicinal plant, used in the treatment of various ailments like skin infections, inflammation, wound healing and as blood purifier and it is also reported for its diverse biological activities such as antitumor, nephroprotective, anti-diabetic activity. The struvite crystal growth inhibitory activity of the leaf extract was examined using in vitro single gel diffusion technique. The crystal growth inhibition of the extract at different concentration was measured using a travelling microscope and the results were found to be significant. The size of the crystals increased gradually in the control tube whereas the crystal size decreased in a dose dependent manner in tubes loaded with extract. This revealed that Tragia involucrata can be effective in treating struvite based urolithiasis condition. The FTIR and XRD analysis were performed to confirm the struvite nature of the crystals. The phytoconstituents present in the petroleum ether extract was

explored using Gas chromatographic Mass Spectroscopy analysis. The analysis revealed terpenoids to be the major phytoconstituent present in the extract.

PCP-05 : Synthesis, Anti-Tuberculosis, Anti-Malarial and Biological Activity of Sydnone Based Quinazoline Derivatives

S. A. Patel[1] and K.C. Patel[2]

[1]Navjivan Science College, Dahod
[2]Department of Chemistry, Veer Narmad South Gujaratu University, Surat
E-mail : shrey.patel84@gmail.com

3-(4-chlorophenyl)-4-(chlorosulfonyl) sydnone on recation with 3-amino-2-substitedphenylquinazoline-4(3H)-one gave corresponding 3-(4-chlorophenyl)-4-{N-[2-(substituted phenyl)-4-oxoquinazoline-3(4H)-yl]sulfamoyl} sydnone. Newly synthesized compounds have been examined on the basis of elemental analysis, IR, ^{1}H NMR spectra. All the compounds were screened against different gram-positive and gram-negative bacteria. Most of these compounds showed better inhibitory activity in comparison with the standard drugs and also screened against anti-tuberculosis and anti-malarial.

PCP-06 : Development and Validation of Stability Indicating Rp-Hplc Method for the Estimation of Bacoside–A from Bacopa Monnieri and its Marketed Formulation Used in CNS Disorders

Patel Samir G.*, Barot Tanvi D. and Sharma Mahavir M.

Pharmaceutical Chemistry and Analysis Department, Ramanbhai Patel College of Pharmacy, Charotar University of Science and Technology, Changa, Anand-388 421, Gujarat
E-mail : samirpatel.ph@charusat.ac.in

A simple, robust, selective and precise. Stability indicating RP-HPLC method has been developed and validated for analysis of Bacoside – A from Bacopa monnieri and its marketed formulation. The drug was separated using a mobile phase Acetonitrile : phosphoric acid, (30 : 70 v/v) on a phenomenex, TC C_{18} (250 . 4.6 mm) 5ìm column at flow rate of 1.5 ml/gradient elution at ambient temperature and detection was performed at 205 nm. The retention time was 17.984, 18.563, 20.271, 21.203 minutes for four different peaks of Bacoside – A. The detector linearity was established in a concentration ranging from 100 – 500 ìg/ml, the regression coefficient was 0.993. The LOD and LOQ for analytical method were 5.23 and 15.84 µg/ml. For stability study the drug was exposed to the stress

conditions such as acidic, basic, oxidation and photolytic as per the recommendation of ICH guidelines Q1(A). The results of the analysis were validated in terms of specificity, limit of detection (LOD), limit of quantification (LOQ), linearity, precision, and accuracy as per ICH guidelines Q2(R1) and were found to be satisfactory. The high recovery and low relative standard deviation confirm the suitability of this methods can employed for the routine analysis of Tablet containing Bacoside – A. The results showed that the rate of degradation was increased with increment in reaction temperature. At the room temperature, as time increases % Drug remain was decreased. Hance, % drug degradation was increased.

PCP-07 : Comparative Evaluation of Protecting Affordability of Flexible Laminates for Bacopamonnieripowder and It's Marketed Formulation

Patel Samir G.[1], Patel Dhaval and Patel Purvish A.[2]

[1]Pharmaceutical Chemistry and Analysis Department, Ramanbhai Patel College of Pharmacy, Charotar University of Science and Technology, Changa, Anand-388 421, Gujarat

[2]Packaging Solutions, Survey No.674, Opp. Satyam Estate - 1, Ahmedabad to Indore National Highway, Village Kubadthal, Daskroi, Ahmedabad, Gujarat-382430

E-mail : samirpatel.ph@charusat.ac.in

Leaf powder of Bacopamonnieri containing an active constituent is Bacoside-A, which is use as brain disorder.Herbal drug are many of time available as over the counter product and used as nutraceuticals. They are often available in flexible packages, but there has been no such authenticated data available in any literature for any plant drug about ability of packages to protect chemical integrity of drug. The major disadvantages of flexible packaging produce sorption, leachable and extractable. In this study, A series of flexible packages made up of variety laminates and its combinations were used to evaluate their relative abilities to preserve chemical integrity of selected plant drug when subjected to accelerated condition. The studies revealed that packaged made up of 1) Polyester+Polyethylene Film 2) Polyester+Metalized Polyester+Polyethylene Film 3) Polyester+Metalized Polyester+ Metalized – Cast Polypropylene 4) Polyester+Aluminum Foil+Polyethylene Film 5) Polyester+Cast Polypropylene and, 6) Polyester+Nylon Film. All those combination were tested for Heat-seal test, puncher strength, lamination bond strength and thickness before starting accelerated studies. The sample of Bramhi Churna and Tablets were stored in different package made up from different

material and its combination for at least 06 months under the controlled condition of temperature and relative humidity (RH) (40°C±0.2°C /80% ± 5% RH). The sample has been withdrawn from 15 Days, 01 Month, 02 Month, 04 Month and 06 Month duration time point and tested for moister content and content for active constituent. Degradation kinetic has been applied to determining rate constant by assuming degradation kinetics and it's order of reaction.

PCP-08 : Chemical and Pharmaceutical Aspects of the Tradition Ayurvedic Drug Samudraphane

Meera Deshmukh[1], Mrudula Wadekar[2], Shivaji Takale[3] and Yogesh Bendale[3]

[1]Tilak Maharashtra Vidyapeeth ,Mukundnagar, Pune-411037
[2]Bharati Vidyapeeth University ,Y. M. College, Postgraduate Department of Chemistry, Paud Road, Pune-411038
[3]Ayurved Rasayani, Amrutkumbh, Navi Peth, Pune-411030
E-mail : m_p_wadekar@yahoo.co.in

Samudraphane is a marine product originated from the cuttlefish bone. It is a white gray coloured hard material floating on sea water. Actually it is the excretion of the sea animal Sepia officinalis which is produced in huge quantities through oceanic calcification process involving biomineralization. The pharmaceutical potential and medicinal utility of Samudraphane has been recognized in ayurvedic medicinal system long ago. Till today, this biomaterial is remained as a purely tradition drug and its use is restricted to few ayurvedic practitioners from India. Literature survey shows that Samudraphane is likely to be interesting biomaterial of applied importance. Its uses in various complaints related to ear is well known in auyrved pharmacy. Apart from this characteristic property, it is claimed to be useful in skin diseases and a better alternative for calcium lactate. It is also found to be an effective adsorbent for dyes and other colouring materials. It has a potential ability to remove fluoride from effluent water. Considering the merits and advantages of this cheaply available bio material, we have undertaken a systematic detail study of Samudraphane. In this communication we would like to present our recent work on the chemical and pharmaceutical aspects of Samudraphane.

PCP-09 : Origin of the Differential and Specific Medicinal Properties of $CaCO_3$ based on Marine Products and their Ayurvedic Formulations

Sonali Dhamal[1], Vividha Dhapte[2], Vinita Bendale[3] and R. W. Jawale[1]

[1]Bharati Vidyapeeth University, College of Engineering, Dhanakawadi-Katraj, Pune-411046
[2]Bharati Vidyapeeth University, Poona College of Pharamcy, Paud Road, Kothrud, Pune-411038
[3]Ayurved Rasayani, Amrutkumbh, Navi Peth, Pune-411030
E-mail : m_p_wadekar@yahoo.co.in

Ayurved pharmacy has introduced different types of drugs and formulations derived from natural resources. Calcium based ayurvedic drugs prepared from marine products is one of these types of drugs. The marine products and corresponding drugs are Conch(shanka bhasma), Conch-shell(shautica bhasma), Cowarie (kapardica bhasma), Coral (praval bhasma) and Pearl (mautika bhasma). Each of these drugs, posseses some common medicinal properties as well as some specific properties. Basically all of these are composed of (a) Calcium carbonate as the major component (more than 95 %) (b) Organic component in the form of protenious network and (c) Several minor as well as trace constituents.

During recent years, the vital importance and practical utility of these drugs is now realized and attempts are being done by researchers to rejuvenate the traditional art and science of the traditional ayurvedic drugs on the basis of modern scientific approach.Through this communication, an attempt will be made to throw some light on the origin of the differential as well as specific medicinal properties of the parent marine products and their ayurvedic formulations using modern techniques like HPLC, IR and UV spectraons copy, XRD, SEM and Thermogravimetry.

PHYSICAL CHEMISTRY SECTION

Sectional President's Address

Complex Equilibria in Aquo-Organic Mixtures-Past, Present and Future

R. Sambasiva Rao

School of Chemistry, Andhra University, Visakhapatnam 530 003
E-mail : rsr.chem@gmail.com

Mother Nature prepared chemical elements during its evolution over billions of years. The animate/inanimate world around as well as inside us contain simple to complex chemical moieties emerged over trillions of interactions under wide range of environment of nature's laboratory. The alchemy, now a history, was around conversion of base metals (lead) into noble (gold) ones. The focus of modern science is to synthesize materials for health, comfort, transport, defense from natural calamities and catastrophes resulting from man promoted activities. The transition of material wealth to information revolutionized pursuits of this century to turn attention to knowledge based approach and physical chemistry is a beacon light in the ocean of chemical processes. The formulation of physical/ chemical models, translation to computational strategies and adopting state-of-art solution algorithms from mathematical sciences is the core activity. The single minded view to predict, perform experiments and iteratively refine activity is now sought after rational approach rather than hit-and-try attempt of yester years' with a belief of 'failures are stepping stones for success'. The analogy is today's mandate in medical sciences that following non-invasive means of 'see and cut if essential' over "cut and see even as exploratory exercise" of earlier only option.

Computer hardware/software/man-machine interfaces for communication peta/exa scale computations/memories are aids for sustained progress in astro-, nano, interfacial chemical outcome in the near future. pKa values for off-the shelf /virtual library/real life chemical species with long cherished traditional experimental procedures and those with latest computational quantum-chemical calculations will be illustrated. A scientific approach of pros and cons of direct/indirect experiments and computational approaches reflecting the unique features and limitations will open vistas in bridging gaps and marching towards nearer and nearer to desired goals of health for all, increased life expectancy, clean environment and understanding brain-mind-consciousness balance

PIL-01 : Design of Functional Materials

G. Narahari Sastry

Centre for Molecular Modelling, CSIR- Indian Institute of Chemical Technology, Tarnaka, Hyderabad 500 607, AP
E-mail : gnsastry@gmail.com

Advanced material design is one of the most important and challenging aspects of contemporary interdisciplinary science. Computational design of molecules and materials have been rapidly advancing and finetuning the non-covalent interactions appear to be an extremely imporat aspect in the advanced material design. In this talk we present our work on CO_2 capture materials, carbaneous materials and will explain the design of advanced materials involving carbon nanostructures. It is crucial that both scientists and technologists work together in an optimal fashion to obtain meaningful results. I will try to explain how chemistry is of fundamental importance in contributing to both these aspects. Some case studies in nano-technology, new material design and computer aided drug design are taken to show how the interplay between basic science and technology have made a significant impact.

PIL-02 : Exceptional Behaviour of Nanomaterials and Architecture of Nanoporous Materials and their Applied Applications

Farid Khan

Nanomaterials Discovery Laboratory, Department of Chemistry,
Dr. Hari Singh Gour central University, SAGAR-M.P.
E-mail : farid.fk@rediffmail.com; faridkhan58@yahoo.com

Materials of length scale 1-100nm belong to nanomaterials of diverse in nature such as carbon nanotubes, fullerenes, nanowires, quantum dots, nanoparticles, photonic crystals, nanoporous materials and so on. These materials have extensive applications in heterogeneous catalysis, sensors, targeted drug delivery, bio-filtration, tissue engineering, power applications, agriculture science, environmental science, and communication technology. Significant progress have been made in porous monoliths however, tuning the morphology of nanoporous materials is a great challenge which can be undertaken by adding the reinforcing agents viz, CNT, GO, nanoparticles, and structural directing agents. This lecture is mainly concerns with synthesis, characterization and applications of nanoporous materials of silver, gold, copper oxide and others using suitable surfactants. Their possible applications as heterogeneous catalysis, sensors and supercapacitors have also been discussed.

PIL-03 : Analytical Sensors Based on Nanoparticles for Low Detection of Toxic Compounds

S. K. Mehta

Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh-160 014
E-mail : skmehta@pu.ac.in

Various organic and inorganic pollutants such as Hydrazine, para-nitrophenol (PNP), 2,4,6 –trinitrophenol (PA), cyanide, trinitrotoluene (TNT) pollute the water system to greater extent. Due the wide use of these inorganic and organic compounds in industries and other activities such compounds are released along with waste water. This may lead serious contamination of groundwater and even drinking water which is harmful to all living beings. In this regard we developed some analytical sensors based on ZnO, α-Fe_2O_3, ZnS and CdS nanoparticles which detect very low concentrations of these toxic compounds in aqueous system. We have also developed an optical sensor based on ZnO QDs for estimation of exact chlorine concentration in water.

PIL-04 : Chemical Biology of human C3a Receptor – Computational Rationale of an Ideal to Model Experiment in Drug Design

Voleti Sreedhara

In-Silico Discovery Research Academic Services Pvt. Ltd., 44-347/66, Tirumalanagar, Moula Ali, Hyderabad -500040, TS
E-mail : sreedhara.voleti@indras.in

Standard definition of *chemical biology* is a scientific discipline spanning the fields of chemistry, biology, and physics. It involves the application of chemical techniques, tools, and analyses, and often compounds produced through synthetic chemistry, to the study and manipulation of biological systems. These fundamental principles applied in identifying novel chemical entities through design, discovery, and developments phases consists of the invention of drugs under chemical biology field for a given disease. Understanding the biological and functional roles of proteins (enzymes, receptors, DNA/RNA) is the biology and normal pharmacology, while the *modulation* of function of biological entities by a set of chemicals (small molecules or small peptides) is the true chemical biology.

While chemistry (organic and inorganic nature) and molecular biology play experimental roles, fundamental involvement of physical chemistry in chemical biology relates to the size, shape, and strength of interactions (static, electrostatic, van der Waal, H-

bonding, long range energetic and thermodynamics) of protein-ligands or protein-proteins. Measurement of such parameters experimentally (structural) is difficult, while computational understanding brings unmatchable rationale. Molecular modeling methodologies and computer-aided drug design tools and techniques are some such physical chemistry knowledge which brings invaluable visualizing help for medicinal chemists, biologists, and pharmacologists in elucidating chemical biology of function of proteins.

In the present talk, implication of human C3a receptor (C3aR) is discussed in inflammation (innate immunity), its chemical biology using various peptides from native is explained, and modulation of activity is achieved through small molecule design. Rational design of structure of human C3aR, computational analysis of interactions of C3aR with C3a and SB28015 validates biologically observed protein-ligand and protein-protein data. Final outcome of rational design in discovery of novel C3aR antagonists is discussed as an elucidative example in detail for chemical biology practice in pharmaceutical industry and academia.

PIL-05 : Thermodynamic Properties of Ionic Liquids with Additives

Harsh Kumar Manchanda

Department of Chemistry, Dr B R Ambedkar National Institute of Technology, Jalandhar - 144011, Punjab
E-mail : h.786.man@gmail.com; manchandah@nitj.ac.in

Ionic liquids are considered as green solvents and they have been considered environmentally friendly and applicable in the development of green technologies. Lots of studies are being carried out on the different properties of ionic liquids with various additives like surfactants, organic salts, amino acids etc. as ionic liquids found variety of applications in all aspects of the life. Our main focus is on the thermodynamic properties of ionic liquids mainly imidazolium based ionic liquid with additives. Thermodynamic properties of ionic liquids with additives give an idea about the characteristics of ionic liquids in variety of mixtures. Conductometric and spectroscopic studies of cetyltrimethylammonium bromide (CTAB) in aqueous solutions of imidazolium based ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate [C_4mim][BF_4] have also been studied. The effect of the addition of the hydrophilic ionic liquid 1-butyl-3-methylimidazolium tetrafluoroborate [C_4mim][BF_4] on the micellization of cetyltrimethylammonium bromide (CTAB) in aqueous solution was studied using electrical conductivity, density, speed of

sound and spectroscopic techniques. From the cmc values and their temperature dependence, various thermodynamic parameters such as standard free energy (ΔG^{o}_{m}), enthalpy (ΔH^{o}_{m}) and entropy (ΔS^{o}_{m}) of the micellization were determined in the temperature range 288.15 K to 318.15 K. Fourier transform infrared spectroscopy (FTIR) and UV-vis spectroscopy were employed to get information regarding the interaction between the surfactant and ionic liquid aggregates. The calculated thermodynamic parameters $|\Delta H^{o}_{m}|$ is smaller than $|T\Delta S^{o}_{m}|$ which suggests that the micellization is entropy driven. Further, in addition we have studied the interactional behavior of citrate salts viz. trisodium citrate, tripotassium citrate, trilithium citrate, triammonium citrate. Volumetric, acoustic and spectroscopic behavior of these salt with 1-hexyl-3-methylimidazolium chloride has been studied [C6mim][Cl]. The experimental densities are used to calculate the apparent molar volume, limiting apparent molar volumes and transfer volumes. Experimental values of the densities and speed of sound were used to estimate apparent molar properties. The structure making or breaking ability of $[C_6mim][Cl]$ has been discussed in terms of sign of partial molar expansibility. Fourier transform infrared spectroscopy (FTIR) and UV-vis spectroscopy were employed to get information regarding the interaction between the citrate salts and ionic liquid. Further another imidazolium based ionic liquid i.e. 1-butyl-3-methylimidazolium tetrafluoroborate $[C_4mim][BF_4]$ with amino acids like L-alanine, L-valine, L-serine, L-threonine.

PIL-06 : Micelle Mediated Techniques Through Physico-Chemical Window

K. Ramakrishna

Department of Chemistry, Institute of Science, GITAM University, Visakhapatnam- 530045
E-mail : karipeddirk@gmail.com

Surfactant mediated techniques viz. Cloud point extraction (CPE), micellar enhanced ultra-filtration (MEUF) and adsorptive micellar flocculation (AMF) have been found applications in concentration/ separation of metal ions, organic/inorganic moieties. All these procedures are simple and inexpensive in removing organic/ inorganic pollutants. They fall under green chemistry category as the surfactants in general are nontoxic, nonvolatile (unlike organic solvents used in liquid–liquid extraction) and only very low concentrations are employed. Further, only a few residues are generated. In this talk, the principles, methodology and applications will be discussed with illustrative test cases from our research and literature reports.

PO-CYSA-01 : Kinetics and Mechanistic Study of Oxidation of Pyrazinamide by Waugh-Type Enneamolybdomanganate (IV) in Perchloric Acid Medium

Bhagwat B. Nagolkar and Sunil G. Shankarwar*

Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431004, Maharashtra
E-mail : bhagwatnagolkar@gmail.com

The kinetics and mechanism of oxidation of tuberculosis drug pyrazinamide in acidic medium was studied spectrophotometrically. The reaction between pyrazinamide and enneamolybdomanganate (IV) in aqueous acidic medium exhibits 1:1 stiochiometry Pyrazinamide : $[Mn^{IV}Mo_9O_{32}]^{6-}$ was carried out under pseudo-first-order conditions keeping large excess of pyrazinamide at a constant ionic strength of 0.3 mol dm^{-3}. The orders in oxidant and substrate were found to be unity and 0.9 respectively. The main oxidative products were identified by spot test, FT-IR, ^1H NMR, LC-MS, and melting point. The effect of $[H^+]$ ion and ionic strength on the reaction have been investigated. The rate constants involved in the different steps of the mechanism are calculated. The activation parameters with respect to slow step of the mechanism are computed and discussed. A mechanism related to this reaction is proposed.

PO-CYSA-02 : Influence of Alkyl Chain of Alcohol on Molecular Interactions of *m*-chlorotoluene and Alcohol : Spectroscopy, Quantum Chemical and Thermodynamic Studies

S. Karlapudi[1], V. Govinda[1], S. Singh[2], I. Bahadur[1,*], K. Siva Kumar[3] and E. E. Ebenso[1]

[1]Department of Chemistry, School of Mathematical and Physical Sciences, Materials Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Agriculture, Science and Technology, North-West University (Mafikeng Campus), Private Bag X2046, Mmabatho 2735, South Africa
[2]Department of Chemistry, Durban University of Technology, P.O. Box 1334, Durban 4000, South Africa
[3]Department of Chemistry, S.V. Arts UG & PG College (TTD'S), Tirupati-517502
[*]E-mail : bahadur.indra@nwu.ac.za

A thorough knowledge of molecular interaction of binary mixtures is essential in many industrial applications such as design involving chemical separations, heat transfer, mass transfer and fluid flow using different techniques.Therefore, the fourier transform infrared spectroscopy (FT-IR)along with quantum chemical calculation and thermodynamic studies have been successfully

employed for pure solvents and their binary liquid mixtures of *m*-chlorotoluene (MCT) and 1-alkanols with different mole fractions, to obtain information about the interactions in liquid mixtures. Furthermore, the excess volumes (V^E), isentropic compressibility (k_s) and excess isentropic compressibility were calculated from experimental data for the binary mixtures at different temperature and at atmospheric pressure.These excess properties were correlated with theoretical model developed by Redlich-Kister. Nonetheless, the recorded FT-IR spectra, derived excess properties and quantum studies are essential to predict the molecular interactions and structural effects between component molecules in binary liquid mixtures.

PO-CYSA-03 : Development of Flexible Pervaporation Membranes by Incorporating Plasticizer into Crosslinked Sodium Alginate Membranes for the Separation of Azeotropic Mixtures

D. D. Achari and M. Y. Kariduraganavar*

Department of Chemistry, Karnatak University, Dharwad-580 003
E-mail : mahadevappayk@gmail.com

Pervaporation (PV), an environment-benign and energy-saving technology, has become a promising alternative to conventional technologies in separation of azeotropic and close boiling liquids [1,2]. In order to make the PV process commercially feasible, membrane and its properties play a vital role. Thus, this paper addresses the preparation of novel flexible PV membranes by incorporating different mass% of dibutyl phthalate as plasticizer into crosslinked sodium alginate. Prior to this, sodium alginate (Na-Ag) was crosslinked with a known amount of polystyrene sulfonic acid-co-maleic acid (PSSAMA) by employing a solution technique. The chemical composition and morphology of the resulting flexible membranes were investigated by various techniques, such as Fourier transform infrared spectroscopy (FTIR), wide-angle X-ray diffraction (WAXD), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM). The developed crosslinked flexible membranes were subjected to PV separation of industrially important azeotropic mixtures, such as water-isopropanol and water-1,4-dioxane at different temperatures. The result demonstrated that plasticizer incorporated crosslinked membranes show higher performance for both water-isopropanol and water-1,4-dioxane mixtures as compared to mere crosslinked membrane. This is mainly attributed to reduction of crystallanity in the membrane metric, which favours higher permeation flux and

separation factor. From the temperature dependent permeation values, the Arrhenius activation parameters were also determined. Based on these data, the performance of the membranes was evaluated and discussed.

PO-CYSA-04 : Synthesis of Mesoporous TiO_2 and its Role as a Photocatalyst in Degradation of Indigo Carmine Dye

Devendra Ahirwar, Mustri Bano and Farid Khan*

Nanomaterials Discovery Laboratory, Department of Chemistry,
Dr. H. S. Gour Central University, Sagar, Madhya Pradesh 470 003
**E-mail : faridkhan58@yahoo.com; devendraahirwar.p@gmail.com*

A modified sol-gel route was used to synthesize mesoporous TiO_2 catalyst that was characterized by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Atomic force spectroscopy (AFM), Optical absorption spectroscopy and Brunauer- Emmitt- Teller (BET) adsorption isotherm technique. The synthesized mesoporous TiO_2 is highly crystalline, pure and consisting very high porosity and surface area 226.25m^2g^{-1}. The catalyst showed an excellent photocatalytic activity against the degradation of indigo carmine in presence of visible light. It was found that 50mL dye solution of 4×10^{-5}M concentration has been completely degraded and decolorized with optimum catalyst dose of 1.5g/L in 150 min, acidic pH and at 25±1°C reaction temperature. The reaction kinetic was studied and it was found that the indigo carmine dye photo catalytic degradation followed pseudo first order reaction kinetics with rate constant, k of 0.007 min^{-1}. Degradation of dye was confirmed by chemical oxygen demand (COD) analysis and UV-Vis spectrophotometry.

PO-CYSA-05 : Fabrication of Novel 3-Dimensional Scaffolds for Bone Tissue Engineering by Incorporating SiO_2 into PCL matrix

Nandini A. Pattanashetti[1], Tania Viana[2], Nuno Alves[2] & Mahadevappa Y. Kariduraganavar*[1]

[1]Department of Studies in Chemistry, Karnatak University, Dharwad 580 003
[2]Centre for Rapid and Sustainable Product Development, Polytechnic Institute of Leiria-2430-028, Portugal
**E-mail : mahadevappayk@gmail.com*

Bone repair or tissue reconstruction has become a challenging topic in the field of tissue engineering and regenerative medicine. Scaffolds made of biodegradable and biocompatible material serves as a temporary skeletal frame to mimic the properties of extracellular matrix (ECM) and induces bone tissue regeneration.

Such porous scaffolds can be developed by various techniques such as solvent casting, particulate leaching, gas foaming, freeze drying and thermally induced phase separation using biodegradable materials. In this paper, BioExtruder was employed for the fabrication of composite scaffolds using polycaprolactone (PCL) and SiO_2 nanopowder. Thermal properties of the scaffolds were determined using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The morphology was analysed using optical microscopy and scanning electron microscopy (SEM). Contact angle meter and universal testing machine (UTM) were employed respectively to measure wettability and compressive modulus of the scaffolds. The *In vitro* cytotoxicity and cell proliferation study was carried out using L929 mouse fibroblasts and MG63 osteoblasts, respectively. It is found that the incorporation of SiO_2 significantly enhanced the mechanical strength of the scaffolds without much compromising the cell viability and proliferation. This suggests that the developed scaffolds are suitable for hard tissues and specifically bone tissue regeneration.

PO-CYSA-06 : Hydrolysis of Di-2,3-dichloroaniline Phosphate in Buffer Media

Nisha Chhetri and S. A. Bhoite*

School of Studies in Chemistry, Pt. Ravishankar Shukla University Raipur, Chhattisgarh-492010
E-mail : nchhetri18@yahoo.com, sa.bhoite10@gmail.com

Hydrolysis of phosphate esters is of crucial importance to biological systems, being involved in energy transduction, biosynthesis, control of secondary messengers and regulation of protein function. In present investigation, kinetic study of hydrolysis of di-2,3-dichloroaniline phosphate has been carried out in pH range from 0.00 to 7.49 in 30% dioxane-water medium at 80°C. The pH log rate profile shows rate maximum at pH 4.11. Neutral and mononegative species have been found to be reactive in pH range from 0.00 to 2.21 and 2.21 to 7.49 respectively. The theoretical rates determined from Debye Huckel equation have been found in close agreement with the experimental rates. Molecularity and Bond fission have been discussed in terms of isokinetic relationship. Probable reaction mechanism has been proposed for the hydrolysis of di-ester *via* its neutral and mononegative species.

PO-CYSA-07 : Development of Fe_2O_3 Nanoparticle Modiûed Carbon Paste Electrode for the Voltammetric Investigation of Paracetamol

Vinay M. M. and Y. Arthoba Nayaka*

Department of Chemistry, School of Chemical Science, Kuvempu University, Shankaraghatta - 577451, Karnataka
**E-mail : drarthoba@yahoo.co.in*

Electrochemical behaviour of paracetamol (PA) has been investigated by cyclic voltammetry (CV), differential pulse voltammetry (DPV) and square wave voltammetry (SWV) using the selective and sensitive iron oxide (Fe_2O_3) nanoparticle modified carbon paste electrode (IOCPE). A quasi-reversible redox process of PA was obtained at modified electrode. The IOCPE exhibited excellent electrocatalytic activity towards PA. The influence of pH was studied and optimized by SWV. The phosphate buffer (PBS) of pH 7.0 was selected as a suitable analytical medium in which PA shows anodic and cathodic peak potential at 0.458 V and 0.088 V (vs Ag/AgCl), respectively. In DPV mode PA gave linear response over the concentration range 3 to 14 µM (r^2 = 0.999) with a limit of detection (LOD) and limit of quantification (LOQ), 0.245 and 0.818 µM, respectively. The proposed method could be successfully validated for the determination of the concentration of PA present in pharmaceutical and urine samples.

PO-CYSA-08 : Development of SBA-15 Templated Mesoporous Reduced Graphitic Oxide Composites for High Performance Supercapacitors

Satishkumar Naik, Anand I. Torvi and M. Y. Kariduraganavar*

Department of Chemistry, Karnatak University, Dharwad -580003
E-mail : mahadevappayk@gmail.com

Among all the energy storage devices, supercapacitors have gained a special been a great attention owing to their fast charge/ discharge rate, long lifetime, and high power density. The capacitive performance of supercapacitors depends largely on the morphology, porosity and crystallinity of the electrode materials. In addition, power density is dependent on the resistance of the ion transport inside the pores. The abundant micropores severely impede the ion transport owing to increased resistance, and thus lower the power density. To optimize this, it is desired to generate mesopores as transport channels with smaller ion transport resistance. Further, the incorporation of graphitic oxide (GO) into porous frameworks has been considered as an effective way to improve the electrochemical properties of the supercapacitors.

Understanding this, we present a novel synthetic route for the synthesis of reduced graphene oxide-mesoporous silica composite by incarporating GO into SBA-15 using P-123 as template and tetraethyl orthosilicate (TEOS) as silica source. Prior to this, GO was prepared through a modified Hummers method. Subsequently, GO was converted into reduced graphene oxide (RGO) through chemical process. The specific interaction between the functional groups of SBA-15 and RGO was confirmed using Fourier transform infrared (FT-IR) spectroscopy. Thermal behaviour was studied using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Surface morphology was investigated by atomic force microscopy (AFM). The resulting composite material was subjected to four probe technique and cyclic voltammetry for the measurement of electrical conductivity and specific capacitance, respectively. From the study, it is found that the resulting material demonstrated an excellent electrochemical performance, and thus the prepared composite could be used as supercapacitor electrode material.

PO-CYSA-09 : Mechanistic Investigations of Oxidation of Ascorbic Acid by Copper(III) Periodate Complex in Presence of Ruthenium(III) Catalyst

Shweta J. Malode and Sharanappa T. Nandibewoor*

Department of Chemistry, K.L.E. Society's K.L.E. Institute of Technology, Gokul, Hubballi- 580030

P.G. Department of Studies in Chemistry, Karnatak University, Dharwad-580 003

E-mail : malodeshweta@yahoo.co.in

Ruthenium(III) catalyzed oxidation of ascorbic acid by diperiodatocuprate(III) has been investigated in aqueous alkaline medium, at a constant ionic strength of 0.10 mol dm^{-3} spectrophotometrically. The catalyzed reaction between ascorbic acid and diperiodatocuprate(III) in alkaline medium exhibits 1:2 stiochiometry i.e., [AA]/[DPC]. The reaction was of first order with respect to [DPC], less than unit order with respect to [AA] and [OH^-], and negative fractional order in [IO_4^-]. The order with respect to [Ru(III)] was unity. The oxidation products were identified by spectral analysis and suitable mechanism was proposed. The reaction constants involved in the different steps of the reaction mechanisms were calculated. The catalytic constant (K_C) was also calculated for the catalyzed reaction at different temperatures. The activation parameters with respect to slow step of the mechanism and also the thermodynamic quantities were determined. Kinetic experimental results suggest that [$Cu(H_2IO_6)(H_2O)_2$] is the reactive copper(III) species and [$Ru(H_2O)_5OH]^{2+}$ is the reactive Ru(III) species.

PO-CYSA-10 : Multi-spectroscopic and Voltam-metric Evidences for Binding, Conformational Changes of Bovine Serum Albumin with Thiamine

Jyoti Bagalkoti and Sharanappa T. Nandibewoor*

P.G. Department of Studies in Chemistry, Karnatak University, Dharwad-580 003
**E-mail : stnandibewoor@yahoo.com, jyotibagalkoti@gmail.com*

The interaction between thiamine hydrochloride (TA) and bovine serum albumin (BSA) was investigated by fluorescence, FT-IR, UV-vis spectroscopic and cyclic voltammetric techniques under optimised physiological condition. The fluorescence intensity of BSA are gradually decreased upon addition of TA due to the formation of a BSA–TA complex. The binding parameters were evaluated and their behaviour at different temperatures was analysed. The quenching constants (K_{sv}) obtained were 2.6×10^4, 2.2×10^4 and 2.0×10^4 L mol^{-1} at 288, 298 and 308 K respectively. The binding mechanism was static type quenching. The values of ΔH^0 and ΔS^0 were found to be 26.87 kJ mol^{-1} and 21.3 J K^{-1} mol^{-1}, and indicated that electrostatic interaction was the principal intermolecular force. The changes in the secondary structure of BSA upon interaction with TA were confirmed by synchronous and 3-D spectral results. Site probe studies reveal that TA is located in site I of BSA. The effects of some common metal ions on binding of BSA– TA complex were also investigated

PO-CYSA-11 : A Novel Modified Exfoliated Graphite Electrode for the Simultaneous Voltammetric Determination of Lead and Cadmium Ions in Contaminated Water Samples

Ganesha Achary[1*], M. N. Kumaraswamy[2], Prathima Mathias D. A.[1] and Y. Arthoba Nayaka[3]

[1]Department of Chemistry, I. D. S. G. Government College, Chikmagaluru, Karnataka
[2]Department of Chemistry, Sir. M. V. Science College, Bhadravathi, Karnataka
[3]Department of Chemistry, Kuvempu University, Shankaraghatta, Karnataka

This work presents a new exfoliated graphite paste electrode, modified by doping with a naphthofuran derivative. The electrode is fabricated for the simultaneous determination of lead (Pb) and Cadmium (Cd) present in the contaminated water samples by differential pulse anodic stripping voltammetry. Under the optimal conditions, Pb^{2+} and Cd^{2+} could be detected in the concentration range from 1×10^{-8} M to 8×10^{-8} M with correlation co-efficients 0.987 and 0.986 for Cd^{2+} and Pb^{2+} ions on modified-EGPE with the linear regression equation, $y= 19.41\times 10^{-6} x + 0.4249\times 10^{-9}$ with correlation co-efficients 0.987 and 0.986 for Cd^{2+} and Pb^{2+} ions respectively. The

sensitivity of modified-EGPE towards determination of Cd^{2+} and Pb^{2+} ions was 0.8×10^{-7}A/µM and 0.5×10^{-7}A/µM respectively. Under the optimized experimental conditions, the lower detection limit (LOD) at modified-EGPE for Cd^{2+} and Pb^{2+} ions was found to be 1.5×10^{-7} M and 3×10^{-7} M respectively. Interferences from other ions were investigated and the proposed method was further applied to the trace levels of Pb^{2+} detection in real samples with satisfactory results.

PO-CYSA-12 : Designing Functional Azeotropic Porous Polymers of 2-(Dimethylamino)ethyl Methacrylate-co-Butyl Methacrylate : Copolymerisation Studies and Application in Strontium (II) Ion Recovery

Kishor S. Rajdeo[1,2], Surendra Ponrathnam[2], Nayaku N. Chavan[2*], Satish K. Pardeshi[1]**

[1]Department of Chemistry, Savitribai Phule Pune University (Formerly Pune University), Ganeshkhind, Pune - 411 007
[2]Polymer Science and Engineering Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411 008
***E-mail : skpar@chem.unipune.ac.in*

Binary copolymerisation studies of 2-(dimethylamino) ethyl methacrylate (DMAEMA), a functional amino methacrylate monomer and butyl methacrylate (BMA) with differing copolymer compositions were studied using solution copolymerisation. The instantaneous copolymer compositions were estimated using gas chromatographic analysis. Binary monomer reactivity ratios and azeotropic copolymer compositions were computed using four terminal linear models: Fineman-Ross (FR), Kelen-Tudos (KT), extended Kelen-Tudos (ext. KT) and Mao-Huglin (MH). The differing surface area beaded polymers with functional amino groups were synthesised using suspension polymerisation with variation in crosslink density. The beaded polymers were well characterized by different analytical characterization techniques including infra-red spectroscopy, x-ray photoelectron spectroscopy, particle size analysis, Brunauer-Emmett-Teller surface area analysis. The application of synthesised porous polymers as functional adsorbents in heavy metal ion recovery were demonstrated with strontium (II) ion. The batch adsorption kinetics was studied with the variable of crosslink density, pH, time, adsorbent dose. These studies reveal that these functional polymers can play a vital role in heavy metal ion recovery and water purification.

PO-CYSA-13 : Fabrication and Characterization of Graphene based Material

Varnika Prakash, Shweta and S.K Mehta

Institute of Forensic Science and Criminology, Panjab University, Chandigarh-160014.
E-mail : varnikaforensics@gmail.com

Graphene based materials exhibit potentially outstanding and amazing features and are employed in scientific arena in the field of sensing, electronics and magnetic device. The derivatives of graphene which are graphene oxide, reduced graphene oxide, modified reduced graphene oxide (metallic nanoparticles, biomolecules, hetereo atom doping) are proven to characteristically exhibit excellent surface properties. The fabrication of these materials is discussed. The graphene oxide is prepared through Modified Hummer' s method which is further reduced by chemical, hydrothermal and electrochemical method. The synthesized product is modified with silver nanoparticles. Finally, the products are characterized by techniques like UV-Vis, FTIR, XRD, SEM, Raman Spectroscopy. The potential of these prepared materials in the field of electrochemical sensing is elaborated.

PO-CYSA-14 : Fabrication of Lanthanide Nanoparticles and their Potential Applications

Aashima[1], S. K. Mehta[1] and S. Singh[2]

[1]Department of Chemistry, Panjab University, Chandigarh
[2]CSIO (Central Scientific Instruments Organization), CSIR, Chandigarh
E-mail : aashisharma664@gmail.com

Lanthanide nanoparticles are well studied because of their wide range of potential uses due to their visible and near-IR luminescent properties. They show more peculiar magnetic properties because of the magnetic anisotropy arising from the large spin-orbit coupling of 4f electrons. Amongst lanthanides nanoparticles, Gadolinium Oxide nanoparticlesis a promising host matrix for upconversion fluorescence because of its good chemical durability, thermal stability, and low phonon energy.In the Present, Gadolinium Oxide Nanoparticles has been synthesized using a reported procedure with slight modification. The resulting nanoparticles were then characterized by different techniques like UV-visspectroscopy, XRD, SEM and TEM etc. The Gadolinium Nanoparticles has been explored in the field of bioimaging, drug delivery, targeted diagnosis and therapeutics. Our future attempts will be carried out to explore their applications in the field of sensing.

PO-01 : A Novel Adsorbent : *Clitoria ternatea* Leaves, for Removal of Crystal Violet Dye from Aqueous Solution

D. J. Borkar[1], N. S. Rajurkar[2*] and P.V. Adhyapak[3]

[1]Department of Environmental Science, Savitribai Phule Pune University, Pune-411007
[2]Department of Chemistry, Savitribai Phule Pune University, Pune-411007
[3]Centre For Materials For Electronics Technology (C-MET), Pune-411008
E-mail : rnilima@rediffmail.com

Textile industry preferentially uses Crystal violet dye for colouring and printing purposes. This dye is toxic and mainly responsible for severe water pollution. The present study focuses on effective removal of crystal violet (C.V.) dye using *Clitoria ternatea* leaves as an adsorbent by batch adsorption process. Adsorption efficiency of *Clitoria ternatea* leaves was found to increase after chemical treatment of the leaves. The study revealed that effective removal of the C.V. dye (15 ppm), was found to be 96.4% at pH 7, contact time 90 min., adsorbent dose 0.01gm and particle size 105µm. The adsorbent was characterized using FESEM, EDX, FTIR, X-RD techniques before and after adsorption. Adsorption process was found to be spontaneous and endothermic in nature. It obeys pseudo second order kinetics and Freundlich adsorption isotherm.

PO-02 : Aqueous Extract of Neem (*Azadirachta Indica*) Leaves as Green Inhibitor for Corrosion of Brass in Nitric Acid Solution

B. B. Patel and R. T. Vashi*

Department of Chemistry, Navyug Science College, Rander Road, Surat-395005, Gujarat,
E-mail : bpatel846@yahoo.com

The inhibition of corrosion of brass in nitric acid Azadirachta Indica (*AI)* leaves was studied by using weight loss, effect of temperature, Polarization and Electrochemical Impedance Spectroscopic methods. Corrosion rate increases with the increase in acid concentration and temperature. As inhibitor concentration increase the percentage of inhibition efficiency (I.E.) increases. The value of Free energy of adsorption (ΔG^0_{ads}), heat of adsorption (Q_{ads}), Energy of Activation (Ea), Enthalpy of adsorption (ΔH^0_{ads}) and Entropy of adsorption (ΔS^0_{ads}) were calculated. The inhibition effect is discussed in view of *AI* molecules adsorbed on the metal surface and it obeys Langmuir adsorption isotherm. Polarization curve indicates that inhibitor act as mixed type and the I.E. was found up to 95.80%. Present study indicates that *AI* extract is a good inhibitor for the corrosion of brass in nitric acid medium.

PO-03 : Green Synthesis, Characterization, Photocatalytic, Fluoroscence and Antimicrobial Studies of Gum Kondagogu Capped Ag_2S NPs

Dasari Ayodhya and Guttena Veerabhadram*

Department of Chemistry, University College of Science, Osmania University, Hyderabad-500007
E-mail : ayodhyadasari@gmail.com

The study describes a simple and green method for the synthesis of silver sulfide nanoparticles (Ag_2S NPs) using gum kondagogu. The synthesized NPs were characterized by TEM, SEM, EDX, XRD FTIR, Fluorescence, UV-vis absorption, zeta potential and TG-DTA techniques. The optical properties and quantum confinement effect of the products were confirmed by means of spectroscopic measurements. Morphologies and sizes were obtained by SEM and TEM. The Ag_2S NPs were spherical in shape with an effective diameter size of 25 nm. The synthesized particles possess photocatalytic activity of various dyes under solar light and temperature effect was studied from 303 to 343 K. The apparent reaction rate was used to calculate the apparent activation energy of the decolouration process, E_a = 13.95 kJ/mol. The activation thermodynamic parameters (ΔG^*, ΔH^* and ΔS^*) were obtained from variable temperature kinetic studies. The photocatalytic property of Ag_2S NPs was also evaluated by the degradation of various dyes under solar light. The effect of Ag_2S on the photocatalytic degradation and influence of parameters such as Ag_2S loading, temperature and light on degradation are evaluated. The degradation reaction follows pseudo-first order kinetics. It was seen that 1.0 g/L of photocatalyst is an optimum dosage of photocatalyst. The interaction between Ag_2S NPs and bovine serum albumin (BSA) was studied by using fluorescence spectroscopic measurements. The synthesized Ag_2S NPs showed good antimicrobial activity against various gram positive and gram negative bacteria.

PO-04 : Kinetics of Base Hydrolysis of Tris(1,10-phenanthroline)Iron(II) Complex in the Presence of Mixed Surfactants of SDS and Triton X-100 : A Probe to Study Synergism and Catalytic Property of Mixed Micelles

V. Srikanth[1], P. Shyamala[2*] and A. Satyanarayana[2]

[1]Department of Basic Sciences & Humanities, Vignan's Institute of Engineering for Women, Kapujaggarajupeta, Visakhapatnam
[2]Department of Physical and Nuclear Chemistry & Chemical Oceanography, School of Chemistry, Andhra University, Visakhapatnam
E-mail : shyamalapulipaka06@gmail.com, shyamalapulipaka@rediffmail.com

Surface tension studies were carried on the binary surfactant mixtures over a wide range of Triton X-100 mole fractions and total surfactant concentrations to obtain critical micellar concentration values(CMC). These CMC values were used to determine the composition of the mixed micelles and the average interaction parameter (β) which contains all the interactions of the mixed surfactants. The method used to determine β is based on Rubingh's theory using a Gauss-Newton iteration technique written in FORTRAN by the authors. The value of β was found to be -0.69 indicating synergistic behavior ie., combined positive catalytic effect of both the surfactants. Hence catalytic property of mixed micelles was investigated by studying the kinetics of base hydrolysis of tris(1,10-phenanthroline)Iron(II) in the presence of Triton X-100/ SDS mixed micellar medium. The reactions have been carried out at various mole fractions of Triton X-100 and at different total surfactant concentrations of Triton X-100 and SDS (C_t). The results show that as $\alpha_{TX\text{-}100}$ increases the rate increases for all values of C_t. Kinetic analysis has been carried out by using a simple pseudophase model and binding constants were determined.

PO-05 : Voltammetric Study of Hydrochlorothiazide on Multiwalled Carbon Nano Tube Modified Carbon Paste Electrode

Purushothama H. T. and Y. Arthoba Nayaka*

Department of Chemistry, School of Chemical Science, Kuvempu University, Shankaraghatta - 577451, Karnataka
**E-mail : drarthoba@yahoo.co.in*

An electrochemical anodic behavior of hydrochlorothiazide (HCTZ) was studied by using multi-walled carbon nano tube modified carbon paste electrode (MWCNTCPE) using cyclic voltammetry (CV), differential pulse voltammetry (DPV) and differential pulse stripping voltammetry (DPSV). Two anodic peaks were observed at peak potential 829 mV and 1070 mV on MWCNTCPE at phosphate buffer (pH 7.0). DPV and DPSV shows good linearity in the concentration range 0.5 to 20 µM and 0.1 to 1 µM, respectively. The limits of detection were found to be 0.5637 μML^{-1} and 0.2398 μML^{-1} respectively. Surface area, sensitivity and electron transfer kinetic parameters were studied. This method can be applied to investigate HCTZ in the pharmaceutical and in urine sample.

PO-06 : Probing the Nature of Molecular Interactions between 1-Ethyl-3-methylimidazolium Methylsulfate and Higher Chain Alcohol : Volumetric and Acoustic Studies

V. Govinda, K. Sreenivasulu, P. Kiran Kumar, E. E. Ebenso and I. Bahadur*

Department of Chemistry and Material Science Innovation & Modelling (MaSIM) Research Focus Area, Faculty of Agriculture, Science and Technology, North-West University Mafikeng Campus, Private Bag X2046, Mmabatho 2735, South Africa
**E-mail : bahadur.indra@gmail.com; bahadur.indra@nwu.ac.za*

The knowledge of molecular interactions of ILs mixture are essential for many of industrial applications due to an amazing and wide variety of desirable properties of ionic liquids. In this regards, present work reported the thermophysical and thermodynamics properties of binary mixtures containing ionic liquid 1-ethyl-3-methylimidazolium sulfate [C_2mim][$MeSO_4$] with higher chain alcohol at various temperatures under ambient pressure using the sophisticated thermodynamic techniques. In this work densities and speed of sound of three binary mixtures such as 1-ethyl-3-methylimidazolium with 1-heptanol, 1-octanol or 1-nonanol were measured in the temperature range from 25 to 35 ^{0}C and under ambient pressure over the entire range of composition. The excess molar volumes (V^E) and excess isentropic compressibilities (κ_s^E) were evaluated by using the experimental data at experimental condition. From all the systems studied, we have observed that positive to negative V^E values for the systems [C_2mim][$MeSO_4$] with 1-heptanol or 1-octanol whereas the positive V^E values observed for the system [C_2mim][$MeSO_4$] IL with 1-nonanol. Negative κ_s^E values obtained for the systems [C_2mim][$MeSO_4$] with 1-heptanol or 1-octanol except higher composition of 1-octanol and positive κ_s^E values for the system [C_2mim][$MeSO_4$] with 1-nonanol at all temperatures. From the obtained results, a discussion was carried out in terms of interactions and structure factors in these binary liquid mixtures.

PO-07 : Synthesis and Characterization of Hexagonal Prism Shaped ZnO Nanoparticle Prepared Through a Microwave Combustion Method

Yathisha R. O. and Y. Arthoba Nayaka*

Department of Chemistry, School of Chemical Science, Kuvempu University, Shankaraghatta - 577451, Karnataka
**E-mail : drarthoba@yahoo.co.in*

The synthesis and study of semiconducting nanostructure

materials have become a considerable interdisciplinary area of research over the past few decades. The present work outlines the synthesis of ZnO nanoparticles via microwave combustion method without using any fuel. The crystal morphology, optical and electrical properties were characterized by X-ray diffraction study (XRD), UV-Visible spectroscopy (UV-Vis), Field emission scanning electron microscopy (FE-SEM), Energy-dispersive analysis using X-rays (EDAX), Transmission electron microscopy (TEM) and Photo-conductivity technique. X-ray diffraction analysis confirms the formation of pure wurtzite ZnO phase with crystallite size in the 38-62 nm range. Scanning electron micrographs shows the hexagonal prism structure of ZnO nanoparticles. EDAX confirms the existence of Zn and O in ZnO. The optical properties and tauc plot studies were performed by UV-Visible spectroscopy. I-V characterization study was performed to determine the electrical property of ZnO films.

PO-08 : Physico-Chemical Studies on Miceller Properties of Dysprosium Soaps in Benzene-Methanol Liquid Mixture

Amit K. Agarwal*, M.K. Rawat and Sandhya Agarwal

Department of Chemistry, Agra College, Agra-282002 (U.P.)
B. R. Ambedkar University, Agra
E-mail : akagarwal.chem@gmail.com

The density, viscosity and conductivity measurements of Dysprosium soaps (Myristate, palmitate and stearate) have been made to study the miceller 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 and atomic number of metal ions. 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 of density an d viscosity measurements have been explained on the basis of the equation proposed by Einstein, Moulik, Vand and Jones-Dole and other well-known equations.

PO-09 : Synthesis and Characterisation of Magnesium, Zinc and Copper Metal Oxide Nanoparticles and their Photocatalytic / Antimicrobial Applications

Manisha Y. Khaladkar[1] and Deepali P. Butala[2]

[1]Applied Science Lab, College of Engg Pune, Pune, Maharashtra
[2]Dept of Chemistry, S. P. College, Pune, Maharashtra
E-mail : myk.appsci@coep.ac.in, deepali.butala@gmail.com

In the present study different metal oxides (Magnesium, zinc and copper) nanoparticles were synthesized using two different methods wet chemical method and hydrothermal method. In the preparation by **wet chemical method** the nitrates of the respective metals were dissolved in 100 ml of water to which NaOH Solution was added dropwise leading to generation of metal hydroxides. These hydroxides are calcined in furnace at 600 and oxide nanoparticles were obtained. In the **hydrothermal** method acetate salt of the metal dissolved in methanol was reacted wih sodium hydroxide in a Teflon lined sealed autoclave and heated at 100 under pressure for 6 hours. These Nanoparticles were characterised using FESEM, EDAX and XRD to investigate their structural and morphological studies. The particles were tested for their antimicrobial and photocatalytic activity.

XRD data was used to calculate the particle size using Scherrers formula and it was found in the nanorange. **SEM** analysis showed metal oxide particles in the nanorange with varying morphology. Zinc oxide nanoparticles were in the range 70-150nm with spherical shape, whereas for MgO most of the nanoparticles are in the range 10-20 nm with spherical morphology. CuO nanoparticles showed rodshaped/ellipsoid morphology. **EDAX** confirms the presence of metals zinc, Mg and Cu in the samples.

The **photocatalytic activity** of ZnO, MgO and CuO nanoparticles were investigated by the degradation of methylene blue dye in aqueous medium under natural sunlight. Results indicate that MgO nanoparticles having better photocatalytic efficiency under natural sunlight irradiation than ZnO and CuO nanoparticles .(may be due to smaller particle size.). Antibacterial study was carried using E coli and S aureus.

Thus a very simple, cost-effective technique for development of nanoparticles was used. No specific conditions need to be maintained.

PO-10 : Vibrational Energy Exchanges at Highly Engineered van der Waals Surfaces

Matukumilli V. D. Prasad[1*] and Baidurya Bhattacharya[2]

[1]Advanced Technology Development Centre, Indian Institute of Technology Kharagpur (W.B.)
[2]Civil Engineering Department, Indian Institute of Technology Kharagpur (W.B.)
[*]E-mail : mvdprasad@iitkgp.ac.in

The phonon is the quantized mechanical vibration describing the fundamental transport mechanism of everyday sound and heat. Precise control of energy exchanges by developing the ability to

manage phonon spectrum is important across various research areas, including themoelectrics, phononic crystals, nanomechanical devices and bio-chemical systems. The nature of phonon propagation and its interfacial scattering are often poorly understood as the control of individual phonons *in situ* remains extremely challenging. The present study is based on classical molecular dynamics, where the phonon pulse is generated on a carbon nanotube either as spatial or spatiotemporal Gaussian wavepacket. We investigate how the propagating phonon of well-defined frequency and polarization interacts with the interfaces such as defects or co-axially placed other nanotube via van der Waals interactions. The computed phonon transmission coefficients and visualized scattering events at different interface scenarios present the mechanistic understanding of non-Fourier type heat conduction. We show that the modified coherent phonon pulse approach provides unprecedented opportunities for simulating coherent phonon excitations in the femto-second laser experiments leading to a potential tool for manipulation of energy transport and better design of functional nano-bio-devices.

PO-11 : C-C Bonding NIR and C-N Bonding Visible Absorbing Squaraines : A Computational Study

Prabhakar[*] and Anuj Thripati

Department of Chemistry, National Institute of Technology
Kurukshetra-136119, Haryana
[*]E-mail : chetti@nitkkr.ac.in

Squaraines are class of novel functional organic dyes and are derived from squaric acid (1, 2-dihydroxy cyclobutene -3,4-dione). These dyes play a crucial role in the design of a variety of photonic materials that are used for applications such as imaging, nonlinear optics, photovoltaics, biological labeling, and photodynamic therapy. In solution squaraine dyes exhibit sharp and intense absorption from visible to near infrared (NIR) region depending on substitution at 1, 3 position of squaric acid. The donor substituent at 1,3 position of squaric acid directly bonded either with Nitrogen (C-N bonding, break in conjugation) or with Carbon (C-C bonding, conjugated back bone). The C-N bonding squaraine dyes are having absorption in visible region (300 - 500 nm) with extinction coefficient ³ 10^4 cm^{-1} M^{-1}. Whereas C-C bonded dyes are having absorption in the range of 600 nm to 900 nm (visible- NIR region) with high extinction coefficient ³ 10^5 cm^{-1} M^{-1}. Larger extinction coefficient and red shifted absorption in later dyes (C-C bonding) when compared with former dyes (C-N bonding) has been studied by

DFT method and are due to presence of diradicaloid character along with extensive conjugation in back bone of the molecule in C-C bonding molecules.

Such as the melting points, glass transition temperatures, crystallinity, moisture/volatile content, thermal/oxidative stability, purity, decomposition temperatures by TG-DTA-DSC modes.

Barium and tin containing sulphate and carbonate are important industrially utility material which was prepared by in situ deposition technique and PVDF containing nanocomposites films by the solution-mixing technique physical properties were obtained by Thermal studies. The thermal properties were investigated using thermogravimetry/differential thermal analysis (TG/DTA) and differential scanning calorimetry (DSC) techniques.

In most of the nanocomposites shows increase in Td, and abnormal behaviour of Tg, which indicates that the physical properties obtained through Thermal analysis provides brief ideas regarding the introduction of filler in the matrix for the suitable properties of the nanocomposites and hence for its industrial applications.

PO-12 : Squarylium Dyes as Molecular Materials : A Case Study Through Computational Chemistry

G. Krishna Chaitanya* and Sandesh U. Mutkule,

School of Chemical Sciences, S.R.T.M. University, Nanded-431 606
E-mail : krishnachaitanya.gunturu@gmail.com

Computational chemistry based on quantum chemical theories, which are replacing the earlier empirical rules, is playing a major role in understanding the dyes post priori experiment or in suggesting modifications, a priori synthesis, suitable to the applications. Recent studies of organic dyes have concentrated in the absorption range greater than 1000 nm, as these are useful in telecommunications, medicine, semiconductor lasers, and so forth. Because these absorb in the near-infrared region, these dyes are also referred to as NIR dyes. Herein, a class of organic functional dyes have been considered as a case study to emphasis on the advantages of Computational Chemistry to the participants. Conventionally, Near Infrared absorbing Squarylium (SQ) dyes dyes were known as D–A–D type of systems and it was believed that the donor (from the side substituent) and acceptor (central four-membered ring and the carbonyl oxygens) abilities will influence their absorption spectrum.In contrast, from our earlier calculations through high level ab initio and density functional theory (DFT)

calculations, the biradicaloid character (BRC) of these dyes has been unveiled and it has been shown that the orbital interactions and the C–C–C angle in the central ring of SQ are playing a major role in their near infrared (NIR) absorption rather than D–A–D phenomenon. Systematic studies on semi-SQ, symmetrical and unsymmetrical SQ and core-substituted (CSQ) derivatives by using ab-initio and DFT methodologies have been presented in this report.

PP-CYSA-01 : Hierarchical Synthesis of Silver Monoliths and their Efficient Catalytic Activity for the Reduction of 4-Nitrophenol to 4-Aminophenol

Mustri Bano* and Farid Khan

Nanomaterials Discovery Laboratory, Department of Chemistry, Dr. H. S. Gour Central University, Sagar – 470003
**E-mail : mustribano1@gmail.com*

A novel catalyst Ag/triton X-705/SiNPs is synthesized by modified sol-gel method without the use of acid or base as catalyst for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) in presence of 0.1M $NaBH_4$ in aqueous media. The reduction time was 30-35 seconds is a function of concentration of 4-NP varied from 0.001M to 0.009M at a constant concentration of Ag/Triton X-705/SiNPs 0.006g. Fe_3O_4NPs, dextran, and trimethylbenzene (TMB) were added separately to Ag/Triton X-705 hydrogel to modify their morphology and catalytic activities against the reduction of 4-NP to 4-AP. The as synthesized monoliths were characterized by FT-IR, TGA, PXRD Analysis, SEM, TEM and (BET) surface area analyzer. Pseudo first order rate constant (k), energy of activation (E_a), and thermodynamic parameters viz. activation enthalpy ($DH^{\ddagger}$), activation Gibbs free energy ($DG^{\ddagger}$) and entropy of activation ($DS^{\ddagger}$) have also been determined. The turn over frequency (TOF) of Ag/Triton X-705/SiNPs catalyst was 9.66 $\times 10^{20}$ molecules/sec and the catalyst used up to nine cycles successfully with greater efficiency claimed to be a potential and leading candidate for the industrial conversion of 4-NP to 4-AP. We claimed that the catalyst Ag/Triton X-705/SiNPs took almost minimum time for the reduction of 4-NP to 4-AP.

PP-CYSA-02 : Synthesis and Florescence Studies on Sulphonic Acids Doped PANi-PVA Thin Films and Quenching with Picric Acid

Parvathi[1] and A.Venkataraman[1, 2*]

[1]Materials Chemistry Laboratory, Department of Materials Science, Kalaburagi-585106, Karnataka
Department of Chemistry, Gulbarga University, Kalaburagi – 585106, Karnataka.

Polyaniline (PANi) doped with sulphonic acids acids has been

prepared by chemical oxidation method. PANi-PVA thin films containing different concentrations of Aniline and organic acids are synthesized through the chemical oxidative polymerization of aniline using ammonium persulphate as an oxidant. The synthesized films are characterized by employing (FTIR) Spectroscopy and X-Ray Diffraction (XRD) for understanding the details of structure of the PANi-PVA thin films. Morphology study was carried out by employing Scanning Electon Microscope (SEM). Thermo gravimetric analyses (TGA) of the films are carried out to study the stability of polymer thin films. Fluorescence of these synthesized films and quenching studies by employing Picric acid (PA) are carried out and the results are reported in this paper.

PP-CYSA-03 : Fabrication, Characterization and Optimization of Cyclodextrin Grafted Soft Assemblyto Study the Stability and Chemo-Effective Effect of Benzyl Isothiocyanate

Shivani Uppal, Khushwinder Kaur and S. K. Mehta

Department of Chemistry, Panjab University -160014, Chandigarh
E-mail : Shivaniuppal21@gmail.com

An innovative process for preparation of inclusion complex (IC) using ultrasonication of Benzyl Isothiocyanate (BITC) has been developed and optimised. The development process included investigation of inclusion behaviour, characterisation and an in-depth study of thermal and UV stability of BITC with β-CD and hp-β-CD. The encompassment in CDs helped to overcome the hindrance of low solubility and high volatility of BITC which is a potential anticancer and antimicrobial agent. The strategy involved exploitation of the process of sonication in laboratory which evidently saved time and energy consumption. Phase solubility along with Gaussian studies proved the formation of 1:1 complex. The physical nature and stability of IC was proved with XRD and UV-visible absorption spectroscopy respectively. TGA analysis showed that the thermal stability of BITC got enhanced in the presence of CDs. Investigations of thermodynamic parameters confirmed the stability of ICs. Both β-CD and hp-β-CD based ICs retained the antimicrobial property of the free BITC, indicating their potential utility as antimicrobial agents.

PP-01 : Preparation and Characterization of Polypyrrole-Tin Oxide Nanocomposite via Interfacial polymerization

Parvati[1], Mahesh D.Bedre[2], Raghunandan Deshpande[3], Arunkumar Lagshetty[4] and A. Venkataraman[1*]

[1]Materials Chemistry Laboratory, Department of Materials Science, Gulbarga University, Gulbarga-585106, Karnataka
[2]Mahesh College of Science, Gulbarga-585103, Karnataka
[3]H.K.E College of Pharmacy, Sedam Road Gulbarga-585101
[4]Appa Institute of Technology, Gulbarga-585101, Karnataka
E-mail : raman_chem@rediffmail.com

Polypyrrole-tin oxide (Ppy-SnO_2) nanocomposites of ~100 nm size were prepared by employing interfacial polymerization method using ammonium persulphate as an oxidizing agent. The bonding nature of the SnO_2 with polymer is understood by the FTIR technique. Crystalline nature of composite is confirmed by the XRD. Morphological studies understood by scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). D.C conductivity suggests the Conducting behavior of composites. The properties of polymer semiconductor materials can easily be tuned to its desired application through the variation of particle size, shape and distribution of nanoparticles.

PP-02 : Study of Oligomeric Structure and Chaperone Activity of α-crystallin Under Heat Stress Condition

Sudipa Saha[*]

Department of Biotechnology, St. Xavier's College, 30 Mother Teresa Sarani, Kolkata-700 016 (West Bengal)
E-mail : sahasudipa74@yahoo.co.in

α-Crystallin is the principal protein constituent of vertebrate eye lens and exists as a large oligomer of two subunits, αA- and αB-crystallin. α-Crystallin exists in solution as a polydisperse high molecular mass aggregate with a molecular weight distribution ranging from 300,000 to over 1 million. It is seen that despite the enormous number of studies on the structure of α-crystallin, the oligomeric sructure of α-crystallin is still the subject of much debate and speculation. Although most chaperones are oligomers, whether oligomerization is absolutely required for protein stability or for chaperone function is not yet established. We studied to determine the relationship between oligomeric structure and chaperone activity of α-crystallin. Gel fitration experiment showed that α-crystallin existed as low and high molecular mass species. Progressive pre-incubation to higher temperatures dissociated the high molecular mass species to the low molecular mass species. We

observed the same finding by the light scattering experiment. Our results also indicate that simple storage of α-crystallin may lead to formation of high molecular weight aggregated α-crystallin which has very low chaperone activity. The loss of chaperone activity may be prevented if its association into larger oligomer can be stopped.

PP-03 : Molecular Interactions in Binary Mixtures Containing Halo-Substituted Carbonyl Compound + n-Alkanols + Alkoxy Alkanols + Amines + Xylenes at Various Temperatures

M. Radha Sirija, N.Gayathri Devi, Ch.Vijayalaxmi, Sd. Kasim Sharif and D.Ramachandran*

Department of Chemistry, Acharya Nagarjuna University, Guntur- 522 510
E-mail : sireeja.maganti@gmail.com, dittakavirc@gmail.com

Densities, viscosities and ultrasonic velocities of binary mixtures containing halo-substituted carbonyl compounds with n-alkanols, alkoxy-alkanols, amines, and xylenes were measured at various temperatures and ambient pressure. From experimental data, parameters were calculated. The obtained values were fitted to the Redlich-Kister equation. The parameters of excess functions are found sensitive for the intermolecular interactions between the binary mixtures. Theoretical values of viscosity of the binary mixtures were calculated using empirical relations and theoretical equations. The relative merits of these relations and theories were discussed.

PP-04 : Chemical Modelling Studies on the Interaction of Succinic Acid Dihydrazide with Some Divalent Metal Ions in Aqueous Medium

Uma Rani Bhagavatula, Shyamala Pulipaka* and Satyanarayana Atreyapurapu

Department of Physical and Nuclear Chemistry and Chemical Oceanography, School of Chemistry, Andhra University, Visakhapatnam -530003
**E-mail : shyamalapulipaka06@gmail.com*

Chemical modelling studies on the metal-ligand binary systems of succinic acid dihydrazide (L) with toxic metal (M) ions Pb^{2+}, Hg^{2+} and Cd^{2+} were carried out potentiometrically using Calvin-Wilson titration technique in aqueous medium at an ionic strength of 0.1M and temperature 303K. The data were analyzed using the Miniquad-75 computer program and species distribution diagrams were generated using the HYSS program. The best-fit models obtained include mononuclear protonated, ML_2H_2, ML_2H, MLH and deprotonated MLH_{-1}, ML_2H_{-1}, ML_2H_{-2} species besides simple ML and

ML_2 type of complexes. In solutions of 2:1 (metal to ligand) molar composition, formation of homo binuclear species of type M_2L and M_2LH_{-2} was observed in which the dihydrazide molecule acts as a ditopic ligand.

PP-05 : Corrosion Prevention of Zinc by Aniline in Sulphuric Acid

S. A. Zele[1] and R. T. Vashi[2*]

[1]Department of Chemistry, B.K.M. Science College, Valsad (Gujarat)
[2]Department of Chemistry, Navyug Science College, Rander Road, Surat – 395009, Gujarat
E-mail : vashirajendra@yahoo.co.in

Corrosion of Zincin sulphuric acid and inhibition efficiency of aniline has been studied by weight loss method, polarization technique and Electro Impedance Spectroscopy (EIS). Corrosion rate increases with the concentration of acid and the temperature. Inhibition efficiency (I.E.) of aniline increases with the concentration of inhibitor while decreases with the increase in concentration of acid. As temperature increases corrosion rate increases while percentage of I.E. decreases. A plot of log (θ/1-θ) versus log C results in a straight line suggest that the inhibitor cover both the anodic and cathodic regions through general adsorption following Langmuir isotherm. Galvenostatic polarization curves show polarization of both anodes as well as cathodes.

PP-06 : Nanoparticles Derived from Metal Functionalized Surfactant : Synthesis, Characterization znd Nucleic Acid Binding Studies

Rekha, S. K. Mehta and G. Kaur

Department of Chemistry, Panjab University-160014, Chandigarh
E-mail : bharrekhasonia@gmail.com

Copper hybridized cetylpyridinium chloride complex (Cu@CPC) has been utilized for the fabrication of copper nanoparticles. Aqueous solution of Cu@CPC and ascorbic acid (greener reducing agent) in appropriate molar ratio was mixed and refluxed overnight at 80°C. Thus synthesized nanoaprticles were well characterized through different spectroscopic and analytical techniques like UV-vis, FTIR, TEM, SEM, DLS and EDX etc. However central aim of the present research work is to study the effect of nanoparticles on calf thymus DNA. Fluorescence quenching of ethidium bromide intercalated DNA and UV-vis absorption behavior of DNA in the presence of Copper nanoparticles indicated that nanoparticles interacted through complex formation. Absorption and fluorescence

data further utilized for evaluation of binding constant, number of binding sites and various thermodynamic parameter like ΔG, ΔH, ΔS. Additionally binding will be explored through DNA gel electrophoresis, cyclic voltammetry and circular dichroism etc.

PP-07 : Inhibition Effect of Potassium Dichromate on the Corrosion of Aluminium in Phosphoric Acid

K. N. Rathod and R. T. Vashi

[*]Department of Chemistry, Navyug Science College, Rander Road, Surat-395005, Gujarat
[*]E-mail : khyatirathod65@yahoo.co.in

The inhibition effect of potassium dichromate on the corrosion of aluminium in phosphoric acid was investigated by weight loss method, potentiodynamic polarisation, Electrochemical impedance measurement and Scanning electron microscope (SEM). It was conclude that inhibition efficiency (I.E.) increased with the increasing concentration of inhibitor. The investigation of adsorption isotherm indicate that the inhibitor fit Langmuir adsorption isotherm, fairly good. The phenomenon of physisorption is attributed to the values of E_a, Q_{ads} and ΔG^0_{ads}. The potentiodynamic polarisation results reveal that the inhibitor act as mixed type and predominantly anodic inhibitor. I.E. of inhibitor was found almost similar by weight loss method, polarisation as well as EIS methods.

PP-08 : The Next Big Thing is Very Small

Veronica Deekala and Rudraraju Ramesh Raju[*]

Department of Chemistry, Acharya Nagarjuna University (AP)
E-mail : rrraju1@gmail.com, veronicakaladhar3@gmail.com

Nanotechnology, one of the cutting-edge technologies of the 21st century, is multidisciplinary and covers many fields, including Chemistry, Physics, Material sciences, Engineering, Biology and even Medicine. One major merit of using Nanotechnology is that one can control and look for tailor made properties in a very predictable manner to meet the need of specific applications. Nanotechnology is an advanced technology, which deals with the synthesis of nanoparticles processing of the nano materials. Nanoparticles can be classified as nanotubes, Nanowires, Nanoshells, Quantumdots, Nanopores, Nanorobots. Nanotechnology research fields require a high degree of precision in both observing and manipulating materials at the atomic level. Nanorobots are nano electrochemical systems designed to perform a specific task with precision at Nanoscale dimensions. The advanced Nanorobotics technology needed to manipulate materials at this scale, a million times smaller than a grain of sand, will be developed in the new

nanorobotics groups. The integration of different technologies to act as simultaneous real-time nanoscale 'eyes' and 'hands', including the advanced nanorobotics, high-resolution ion/electron microscopy, image processing/vision control and sophisticated sensors, will lead to the ability to manipulate matter at the scale of atoms(or) molecules. The main element used will be carbon in the form of diamond /fullerene nanocomposites because of the strength and chemical inertness of these forms. Nanorobots could also carefully scan the structure of our brain, providing a complete readout of the connection. Nanorobots are tiny machines used to cure disease in human or in any organism performs task at nanoscale dimensions.

PP-09 : The Behaviour of Physical Parameters Due to Nano-filler in Polymer Nanocomposites Through Thermal Studies

Gautam Jaiswar

Department of Chemistry, Dr. B.R. Ambedkar University, Agra
E-mail : gjaiswar@gmail.com

Polymer nanocomposite (PNCs) and conventional reinforced polymer both are different, microscopic organic and inorganic filler are incorporated in polymer matrix. PNCs are the combinations of strength, stiffness, and weight that cannot be expressed separately from the individual components. PNCs properties are directly depends on the polymer matrix properties, the interaction between polymer matrix and nano filler, properties of nano fillers and their surface free energy and surface area of the interfacial bonds. The aspect ratio of the dispersed nano fillers in polymer matrix and the loading level of nano filler define the area of interfacial bond. Thermal method of characterisation provides important role in choosing the nanoparticle in the matrix for the suitable properties of polymer nanocomposites, by determining the physical parameter

PP-10 : Variation of Physical Parameters of Infected Blood Samples with Combination of Different Medicinal Plants

Supriya Kate

Research Scolar JJT University Jhunjhunu, Rajsthan

Medicinal plants are those plants that are used (parts, extracts etc) in treating and preventing specific ailments and diseases that affects human being. There are several species of medicinal plants in that basil, zinzeber, azardica indica, curcuma longa, cerica papaya, Allium staviumum are having very unique medicinal properties. These all species individually differ in their medicinal as well as

chemical properties. This research is on comparative study of different physical parameters like pH, critical solution temperature, and boiling point ets with their different combinations. Also the comparative study of these parameters with combination of infected blood samples.

PP-11 : Densities and Viscosities of Binary Mixtures of 1, 4-Dioxane with 1-Propanol and 2-Propanol at 25 and 35^{0}C

Prashant Pachauri, M. K. Rawat and Rita Dixit

Dept. of Biotech, Agra College Agra- 282002
E-mail : prashantaca2013@gmail.com

Densities and Viscosities for 1,4-dioxane with 1-propanol and 2-propanol mixtures have been measured as a function of mole fraction at atmospheric pressure at 25 and 35^{0}C. The calculated excess volume (V^E) are positive over the entire range of composition in both systems. The V^E data were fitted by means of a Redlich-Kister type equation. The magnitude of these experimental quantities is discussed in terms of the nature and type of intermolecular interactions in binary mixtures. When available, the results have been compared with literature values.

PP-12 : Ocimum basilicum (Tulsi) Leaves Extract as Corrosion Inhibitor for Corrosion of Aluminium in Hydrochloric Acid

N. I. Prajapati* and R. T. Vashi

Department of Chemistry, Navyug Science College, Rander Road, Surat-395005, Gujarat
E-mail : 6haprajapati@gmail.com

The corrosion of Aluminium in hydrochloric acid and its prevention by Ocimum basilicum has been studied. Corrosion behaviour of aluminium was stuied in absence and presence of hydrochloric acid using Ocimum basilicum as green inhibitor by applying various methods like weight-loss, effect of temperature, galvanostatic polarization, electron impedance spectroscopy. Corrosion loss increases with the increase in acid concentration and with increase in temperature. The inhibition efficiency (I.E.) of inhibitor was increases with increases in inhibitor concentrations. As temperatures increases percentage of I.E. decreases. The values of activation energy (E_a), free energy of activation (ΔG_a), Heat of adsorption (Q_a), enthalpy of adsorption (ΔH_a) and entropy of adsorption (ΔS_a) were calculated. Polarization study indicates that inhibitor act as cathodic typed inhibitors.

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