ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

Sectional President's Address

AIL-01 : Mesoporous Materials : Chemistry Perspective

I. Ajit Kumar Reddy
Department of Chemistry, National Institute of Technology Warangal, Warangal - 506004
E-mail : iakreddy@nitw.ac.in

Porous materials are classified according to IUPAC standards based on the range of pore diameter as Microporous Materials (< 20 Å), Mesoporous Materials (20 Å to 500 Å) and Macroporous Materials (> 500 Å). Due to smaller pore diameter microporous materials have limited applications. Mesoporous materials have special features like very high surface area (200-1000 m^2g^{-1}) and tunable pore characteristics and hence have been subject of intense research by chemists and physicists world over. Large number of chemists are currently engaged in investigating the applications of mesoporous materials in various green procedures particularly as adsorbents and catalysts. Our group is involved in synthesizing functionalized mesoporous materials, characterizing them and studying their catalytic applications towards degradation of dyes, gas and liquid phase oxidation conversions and synthesis of organic compounds. Major advantage of these materials is their heterogeneous nature. They can be easily separated from the reaction mixture by simple filtration at the end of the reaction.

Mesoporous aluminosilicates produced by the mobil oil corporation, called MCM with their high surface area and nanometer sized pores make them ideal candidates for catalytic applications. Keeping this in view, we have synthesized various metal incorporated mesoporous MCM-41 and amino phosphate molecular sieves and characterized them by various analytical techniques such as PXRD, SEM, FTIR and N2 adsorption-desorption studies. These techniques reveal the mesoporous character of the synthesized materials with regular arrangement of pores.

Pollutants from the industrial effluents cause serious damage to the environment. It is important that chemists find ways to reduce and eliminate these pollutants by environmental friendly methods. In this direction, we have investigated the applications of functionalized mesoporous materials towards degradation of textile dyes such as Crystal violet and Rhodamine B. Effect of parameters such as pH, concentration of the oxidant and catalyst dosage on the degradation is studied for establishing the optimum conditions for dye degradation. Studies on reusability of these materials as catalysts for dye degradation revealed that they can be employed for several cycles without loss of activity.

AIL-02 : National Facility for Analytical Instrumentation : A growth Marker for Small and Medium Pharma Industries

Anamik Shah

National Facility for Drug Discovery through New Chemical Entities (NCE's) Development and Instrumentation Support to Small Manufacturing Pharma Enterprises, Saurashtra University, Rajkot, Gujarat
E-mail : anamik_shah@hotmail.com

The globalization, particularly in pharma, chemical, and other allied industries has created a new challenge predominantly for small and medium scale industries. And though they have contributed a lot in GDP of Gujarat state and nation as well, their survival has become a big challenge in last decade. Looking to the scenario, Saurashtra University has taken several initiatives with augmenting resources from Department of Science & Technology - New Delhi, Government of Gujarat and Government of India. The current talk will be a sharing of pleasant innovative experiences done successfully at Saurashtra University for training human manpower, improving curriculum activities and helping small & medium scale industries in the critical area of R&D, Process Chemistry, and Analytical Support. Few case studies about managing resources in more plausible manner will be discussed in the talk.

AIL-03 : Photocatalysis : An Emerging Technology with Green Chemical Approach

Rakshit Ameta

Department of Chemistry, Pacific College of Basic & Applied Sciences, PAHER University, Udaipur - 313024 (Raj.)
E-mail : rakshit_ameta@yahoo.in

Water is utmost necessary for the survival of the mankind on this planet Earth, but it is being contaminated by rapidly increasing urbanization, transportation, industrialization, etc. It is further supported by pressure of increasing population. Many industries discharge their effluents either without treatment or with some very simple treatment into the nearby water resources. This has resulted into contamination of water creating scarcity of potable water. Various methods have been tried for the decontamination of this polluted water. Here, photocatalysis has entered the scene and emerging as an eco-friendly pathway to solve this problem.

Basics of photocatalysis will be discussed along with its multi-faceted applications covering a wide range like purification of water, synthetic applications, disinfections, combating against dreadful diseases, solving the problem of energy crisis, etc. Photocatalysis provides a simple way to generate electron-hole pair, which can serve the purpose of oxidation and/or reduction. Such a condition is very difficult to obtain otherwise. It is emerging as a prospective technology and the time is not far-off when this process will become economically viable. Some countries have already started commercializing applications of photocatalysis for different useful purposes.

AIL-04 : Analysis of Water Parameters and Study of Removal of Fluoride Using Mesoporous Materials

K. K. Tiwary and R. R. Jha

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

Physico-chemical studies of ground water samples both from bore wells and dug wells of Daltonganj block areas of Palamau district of Jharkhand have been carried out for various parameters in general and that of fluoride concentration in particular in pre-monsoon season of 2009. Though, generally ground water of both types of wells are of good quality but in certain areas it is confronted with slightly high concentration of fluoride causing dental fluorosis among children. In dug well fluoride concentration in 7 samples area are bit on higher side while in bore wells too, 7 samples are on higher and rest 7 are within lower limit. The other variables so far analysed are within permissible limit of WHO for portable water in both types of wells samples. The variation observed in various parameters are due to its geogenic origin, of the various parameters and also of the nature of depth of wells of different places in the present area.

A new type of mesoporous Zr-Phosphate was prepared for the removal of fluoride. The mesoporous material prepared is confirmed by its characterization by XRD which give its surface area and pore size distribution was confirmed by TEM. NMR and FTIR also confirmed its structure. A batch adsorption technique for investigating adsorption kinetic and equilibrium parameters and determining pH adsorption edges is applied. It is shown that the adsorption properties of mesoporous material for fluoride ion depend on the pH value and anion concentration. The adsorption of fluoride on the mesoporous material is found to be 90.4% at pH 3.0 the Frendlich model can describe the adsorption equilibrium data of fluoride. The sorption of the anions on the mesaporous material is a rapid process and the adsorption kinetic data can be simulated very well by the pseudo second order rate equation. The column performance is carried out to assess the applicability of the mesoporous material for the removal of fluoride ion from ground water with satisfactory removal efficiency. The desorption experiment shows that fluoride ion sorbed by the mesoporous column can be quantitatively desorbed with 5 ml of 0.50 mol/L NaOH at elution rate of 1 ml/min.

AIL-05 : *Chlorella sp.* based Biosensor for Selective Determination of Mercury in Presence of Silver Ions

Susheel K. Mittal and Jasminder Singh

[*]School of Chemistry & Biochemistry, Thapar University, Patiala, 147004
E-mail : smittal@thapar.edu

Whole cell biosensors are the focus of increasing interest worldwide as methods for detection of various pollutants like heavy metals, pesticides etc. In the present workwhole cell based biosensor is prepared by immobilizing *Chlorella* sp. microbes over glassy carbon electrode for determination of mercury in presence of potential interferents like silver and other heavy metal ions. Algae, *Chlorella* sp. was identified, cultured and sub-cultured, harvested by centrifugation and starved to induce maximum alkaline phosphatase activity, before immobilizing it on glassy carbon surface using bovine serum albumin as matrix and glutaraldehyde as crosslinker.The prepared biosensor was studied as working electrode using chronoamperometric and cyclic voltammetry with a potentiostat using platinum electrode and a saturated Ag/AgCl electrode as counter and reference electrodes, respectively. Mercury and silver were used for testing in this work.Studies for interference was carried out by adding metal ions like Silver, zinc, sodium, magnesium etc., in fixed concentration i.e 1×10^{-6} M to different concentrations of Hg^{2+} ions and their effect on the slope of Hg^{2+} ions was noted.

The proposed biosensor is optimized for characteristics like; substrate concentration, pH, response time, durability, etc. by immersing algae modified glassy carbon electrode in p-nitrophenyl phosphate as substrate with constant stirring. Entrapment of biomass in bovine serum albumin was confirmed using scanning electron microscopy. APA causes the production of electroactive p-nitrophenol from electroinactive p-nitrophenylphosphate which gets oxidized at glassy carbon electrode leading to the flow of current. The decrease in magnitude of the current generated for a given concentration of microbial cells can be related to the concentration of heavy metal ions. The electrode responds linearly in concentration range of 10^{-14} M to 10^{-6} M for mercury and showed the rare selectivity for it over silver, alkali metals, alkaline earth metals and transition metals with an expected life of 14 days.

AIL-06 : Development of Portable On-site Biosensors for Detection of Trace Levels of Small Molecular Weight Medical Diagnostic Markers, Endocrine Disruptors and Food Additives

K. Vengatajalabathy Gobi, K. Koteshwara Reddy, M. Satyanarayana and V. Rakesh

Department of Chemistry, National Institute of Technology, Warangal-506 004(A.P.)
E-mail : drkvgobi@gmail.com

Detection of small molecular weight analytes at trace levels has become increasingly important in a wide variety of fields such as industrial safety, quality control, food preservative and adultration, stimulant drug use and trafficking, military defence and medical diagnostic applications. Portable on-site analytical capabilities are essential to effectively manage the present day requisites. Biomolecular recognition elements were coupled with various physicochemical transduction elements to fabricate highly sensitive and selective biosensors capable of lab-on-chip, on-site portable analysis.

We have investigated electrochemical and surface plasmon resonance (SPR) methods to fabricate biosensors because of their potential advantages such as disposable sensor chips, low-cost transduction materials and portable miniature instrumentation. Enzymes, antibodies and molecular imprinted polymers were coupled with transducers as biomolecular recognition elements to fabricate the sensor systems. Surface modification of transducer elements with nanomaterials and nanoensembled surfaces to anchor the biomolecular recognition elements was optimized for better sensor performances. Electrochemical and SPR sensors for the detection of biomedical diagnostic markers, superoxide dismutase, cholesterol, creatinine and insulin, were developed for detection of trace levels of physiological concentrations. Interference due to the presence of homologous compounds, proteins and potential electroactive molecules were investigated and controlled to achieve better sensor performances. Surface modification techniques, analytical range, sensitivity, selectivity, strategies and analysis in artificial physiological samples would be discussed in detail.

AIL-07 : New Reversed–Phase Thin Layer Chromatography System for Resolution of Coexisting Nickel Cobalt and Copper Ions from Aqueous Solution

Ali Mohammad

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

A novel thin layer chromatography (TLC) system comprising of stannic arsenate ion exchanger gel mixed with silica gel in 10:1 ratio by weight impregnated with tributyl phosphate (0.2M) as stationary phase and aqueous potassium thiocyanate (0.1M) as mobile phase has been identified most favourable for providing well resolved spots of Co^{2+}, Ni^{2+} and Cu^{2+} from their mixture. Semiquantitatively determination of Ni^{2+} in industrial Waste water was also possible.

In search of efficient layer materials for thin layer chromatographic studies of transition metal cations inorganic ion exchanger gels have been blended with silica gel. The mixed gels have been tested on-plate identification of coexisting heavy metals with preliminary separation by reversed-phase thin layer chromatographic procedures. The experimental conditions were optimized for getting best possible results in terms of detection clarity, spot compactness and separation efficiency. The comparison of results obtained by normal phase-TLC using silica gel, inorganic ion exchanger and mixed silica-ion exchanger, flat bed clearly demonstrate the effectiveness of mixed phase. Further the better chromatographic performance of mixed silica gel- inorganic ion exchanger gel impregnated with tributyl phosphate shows the superiority of reversed- phase in chromatography / TLC.

The essential requirements for better resolution were identified as:

(a) Mixed – bed composed of inorganic ion exchanger and silica gel.

(b) Presence of tributyl phosphate in stationary phase instead of its presence in mobile phase.

Presence of SCN^- ion in water was used as mobile phase for chromatography.

AO-CYSA-01 : Voltammetric Oxidation and Determination of Atorvastatin based on the Enhancement Effect of Cetyltrimethyl Ammonium Bromide at a Carbon Paste Electrode

Jyothi C. Abbar[1] and Sharanappa T. Nandibewoor[2]

[1]Dept. of Chemistry, Gogte Institute of Technology, Udyambag, Belgaum 590008
[2]P.G. Dept. of Studies in Chemistry, Karnatak University, Dharwad 580003
E-mail : jyothiabbar@gmail.com

The voltammetric behavior of an antihyperlipoproteinemic drug, atorvastatin (ATOR), at a carbon paste electrode (CPE) in the presence of an enhancing agent, cetyltrimethyl ammonium bromide (CTAB) has been investigated using cyclic and differential pulse voltammetry. The results indicated that the voltammetric response of ATOR was improved distinctly in the low concentration of CTAB suggesting that CTAB exhibits noticeable enhancement effect to the determination of ATOR. The dependence of the current on pH, concentration and scan rate was investigated to optimize the experimental conditions for the determination of ATOR. The anodic peak was characterized and the process was adsorption controlled. In the range of 0.05 µM to 10 µM, the current measured by differential pulse voltammetry presents a good linear property as a function of the concentration of ATOR with a detection limit of 4.08 nM with good selectivity and sensitivity. The proposed method was successfully applied to ATOR determination in pharmaceutical samples and for the detection of ATOR in urine as a real sample. This method can be employed in clinical analysis, quality control and routine determination of drugs in pharmaceutical formulations.

AO-CYSA-02 : Rapid Purity Determination of Some Commercial Drugs by Proton NMR Using Internal Standard Method

Chandu N. Potangale and Satish K. Pardeshi*

Department of Chemistry, University of Pune, Ganeshkhind, Pune-411007
E-mail : skpar@chem.unipune.ac.in

Proton NMR is used for the quantification of drugs by using internal standard method. In present study 1, 4-bis-trimethylsilanyl-benzene is used as an internal standard for analysis. This method demonstrated for quantification of some commonly used drugs like metaprolol, labetalol, methyl paraben etc. The drug samples were prepared in the 10-40 mM range and dissolved 600 µl in various NMR solvents with internal standard and proton NMR experiments were carried out. Simultaneously purity of drug samples was determined by HPLC analysis using method development for each sample. Results show that it is a good quantitative estimation method for drug purity,

and complies less than 1% deviation with HPLC analysis. This is quick quantification method for the determination of impurities within few minutes in drug molecules than HPLC under appropriate conditions. The method is also suitable for quantification of agrochemicals, fine chemicals, organic reaction intermediates, etc.

AO-CYSA-03 : Solid-Phase Extraction and Gas Chromatography-Mass Spectrometry for Trace Analysis of Organochlorine Pesticide Residues in Environmental Water Samples

K. Rama Mohan* **and K. Manohar**[1]

CSIR-National Geophysical Research Institute, Uppal Road, Hyderabad-500007
E-mail : krenviron@ngri.res.in, krngri@rediffmail.com

This study describes simple and suitable methodology for trace analysis of organochlorine pesticides (OCPs) in environmental water samples based on solid phase extraction (SPE) and gas chromatography-mass spectrometry (GC-MS). For this study, both parent compounds and degradation products were selected in order to understand their persistence and extent of contamination in the aquatic environment. The pesticide residues are detected in the low to sub-ppb range (0.001-0.004 µg/L) with good precision (average 6.5% RSD) and excellent extraction efficiency (81-96%, average 89.9%) for the majority of analytes. The developed methodology has been applied in a monitoring program of groundwater and surface water samples from Kazipally watershed, north-western Hyderabad city. The pesticides detected in the sampling program are HCHs, DDTs, and Cyclodienes. Pesticide contamination was investigated in both surface and ground water samples to assess their distribution trends in the study area. Among the ground water samples analyzed, 91% samples for DDT and 84% samples for HCH exceeded WHO recommended drinking water limits which is a matter of great public health concern.

AO-CYSA-04 : An Experimental and Theoretical Study on the Structural Properties of *N*'-[(*E*)-(5-chloro-2-hydroxyphenyl)methylidene] aceto-Hydrazide

A. V. Aparna [a], **Ch. Sarala Devi**[b]* **and D. A. Padmavathy**[c]

[a]*Department of Chemistry, Nizam College, Osmania University, Basheerbagh, Hyderabad*
[b]*Department of Chemistry, University College of Science, Osmania University, Hyderabad*
[c]*Department of Chemistry, Post Graduate College of Science, Saifabad, Osmania University, Hyderabad*
**E-mail : dr_saraladevich@yahoo.com*

The structural properties of N'-[(E)-(5-chloro-2-hydroxyphenyl-methylidene]acetohydrazide (NClHMAH) have been investigated by spectro-analytical and computational studies. ChemAxon and HyperChem 7.5 tools were employed to generate energy parameters, heat of formation and dipole moment values. Molecular orbital calculations were performed with quantum mechanics based semi empirical method at Parametric Method 3 (PM3) level. The compound NClHMAH was characterized by elemental analyses IR, ^1H – NMR, ^{13}C – NMR, DEPT and Mass spectral data. The equilibrium studies were carried out to determine the dissociation constant of NClHMAH in 70% v/v DMF – water medium at 303 K and 0.1 M (KNO_3) ionic strength adopting pH-metric technique. The dissociation of two protons is evident from these studies indicating it as a dibasic acid. The microbial studies suggest that moderate antibacterial activity was shown by NClHMAH against S. aureus and the compound is resistant to E.Coli. The copper complex has exhibited great anti – bacterial activity for both the cultures.

AO-CYSA-05 : Multiresidue Method for the Analysis of Pesticide Residues in Vegetables using Ultra Pressure Liquid Chromatography /time-of-flight Mass Spectrometry (UPLC/TOF-MS)

Sivaperumal P.[1]*, Anand P.[1] and Riddhi L.[1]

[1]National Institute of Occupational Health, ICMR, Ahmedabad-380 016
E-mail : sivaperum2003@yahoo.co.in

The principal objective of this study was to develop a simple multiresidue method involving a quick, easy, safe extraction and environment friendly method for the identification and quantification of pesticide residues in vegetables using UPLC/TOF-MS. The samples were extracted with acetonitrile and acetic acid (95:5, v/v) and cleaned up with florisil solid- phase extraction (SPE). The quantitation of individual pesticides was based on external calibration curves with a correlation coefficient in excess of 0.996 for the all pesticides selected. The method detection limits (MDLs) and lower limit of quantifications (LLOQs) range from 0.8 to 9.0 and 3.0 to 30.0 ng/g, respectively. The developed procedure gave satisfactory recovery (73-112%) and relative standard deviation values (<13%) for the studied pesticides. The method of detection limit was 5–10 times lower than the prescribed tolerance limit established by the regulatory authority. Uncertainty measurements were evaluated at the concentration of below tolerance limit and the measurement was not more than 15%. The method was successfully applied to determination of pesticides in vegetable samples and the result shows that are safe for human consumption.

AO-CYSA-06 : Development and Validation of New HPTLC Assay Method for Determination of Terazosin in API

Yashwantsinh Jadeja*, **Jabal Thanki***, **Darshana Pandya***
and Ranjan Khunt

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : yashwant_9274@yahoo.com

The aim of this study was to develop and validate a method for the determination of Terazosin, by using HPTLC, which gives better results and time saving than other methods. Terazosin acts to lower the blood pressure and is therefore a drug to choice for men with hypertension and prostate enlargement. In present method HPTLC separation was achieved on precoated silica gel G60-F254 Aluminum Sheet (E.Merck, Germany) using mobile phase of methanol : methylene dichloride (15:85 v/v) and the determination were carried out at 254 nm by using UV-scanner. For the validation purpose accuracy, precession, linearity, LOD, LOQ & robustness was also determine for this method and satisfactory results were obtained.

AO-CYSA-07 : Spectral Characterization of the Binding and Conformational Changes of Bovine Serum Albumin upon Interaction with an Antihistamine Drug, Ketotifen Fumarate

Kirthi S. Byadagi and Shivamurti A. Chimatadar*

P. G. Department of Studies in Chemistry, Karnatak University, Pavate Nagar, Dharwad -580003
**E-mail : schimatadar@gmail.com, ksbyadagi@gmail.com*

The binding of ketotefin fumarate (KF) to bovine serum albumin (BSA) was investigated by spectroscopic techniques. The binding parameters have been evaluated by fluorescence quenching method. The thermodynamic parameters, $\Delta H°$, $\Delta S°$ and $\Delta G°$ calculated at different temperatures indicated that the hydrogen bond and hydrophobic forces played a major role in the interaction of ketotifen fumarate with BSA. Based on the Förster's theory of non-radiation energy transfer, the binding average distance, *r* between the donor (BSA) and acceptor (ketotifen fumarate) was evaluated. Spectral results observed showed that the binding of ketotifen fumarate to BSA induced conformational changes in BSA. The effect of common ions on the binding of ketotifen fumarate to BSA was also examined.

AO-CYSA-08 : Investigation of the Interaction between a New Antiarrhythmic Drug-procainamide Hydrochloride with Bovine Serum Albumin and the Effect of Some Common Ions on the Binding : A Fluorescence Quenching Study

Manjunath D. Meti and S. A. Chimatadar*

P. G. Department of studies in chemistry, Karnatak University, Dharwad 580003
**E-mail : schimatadar@gmail.com, manjunathmeti4@gmail.com*

This study is designed to examine the interaction of procainamide hydrochloride(PAH) drug with bovine serum albumin(BSA) using fluorescence spectroscopy(FS) and ultraviolet spectroscopy(UV) under simulated physiological conditions. The experimental results showed that a static quenching mechanism in the interaction of PAH with BSA. The number of binding sites close to unity for PAH–BSA indicated the presence of single class of binding site for PAH in protein. The binding constants, K, and the number of binding sites, n, are calculated at different temperatures according to the Stern–Volmer equation. The thermodynamic parameters, ΔG°, ΔH° and ΔS° calculated at different temperatures according to van't Hoff equation indicate that the hydrogen bonds and van der Walls forces played major role in the binding of PAH to proteins. The calculated distance r between PAH and the protein is evaluated according to the theory of Förster energy transfer. The effects of common ions on the binding constants of PAH-BSA complexes are also examined. The result of fluorescence spectra and UV-Vis absorption spectra shows that the secondary structure of the protein has been changed in the presence of PAH.

AO-CYSA-09 : Efficient Synthesis of Polysubstituted Cyclohexene Derivatives by Using Lipase in Biodegradable Solvent

Vasant S. Borude and Sanjeev R. Shukla*

Department of Fibre and Textile Processing Technology, Institute of Chemical Technology, N. Parekh Marg, Matunga, Mumbai-400 019
E-mail : srshukla19@gmail.com, borudevasant@gmail.com

A simple and efficient method for the synthesis of polysubstituted cyclohexene derivatives has been developed. One-pot multicomponent reactions (MCRs) between aromatic aldehydes, malononitrile and nitromethane by using *Rhizopus oryzae* lipase as a biocatalyst in a biodegradable deep eutectic solvent (DES) were carried out. The simple quaternary ammonium DES, easily synthesized from choline chloride and urea was used in the reaction which is easily available, cheap and environment friendly. This method provides access to pharmaceutically

relevant products using environmentally friendly reaction conditions in excellent yields. The remarkable catalytic activity and reusability of lipase and DES widen their applicability in MCRs for the synthesis of polysubstituted alkenes with better yields.

Lipase as a biocatalyst provides excellent alternative to organic transformations because of their stability, selectivity and easy availability. It has been applied in mannich reaction, transesterification and ester hydrolysis. The ability of a DES as solvent has not been extensively explored in the field of organic chemistry. DES is eutectic mixture of a solid ammonium salt like choline chloride and a hydrogen-bond donor like urea, glycerol, malonic acid, etc. Deep eutectic liquid have similar properties to other conventional ionic liquids. These eutectic mixtures are easily available, cheap and environment friendly.

AO-CYSA-10 : Greener and Efficient Synthesis Protocol for Selective Decahedral Palladium Nanoparticles and its Catalytic Performance for Suzuki Coupling Reaction

Aniruddha B. Patil and Bhalchandra M. Bhanage

Department of Chemistry, Institute of Chemical Technology, Matunga,
Mumbai- 400019
E-mail : aniruddhapatil135@gmail.com, bm.bhanage@ictmumbai.edu.in

A convenient, mild, cost-effective and environmental benign synthesis of decahedral palladium nanoparticles (PdNPs) by exposing aqueous $PdCl_2$ solution to the sunlight in the presence of citric acid as a reducing agent and PVP as a capping agent was reported. The obtained nanoparticles were characterized using techniques like TEM, SAED, FEG-SEM, XRD and EDAX. It was observed that up to 70% of the PdNPs have decahedron shape while remaining 30% consists of all other different shapes. The citric acid helps in shapes selective synthesis whereas concentrated solar energy supplies duel energy which helps to speed up the reduction process. The aqueous reaction mixture of PdNPs was directly employed for the Suzuki coupling reaction and hence centrifuging efforts and cost of reagents required for the isolation of nanoparticles were avoided. The methodology is applicable to diverse substrates providing excellent yields. Notably, the obtained yields with lowest catalytic loading resulting in highest TOF (0.05 mol% catalyst loading and TOF of 1960 h^{-1}) were among the best ever reported for the Suzuki coupling reaction. The catalyst was reused for three consecutive recycles. The effectiveness of present new protocol for the PdNPs synthesis was also compared with PdNPs prepared using conventional heating method.

AO-CYSA-11 : Urinary Iodine Excretion : The Most Appropriate Outcome Indicator for Iodine Deficiency in Pregnant Women

N.S. Rajurkar*[1,2], Neeta Zatakia[2] and S. F. Patil[3]

[1]Department of Chemistry, University of Pune, Pune 411007
[2]Department of Environmental Science, University of Pune, Pune 411007
[3]Bharati Vidyapeeth, Pune 411030
E-mail : rajurkar@unipune.ac.in

Iodine deficiency is a major health problem worldwide with more than 1600 million people at the risk of iodine deficiency disorders (IDD). As most of the iodide is excreted in the urine, urinary iodide excretion is currently the most convenient laboratory marker of iodine deficiency and plays an important role in public health surveillance in many countries. The present investigation deals with the urinary iodine estimation of pregnant women from rural area around Pune city. The analysis of the samples was done by using Sandell-Kolthoff reaction which is iodide catalysed reaction between As(III) and Ce(IV). The obtained data are examined in the light of classification recommended by WHO / UNICEF based on urinary iodine concentration. It is revealed that out of 71 pregnant women, 33 pregnant women showed moderate iodine deficiency and 38 showed mild iodine deficiency.

AO-CYSA-12 : A Novel Titanium n-Propylamino Phosphate Catalyst : Synthesis, Characterization and Crystal Violet Catalytic Degradation Studies

A. Rajini[1], M. Nookaraju[1], K. Selvaraj[2], I.A.K. Reddy[1] and N. Venkatathri[1*]

[1]Department of Chemistry, National Institute of Technology, Warangal 506 004, Andhra Pradesh
[2]Catalysis division, National Chemical Laboratory, Pune 411 008, Maharastra
E-mail : venkatathrin@yahoo.com

Titanium n-propylamino phosphate (TNPAP) catalyst has been synthesized at room temperature using n-propylamine as template. The synthesized catalyst morphological and structural properties are characterized. Catalytic application of the material towards the catalytic degradation of crystal violet in presence of hydrogen peroxide at room temperature is carried out. Even though, hydrogen peroxide acts as a good oxidizing agent for the degradation of the dye, it is found that the presence of TNPAP with sunlight increases the degration rate to a maximum extent. Influence of various parameters such as effect of pH, concentration of hydrogen peroxide, dosage of catalyst and concentration of crystal violet on the degradation has been investigated.

The optimum conditions required for the degration have been established. We have found that about 91% of crystal violet has been degraded in 150 minutes.

AO-CYSA-13 : Recovery of Copper Ions from Loaded Commercial Activated Alumina

Nilima S. Rajurkar*[1, 2], Kumaree Dimya[2] and Ashok N. Gokarn[2]

[1]Department of Chemistry, University of Pune, Pune 411007
[2]Department of Environmental Science, University of Pune, Pune 411007
E-mail : rajurkar@unipune.ac.in

Treatment of waste water containing heavy metal pollutants is one of the most important environmental issues facing every country today. Adsorption has emerged one of the most effective technologies for removing heavy metals present in trace amounts from water and wastewater. Furthermore, this process facilitates recovery of the metal ions adsorbed on the adsorbents. The present work explores regeneration potential of loaded commercial activated alumina (CAA). Copper ions were significantly adsorbed on CAA and the recovery of metal ions was carried out by using column process. This was done in two steps viz. optimization of different solvents to elute copper ions from the loaded adsorbent and optimization of volume of the optimized solvents. HCl, KCl, NaOH and HNO_3 each of 1M concentration were used as eluents. It was found that 61.71% of copper ions was recovered using HCl solvent. The results show that the spent metal ions can be effectively recovered.

AO-CYSA-14 : Assessing Impacts of Ozone on Agricultural Crops in a Semi Arid Region in Agra

Renuka Saini and Ajay Taneja

Department of Chemistry, Dr. B.R. Ambedkar, University, Agra
E-mail : renukasaini@gmail.com

Ozone (O_3) is present both in the troposphere and the stratosphere. Tropospheric O_3 is predominantly produced by photochemical reactions involving precursors generated by natural processes and to a much larger extent by anthropogenic activities. There is evidence for a trend towards increasing tropospheric O_3 concentrations. However, tropospheric O_3 is known to account for only 10% of the vertical O_3 column above the earth's surface. The stratosphere accounts for an additional 90% of the O_3 column. Ozone in these two regions are chemically identical (both consist of three oxygen atoms and have the chemical formula "O_3"), the ozone molecules have very different effects on humans and other living things depending upon their location. Tropospheric O_3 is known to be highly phytotoxic. Appropriate exposures to O_3 can result in both acute (symptomatic) and chronic (changes in growth, yield or productivity and quality) effects. Chronic effects are of great concern in terms of both crops and forests. Systems theory provides the required conceptual framework for linking exposure science and toxicology in order to study, characterize and predict the complex interactions between vegetation and pollutants that lead to adverse effects on plants and crops using exposure indices like AOT 40 and SUM 60. In the present study, risk analysis on O_3 levels at Agra has been evaluated on wheat crop.

AO-01 : Thermal and Biological Studies of 4-Hydroxybenzaldehyde – Formaldehyde - Phenyl hydrazine Terpolymer Ligand and its Transition Metal Complex

Vaishali R. Bisen and Wasudeo B. Gurnule

Department of Chemistry, Kamla Nehru Mahavidyalaya, Nagpur- 440 009
E-mail : wbgurnule@yahoo.com

A new terpolymer ligand involving 4- hydroxybenzaldehyde, phenyl hydrazine and formaldehyde (4-HBFPH) has been synthesized in the presence of HCl medium. The 4- HBFPH ligand was characterized by elemental analysis and various spectral techniques like FTIR, UV – Visible, ^{1}H and ^{13}C NMR to elucidate the structure and properties of the terpolymer ligand. The 4-HBFPH metal complex were prepared using 4-HBFPH ligand with some transition metal ion such as Cu^{2+}, Ni^{2+} and Zn^{2+} ion in the presence of ethanol medium. The prepared complexes have been characterized by elemental analysis, FTIR, electronic, ^{1}H and ^{13}C NMR spectral studies. The molecular weight of 4-HBFPH ligand and its metal complexes was determined by gel permeation chromatography (GPC). The surface feature and crystalline behavior of the ligand and its complex were analyzed by scanning electron microscope (SEM) and X-ray diffraction (XRD) methods. Thermal stability of the ligand and its metal complexes was studied by thermo gravimetric analysis(TGA). Kinetic parameters such as activation energy (E_a) and order of reaction (n) and thermodynamic parameters viz. ΔS, ΔF, s* and Z were calculated using Freeman-Caroll (FC), Sharp- Wentworth (SW) and Phadnis- Deshpande(PD) methods. Thermal degradation model of the terpolymer ligand and its metal complexes was also proposed using PD method. The antibacterial activities of the 4-HBFPH ligand and its metal complexes were checked against chosen microbes such as *Shigella sonnei, Escherichia coli, Klebsiella species, Staphylococcus aureus, Bacillus subtilis and Salmonella typhimurium.*

AO-02 : HPTLC Method for Estimation of Modafinil in the Bulk and Tablet Formulation

Hitendra S. Joshi

Sophisticated Analytical Instrument Lab, Department of Chemistry, Saurashtra University, Rajkot-360 005, Gujarat
E-mail : drhsjoshi49@gmail.com

A simple and rapid HPTLC method for analysis of Modafinil in bulk drug as well as tablet formulation has been developed and validated. Aluminum foil TLC plates precoated with silica gel 60F 254 were used as stationary phase ethyl acetate, acetone and methanol in the volume ratio of (7:2:1 v/v) respectively as mobile phase. A compact band (R_f 0.42±0.02) was obtained for modafinil. Densitometric analysis was performed in absorbance mode at 232 nm. Stastistical analysis revealed a good fit of quadratic calibration curve with regression coefficient r=0.999 between peak area and concentration in the range of 40-160 µg/ml. The percentage recovery of drug was found in range of 99.38-100.33% with standard deviation less than 2.0 specify good accuracy of method. Modafinil was subjected to acid and alkaline hydrolysis, oxidation, photochemical and thermal degradation and checked that drug peak is well resolved from degraded product. Statistical analysis proved the method enables repeatable, selective, and accurate analysis of the drug. It can be used for identification and quantitative assay analysis of Modafinil in the bulk drug and in tablet formulations.

AO-03 : Synthesis, Characterization and Determination of [Di (4-amino N-acetyl) phenoxy] Methyl Ketone in Biological Fluids by Spectrophotometry

Bhavna A. Shah[a*], Pravin S. Patil[a] and Hirva A. Shah[b]

[a]Department of Chemistry, Veer Narmad South Gujarat University,*
Udhana Magdalla Road, Surat, 395007, Gujarat
[b]S K Patel College of Pharmaceutical Education and Research,
Ganpat University, Kherva, Mehsana, 384012, Gujarat
E-mail : bhavna606@gmail.com

A new acetaminophen derivative; [Di (4-amino N-acetyl) phenoxy] methyl ketone (DPMK) was synthesized by condensation reaction between (4- amino N- acetyl) phenoxy acetyl chloride (APAC) and (4-amino N- acetyl) phenol. The compound has been characterized by FTIR, ^{1}H NMR, LCMS and elemental analysis. A simple, rapid and accurate spectrophotometric method has been developed for quantification of DPMK. The procedure is based on a nitroso-compound formation and generates an instant reddish yellow color, having an absorption maximum at 433 nm with a molar absorptivity of 6.949 × 10^3 L/(mol cm). Beer's law is obeyed in the concentration range of 5 to 65 μg mL^{-1}. Optimization of temperature and time revealed 30 °C and 5 min as the best conditions for optimal color formation. The proposed method has been successfully applied for the determine of the spiked DPMK in biological fluids.

AO-04 : Differential Complexations : An Analytical Probe for Separation of Some Metals in Solution

Eknath Nirapure, Gopal Sahu and Subhash Lavale*

Chemical Research Laboratory, J.H.Govt.P.G. College, Betul (M.P.) 460001

Chemists usually requires to analyse mixtures of complex material viz. organics, cis-trans, metals, metaloids, non metals, multi-component system and bio-products. An analytical probe, differential complexation are based on the differences in the stability constants of complex formed in - situ. Suitable complexation for reproducible separation have been searched out for some cases. Polarographic waves of mixture of Cd(II), Sn(II) and Pb(II) in bicomponant mixture & tricomponant solutions have suitably been separated using salycillic acid, Bivalent Cd, Sn and Pb have got $E_{½}$ = - 0.50 V Vs SCE, - 0.41 V Vs SCE and - 0.71 V Vs SCE and hence polarographic separation and simultanious determination not possible without suitable complexation. Present investigation revealed the simultanious determination of three metal in the ratio of 1:10 and 10:1, the polarographic wave was not superimposed. Ternary system is also possible and revealed that their separation are due to difference of stability constant of complexes formed in test polarographic solution. The polarograms in distinct condition of pH, μ, SE, complex, stable constants are recorded, interpreted and highlighted as a successful probe for chemists.

AO-05 : Obesity is Morbid not only for Adult but also for Child

Kamal Kishor Singh and Shyam Kumar

Chemistry Department A.N. College, Patna
E-mail : kksancmail@gmail.com

According to latest studies, it is reported that the worst problem due to obesity are heart ailments or heart attacks and statistics shows that heart disease is the number one killer across the country The main reason why there is an increase in the number of heart ailments is a sedentary life style. The body is like a bank. The more you put in the bank and the less you remove, the more the balance increases. Since there is more calorie intake and fewer workouts, fat in the body accumulates over time and it causes trouble in the most sensitive area of the body that is Heart.

The creation of an obeso-genic environment is a concern particularly for young girls who undergo the physiological transition to enter puberty and may have a tendency to gain weight junk food, irregular food intake, lack of exercise and sleep deficiency are the main culprits. Festive season adds to people fat in take under the guise of religion and festivities people eat richer food. People get an excuse to skip exercise in monsoon season due to rain and due to cold in winter. It adds up to the slow procedure of adding fat to the body.

Eating habits of children act as another important cause of child obesity. The children today have greater reliance on unhealthy and calorie rich fast foods like cheese burger, hamburger, milk shakes, French fries, pizza, chips and chocolates rather than healthy foods like fruits, vegetables, spinach and grains – all these add as a factor for causing child obesity.

AO-06 : Method Development and Validation of RP-UPLC Method for Rapid Quantification of Deflazacort in Pharmaceutical Tablets

Madhavi Patel, Hetal Jebaliya, Batuk Dabhi, Yashwantsinh Jadeja and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005.
E-mail : Patel_madhavi25@yahoo.com; hetal_jebaliya@yahoo.com; anamik_shah@hotmail.com

The intent of this study was to develop a simple, precise, reliable and accurate isocratic reversed-phase UPLC assay method. The method is developed for the rapid quantification of Deflazacort in bulk drug. Chromatography was carried out on an equity UPLC BEH C18 column (50×2.1 mm, particle size 1.7 µm) using mobile phase methanol and water (70: 30 v/v) at a flow rate of 0.25 ml/min at 30° C temperatures. The detection was achieved at 245 nm by using photo-diode array detector. The method was validated for specificity, linearity, precision, accuracy, robustness and solution stability. The method was linear in the drug concentration range of 20-80 µg mL^{-1} with a correlation co-efficient 0.999. The accuracy was between 99.22 % to 100.43 %. The method validation performed according to the ICH guideline, where all results met to acceptance criteria

AO-07 : Detection and Identification of Organics Present in Industrial Waste Amended Soils by FTIR and GC – MS Techniques

B. H. Patil

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar-425412

The industrial waste amended soil samples from coastal area of Surat(Gujrat) were collected. The samples were extracted in dichloromethane and recorded for FTIR and GC-MS. Several organic compounds have been found and these compounds ultimately affect the soil and water quality of the area.

AO-08 : Use of Photo-Fenton Reagent for the Degradation of Basic Orange 2 in Aqueous Medium

Dileep Kumar and Rameshwar Ameta*

Pacific College of Basic and Applied Sciences, Pacific University, Udaipur-313024 (Raj.)
E-mail : dhkhandelwal@gnfc.in, ameta_ra@yahoo.com

Photocatalytic decolourization of dyes using AOP is a new concern among researchers since it offers an attractive method for decolorization of dyes and breaks them into simple mineral form.

The oxidation using Fenton Reagent has been found to be a promising treatment method for the effective decolorization and degradation of dyes. A detailed investigation of photodegradation of basic Orange-12 (BO2) using H_2O_2/Fe^{+3} have been carried out. Results indicate that dye degradation is dependent on concentration of dye (BO2), photocatalyst (Fenton reagent), H_2O_2 and pH of the experimental solutions. The optimum conditions for the photobleaching of dye had been established. The kinetics of degradation of the dye in the dilute aqueous solutions follows first order kinetics. The results indicated that the treatment of the dye by Photo-Fenton reagent was efficient at optimum conditions.

AO-09 : A Comparative Study of Effect of Surface Charge on Photocatalytic Degradation of Cationic and Anionic Dyes using Zinc Oxide Powder

Ritu Vyas and Suresh C. Ameta

Department of Chemistry, Pacific Institute of Technology, PAHER University, Debari, Udaipur – 313024 (Raj.)
E-mail : ritu24vyas@gmail.com

The photoreduction of cationic and anionic dyes (Brilliant green and Erythrosin B) has been carried out using ZnO as photocatalyst. This photochemical reaction was monitored spectrophotochemically.

The effect of different parameters like pH, concentration of dyes amount of semiconductor and light intensity on the reaction rate was observed. The effect of charge of different cations, anions and ligands on the reaction rate was also studied by taking cations like Na^+, Ba^{2+}, Al^{3+} ; anions Cl^-, SO_4^{2-}, PO_4^{3-}, and ligands like EDTA and NTA. Further behavior of photocatalytic degradation was also studied by varying the concentration of cation (Ba^{2+}), anion (PO_4^{3-}), and ligand (EDTA). A tentative mechanism of the photocatalytic degradation of these dyes was also been observed

AO-10 : Highly Selective, Effective and Reusable Method for Conversion of Glycerol into 1, 4-dioxanol using Cesium Doped Dodecatundustophosphoric Acid Supported on Clay K 10 as Nanocatalysts

Ganapati D. Yadav* **and Akhilesh R. Yadav**

Department of Chemical Engineering, Institute of Chemical Technology, Matunga, Mumbai-400 019
E-mail : gdyadav@yahoo.com; gdyadav@ictmumbai.edu.in

Selective transformation of glycerol into value added products remains a challenging task due to its polyfunctional nature. Acetalization of glycerol to 5-membered [1, 4] dioxan-4-yl)-methanol was efficiently catalyzed by cesium doped dodecatungstophosphoric acid supported on clay K10. 100% selectivity toward desired product was achieved. The influence of solid-liquid mass transfer resistance and absence of the intra-particle diffusion resistance was calculated to ascertain the kinetic aspect of the reaction. The effect of various parameters such as speed of agitation, catalyst loading, mole ratio and temperature on selectivity and conversion of glycerol was investigated in detail. Suitable kinetic model was developed and reaction was found to follow pseudo first order regime with energy of activation 11.64kcal/mol. Catalyst was found to be active and reusability was studied up to seven runs. The result clearly shows effectiveness of catalyst for selective synthesis of [1, 4] dioxan-4-yl)-methanol for an environmentally benign process.

AO-11 : Synthesis and Characterization of Nanocrystaline CdS/PVA Composite Thin Film and its Application in Photocatalytic Reduction of Pb(II)

Praful S. Patil, Manohar R. Patil , Yogesh V. Marathe and
V. S. Shrivastava*

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

The work reports the preparation, characterization and application of nanocrystaline CdS thin film in PVA matrix. The composite is prepared by the association between poly vinyl alcohol and CdS using chemical bath deposition method .The structural characterization of prepared nanocrystaline thin film was performed by SEM and XRD techniques. Optical characterization of thin film was performed by UV-Visible spectroscopy. The XRD study shows evidence for the formation of nano sized crystals with crystallite size 45 nm while the optical band gap of chemical bath deposited thin film is found to be 2.84 eV. This film is better photocatalyst for industrial waste water decontamination mediated by visible light radiation than alone CdS. The obtained CdS/poly vinyl alcohol composite thin film were employed in experiment of photoreduction of Pb(II).The results shows that the Pb(II) successfully removed from aqueous solution in photocatalytic system. The photocatalytic activity of the prepared thin film exhibit comparable removal efficiency with CdS powder. The optimum conditions for removal of Pb(II) was pH=5, Contact time 30minutes, Temparature 210 °K and Metal ion concentration 30mg/L.

AO-12 : 2-(2-E-(2-Hydroxy Phenyl)Ethlidene) Amino ethyl) Ethane-imidoyl)phen as a New Analytical Reagent for Extractive Determination of Cobalt

Jayashree S Patil[1], R S Lokhande[2], S B Dharap[3], Poonam Shevade[4] and Sonali S Patil[5]

[1]JSM College Alibag, Raigad
[2]School of Basic Science Jaipur National University
[3]Bhausaheb Nene College, Pen Raigad
[4]Department of Chemistry University of Mumbai
[5]JSM College Alibag, Raigad

A 2-(2-E-(2-hydroxy phenyl)ethlidene)amino ethyl)ethane-imidoyl)phen was synthesized subjected to FTIR, NMR, elemental analysis and Mass Spectroscopy for characterization. The synthesized reagent was then applied for liquid – liquid extraction and spectrophotometric determination of cobalt metal forms light pink coloured complex, which can be extracted in chloroform at pH 6.6 having absorption maxima at 450 nm. The molar absorptivity and Sandell's sensitivity was calculated on the basis of total cobalt (II) taken. The developed method is highly sensitive, selective, simple, rapid, accurate and has been satisfactorily applied for the determination of cobalt in the synthetic mixtures.

AO-13 : A Preliminary Study of Sediment Pollution Along the Mahim Creek of Mumbai

Pravin U. Singare*, **Sunny Ferns, Deepak D. Dagli and Vijay G. Bhawe**

Department of Chemistry, Bhavan's College, Munshi Nagar, Andheri (West), Mumbai 400 058
**E-mail : pravinsingare@gmail.com*

The present preliminary study was therefore performed to understand the pollution status due to accumulation of toxic heavy metals like *Pb*, *Fe, Zn*, *Cu* and *Hg* in the sediments of Mahim Creek of Mumbai. The analysis of these toxic heavy metals was done by *AAS* technique coupled with cold vapour technique (for *Hg* analysis). The maximum tolerable limit set by *CPCB* for the above toxic heavy metals is 0.1, 3.0, 5.0, 3.0, 0.01 ppm respectively for inland surface water; and that for marine coastal areas the limit set is 2.0, 3.0, 15, 3.0 and 0.01 ppm. However it was observed that the concentration of these toxic heavy metals in the creek sediments where 7.33 ppm, 0.78%, 71.18 ppm, 18.16 ppm and 0.02 ppm respectively, which was above the maximum tolerable limit. It is expected that these heavy metals accumulated in the creek sediments may enter the water creating threat to aquatic life. It is expected that in addition to the water analysis practiced for years, sediment analysis performed in the present investigation will help in evaluating quality of the total ecosystem of the creek and will provide environmentally significant information about natural and anthropogenic influence on the water body.

AO-14 : Studies on Effect of Fly Ash (VSTP, Singrouli) on Surrounding Environment

Neeraj Verma, Alok Singhai and Harish Wankhade

Regional Office, MP Pollution Control Board, Paryavaran Parisr,
E-5 Arera Colony, Bhopal-16 (MP)
E-mail : neeraj_v22@rediffmail.com

A considerable part of electricity in India is produced from thermal power plant in which coal is utilized as fuel. Fly ash is the residue produced from combustion of coal. Fly ash is subsequently removed, transported and deposited in open storage areas (ash dams) where it is accumulated in large amount and thus create environmental problems. When coal is burnt, the sulfur contents present in the coal are converted to sulfur dioxide and oxides of nitrogen. These pollutants escape in the atmosphere and pollute the environment.

NTPC has three Super Thermal Power Plants in the area including Vindhyachal project VSTP which is one of the major oldest and important established units in the field of power generation in M.P. This type of industry causes heavy air pollution in the system.

The generated variables of chemical compounds affect all the components of the ecosystem. The plants being the primary are the worst sufferer of producers depending much on gaseous exchange and remains exposed to these pollutants, attract the pollutants generated in the production process of thermal power plants. In order to recognize and predict hazardous effects of pollutants, the scientific monitoring of these environmental components is essential. For this purpose, the quantitative characterization of air is the prerequisite. It gives us an idea about the seriousness of pollution problem in environmental components. An approach during 2009-10 has been made to study the impact of air pollutants on surrounding environment with some specific monitoring at Singrouli, Madhya Pradesh. Study clearly indicates that there was an adverse impact on the surrounding atmosphere of the area in the form of heavy suspended particulate matter. SPM varied between 221 to 465{however most of the time it exceeded the norms (200 µg/cubic meter)}, particulate matter PM2.5 between 39 to 104.7 µg/cubic meter.

AO-15 : Development of a Reliable Analytical Method for Extraction Spectrophotometric Determination of Ruthenium (III) from Catalyst and Fissium Alloy using o-Methylphenyl Thiourea as a Chromogenic Chelating Ligand

Shashikant R. Kuchekar[a, *], Sung H. Han[b] and Yogesh S. Shelar[a]

[a] *Analytical Chemistry Laboratory, Department of Chemistry, A. C. S. College, Satral, At Post. Satral, Taluka. Rahuri, District. Ahmednagar, Maharashtra state 413711*

[b] *Inorganic Nano materials Laboratory, Department of Chemistry, Hanyang University, Seoul 133-791, South Korea*

A simple and selective spectrophotometric method is developed for the extraction spectrophotometric determination of ruthenium(III) using o-methylphenyl thiourea (OMPT) as a chromogenic chelating ligand. The basis of proposed method is ruthenium(III)-OMPT complex formation in aqueous media at 3.0 mol L^{-1} hydrochloric acid concentration after 5.0 min heating in a boiling water bath and the complex formed is extracted in to chloroform. The absorbance of green colored organic layer is measured at 590 nm against the reagent blank. The beer's law was obeyed up to 42.5 µg mL^{-1} of ruthenium(III) and the optimum concentration range is 7.56 – 39.81 µg mL^{-1} of ruthenium(III) as evaluated by ringbom's plot. The molar absorptivity and sandell's sensitivity of ruthenium(III)-OMPT complex in chloroform are 2.34×10^3 L mol^{-1} cm^{-1} and 0.043 µg cm^{-2} respectively. The composition of ruthenium(III):OMPT complex (1:2) was established from slope ratio method, mole ratio method and job's continuous variation method. The binary complex is stable for more than 48 h. The interfering effect of various cations and anions are also studied. The suitable masking agents are used wherever necessary to enhances the sensitivity of method. The method is successfully applied for determination of ruthenium(III) from binary and ternary synthetic mixtures, synthetic mixtures corresponding to fissium alloy and ruthenium catalyst. The repetition of method is checked by finding relative standard deviation (R.S.D) for ten determinations which is 0.23 %. A scheme for sequential separation of ruthenium(III), palladium(II), rhodium(III) and platinum(IV) has been developed.

AO-16 : Chemionics Study of Newly Synthesised Photochromic Schiff base Compound

Bhavna A. Shah[*a], Pratima R. Surati[a] and Ajay V. Shah[b]

[a]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat,
[b]Science and Humanities Department, Polytechnic, Vidyabharti Trust, Umrakh, Bardoli, Gujarat,
[*]E-mail : bhavna606@gmail.com

A new Schiff base compound 4((o-tolylimino)methyl)-3-methyl-1-phenyl-1*H*-pyrazol-5-ol(4TM-MPP) was synthesised and characterized by elemental analyses, LC-MS, FTIR and ^{1}H-NMR spectra. The compound exhibit photochromic property under 365 nm UV-light irradiation, which can be observed with solid state reflectance and fluorescence spectra. It suggests that the photoisomerization is due to photoinduced intermolecular hydrogen bond which results in enol to keto transformation. The chemionics study is carried out using (Ni^{+2}, H^+), (Ag^+, H^+), and (Na^+, H^+, and OH^-) using the UV absorption spectra in solution, which shows logic behaviour of INHIBIT, NOR and XOR respectively.

AO-17 : Simultaneous RP-HPLC Determination of Four Main Ingredients in Cough Syrup Containing Chloropheniramine Maleate, Pseudoephedrine HCl, Ambroxol HCl and Guaiphenesin as Active Ingredients

Sandip Surve, Rama Lokhande, Rajiv Sutar, Surekha Kolhal, Sanjay Pednekar and Sanket Gudekar

Department of Chemistry, Jaipur National University, Jaipur, Rajasthan

A novel and single RP-HPLC method was developed for the determination of four active ingredients (chloropheniramine maleate, pseudoephedrine HCl, ambroxol HCl and guaiphenesin,) in pharmaceutical dosage form and validated the method as per ICH and FDA guidelines. The separation was achieved on Nucleosil CN column, 25 cm × 4.6 mm, 7 µ in the simple isocratic mode using buffer containing Glacial acetic acid, dibutylamine and hexane sulphonic acid sodium salt. Mobile phase prepared contained the mixture of Buffer: acetonitrile: THF (90:2:8) with flow rate of 1.0 mL per min. Column oven temperature maintained at 25°C and performed the analysis on UV detector using 254 nm. Quantification was achieved with 20 µg per mL of Chloropheniramine maleate, 300 µg/ml of psudoephedrine, 500 µg/ml of guaiphenesin and 150 µg/ml of Ambroxol with 100 ± 3.0% recovery. The method was validated by determining its sensitivity, linearity, accuracy and precision. The proposed method is single, shorter runtime, accurate and reproducible. This method can be applied for routine analysis of all four active ingredients quantification in pharmaceutical dosage form

AO-18 : Removal of Acidic Dye from Aqueous Solution by Leucaena Leucocephala Seed Pods

A. K. Patil[a] and V. S. Shrivastava[b]

[a]Department of Chemistry, Dhanaji Nana Mahavidyalaya, Faizpur-425503 (M.S.)
[b]Center for P.G. Research in Chemistry, G.T.P. College, Nandurbar-425412 (M.S.)
E-mail : akpatildnm@yahoo.co.in.

Adsorbent prepared from *Leucaena leucocephala* seed pods was successfully used as a low cost adsorbent for the removal of Congo red (acidic dye) from aqueous solution. Adsorption of Congo red was dependent on pH, initial concentration, adsorbent dose and contact time. The result indicated that, the adsorption of Congo red was 91 % at the optimum pH of 5. The optimum contact time was 120 minutes and the adsorbent dose was 2 g/l of *Leucaena leucocephala* seed pods.

The Freundlich and Langmuir isotherm equations were applied for the equilibrium adsorption data and the various isotherm parameters were evaluated. The Congo red adsorption on the *Leucaena leucocephala* seed pods follows pseudo second-order rate kinetics.

AO-19 : Gamma Induced Modifications on Physico -chemical Properties of Polymeric Track Detectors

Dipak Sinha

Department of Chemistry, Nagaland University, Lumami Campus-798627, Nagaland

Gamma exposure in the dose range of 10^1 Gy to 10^6 Gy, is found to modify the physico- chemical properties of different track detectors at higher doses. For PADC detectors, the track etch rates are greatly enhanced at the highest dose. However for polycarbonates, the etch rates are not influenced to significant extent. The thermal stability of the detectors is also modified for some polymers like PADC, PVC and PP. The thermal stability decreases for most of the films with an exception of polypropylene. Due to chemical etching, the thermal stability of PADC (American-Acrylics) decreases unlike the un-etched one. For polycarbonate detector, due to gamma exposure, crystalinity of the polymer increases. The dielectric constant of PADC (Homalite) detector increases at a dose higher than 10^4 Gy, signifying the fact that polarization of the detector increases at doses higher than 10^4 Gy.

AO-20 : A Sensitive Spectrophotometric Determination of Paraquat Residue in Environmental Samples

J.S. Thakur[1], R.S. Dhundhel[2] & R.M. Patel

[1] *Department of Chemistry, Shri Shankracharya Institute of Professional Management and Technology, Raipur, (C.G.)*
[2] *Department of Chemistry, Shri Shankracharya College of Engineering and Technology, Bhilai, (C.G.)*

A sensitive spectrophotometric method is developed for the determination of paraquat residue in environmental samples. The method is based on alkaline hydrolysis of paraquat to stable blue colour free radical, which is reduced by sodium borohydrirde. The method is based on involved three steps : extraction of residue from the palm oil, clean up procedure using amberlite resin and spectrophotometric determination of the purified material. The percentage recoveries were greater than 98% for 0.01 μg ml^{-1} level of concentration. Beer's law is obeyed over the concentration range of 2 - 30 μg of paraquat per 25 ml of the final solution (0.08 - 1.2 ppm) at 575 nm. The molar absorptivity and Sandell's sensitivity were found to be $2.2\times10^4 \pm 100$ 1 mol^{-1} cm^{-1} and 0.004 μg cm^{-2} respectively. The lower limit of determination of paraquat is 0.06 ppm. The method is highly reproducible, selective and has been applied to determination of paraquat in palm oil and various environmental samples.

AP-CYSA-01 : Chemical and Morphological Composition of Fine Particulate Matter in Low, Middle and High Income Neighbourhoods in Agra Region

Pradyumn Singh, Saurabh Yadav and Ajay Taneja

Department of Chemistry, Dr. B. R. Ambedkar University, Agra-282002
E-mail : singh.pradi@gmail.com

The massive growth in socioeconomic status and the size of cities over the past few decades has led to serious deterioration in the indoor air quality. One of the important constituents of airborne pollutants which has major health hazard is fine particulate matter ($PM_{2.5}$). The present study shows the current scenario of aggregate relation between income and pollution at household level. We measured indoor fine particulate matter ($PM_{2.5}$) concentration in three different socioeconomic neighbourhoods in Agra, the north central region of India. Fine particulate matter ($PM_{2.5}$) samples were collected on polytetraflouroethylene (PTFE) filter papers with the help of fine particulate sampler (APM 550- Envirotech, New Delhi) from different income groups in Agra region. Scanning electron microscopy coupled with energy dispersive spectrometer (SEM-EDS) was used to understand the difference in terms of shapes, morphology and elemental composition of fine particulate matter ($PM_{2.5}$) and to further link them to potential sources. Some measures will also be suggested for improving the indoor air quality.

AP-CYSA-02 : New Stability Indicating Assay Validation of Agomelatine in Tablets and Determination of Content Uniformity by RP-HPLC

Reema H. Rupareliya and H.S. Joshi

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : drhsjoshi49@gmail.com

A simple, précised, and accurate RP-HPLC method has been developed and validated for assay of agomelatine in tablets and for determination of content uniformity. Isocratic RP-HPLC method was developed on Waters C18 2504.6mm, 5µm column using mobile phase as Methanol: Water (70:30) at a flow rate of 1.0 mL/min and the detection was carried out at 230 nm using photo-diode array detector. Forced degradation study was carried out by oxidation, hydrolysis, photolysis and heating the drug. The method was validated for specificity, linearity, precision, accuracy, robustness and solution stability. The method was found to be linear in the concentration range of 20-80 µg/mL with correlation coefficients of 0.9991. The precision (relative standard deviation: RSD) among a six sample preparation was 0.09% and 0.22%. The accuracy (recovery) was between 97.68% and 99.78%. Degradation products produced as a result of stress studies did not interfere with the detection of agomelatine. Therefore, the assay can be considered to be stability-indicating and was found suitable for determination of content uniformity.

AP-CYSA-03 : HP-TLC Analysis and Method Validation of Famotodine

Pinakin Kathiriya*, Ravi Ghediya* and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : yashwant_9274@yahoo.com

Famotodine is a well known pharmaceutical active compound and used as a anti-ulcer agent i.e. histamine H_2 antagonist. In pharmaceutical industries and research organization most of the analysis and identification is done by HPLC and UPLC due to various advantages like accuracy, precision, rapidity, and reproducibility of the results, similar results can be obtained with HP-TLC. HP-TLC has a advantage compare to HPLC and UPLC as cost of analysis is much smaller due to fact that cost of instrumentation for HPLC and UPLC is much higher and no special class of solvent are required for HP-TLC and hence can be afford by small organization and industries. Famotodine was analyzed with HP-TLC and method was validated by means of statistical analysis of the collected data.

AP-CYSA-04 : Determination of Lafutidine in Human Plasma and Dosage form using HPLC with a Photodiode Array Detector

P. P. Vekariya and H. S. Joshi*

Department of Chemistry, Saurashtra University, Rajkot- 360 005
E-mail : drhsjoshi49@gmail.com

Lafutidine is histamine H_2 receptor antagonist drug. Determination of Lafutidine in human plasma and dosage form, a rapid, sensitive and specific HPLC method was developed and validate using Photodiode array detector. Lafutidine was extracted from human plasma by solid phase extraction procedure using strata x SPE cartridge, the analyte was chromatographically separated by symmetry waters c_{18} column (5µm, 4.6 × 250 mm), using mobile phase 65:35 v/v methanol: 25 mM Ammonium acetate (pH-4.5). Calibration curve showed good regression ($r^2 > 0.999$). Linearity range for Lafutidine 50ng to 1000 ng/ml. Method was successfully applied the dosage form of Lafutidine.

AP-CYSA-05 : Development and Validation of Stability Indicating HPLC Assay Method for Determination of Tapentadol in Tablet Formulation

Gaurang P. Pandya[a] and Hitendra S. Joshi[a]*

[a]Sophiticated Analytical Instruments Lab, Department of Chemistry,
Saurashtra University, Rajkot-360 005, Gujarat
E-mail : drhsjoshi49@gmail.com

The purpose of the research described herein was to develop simple, precise and accurate isocratic stability indicating reversed phase HPLC assay method for determination of Tapentadol in bulk drug as well as solid dosage forms. Isocratic RP-HPLC method was developed on Phenomenex C8 1504.6mm, 5µm column using mobile phase as Acetonitrile:Water:Formic acid(60:40:0.1) at a flow rate of 1.0 ml/min and the detection was carried out at 272 nm using photo-diode array detector. The drug was subjected to oxidation, hydrolysis, photolysis and heat to apply stress condition. Linear calibration curve with regression coefficient r=0.999 was obtained in the range of 40-160 µg/ml. The validation element investigated showed that the method has acceptable specificity, accuracy, linearity, solution stability, precision and robustness. Thus developed method can be used in routine assay analysis as well as stability study of Tapentadol.

AP-CYSA-06 : Method Development and Validation for Quantitative Analysis of Cinnarizine in Pharmaceutical Dosage Form by HPTLC

Yashwantsinh Jadeja*, Batuk Dabhi, Madhavi Patel, Hetal Jebaliya and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : yashwant_9274@yahoo.com

A new rapid, accurate, precise and economic method developed for the quantitative analysis of cinnarizine by High Performance Thin Layer Chromatography using 10 × 10 aluminium sheet silica gel 60F254 and mixture of chloroform : acetone (8:2v/v) as an eluent at 228 nm wavelength. The calibration curve for cinnarizine was found to be linear (r^2=0.999) at concentration between 1.25 to 8.75 µg/spot with a limit of detection and quantification of 0.25 and 1.25 µg/spot respectively. This method was also anticipated can be effectively used to establish marketed formulation.

AP-CYSA-07 : Electro-oxidation of Nimesulide at Gold Electrode and its Determination in Pharmaceutical Dosage Form and Human Biological Fluid

Shweta J. Malode and Sharanappa T. Nandibewoor*

P.G. Department of Studies in Chemistry, Karnatak University, Dharwad-580 003
E-mail : stnandibewoor@yahoo.com, malodeshweta@yahoo.co.in

The electro-oxidation of nimesulide has been investigated by cyclic and differential-pulse voltammetry at different pH at gold electrode. Cyclic voltammetric studies were performed in a wide range of sweep rates and various concentrations of nimesulide. The oxidation process was irreversible and exhibited a diffusion-controlled behavior. According to the linear relation between the peak current and the nimesulide concentration, differential-pulse voltammetric method for the quantitative determination in pharmaceuticals was developed. The recovery was determined to be 97.3 to 100.2 % by means of standard addition method. The linear response was obtained in the range of 2.0×10^{-7} to 1.2×10^{-6} M with a detection limit of 1.11×10^{-9} M with good selectivity and sensitivity. The electrochemical behaviors of nimesulide were studied and electron-transfer coefficient ($\alpha = 0.5$), proton number ($X = 1$) and electron transfer number ($n = 2$) have been determined. The proposed method was also applied for the detection of nimesulide in urine as a real sample.

AP-CYSA-08 : Method Development and Validation of Stability-Indicating RP- HPLC Method for Quantitative Analysis of Dronedarone Hydrochloride in Pharmaceutical Tablets

Batuk Dabhi*[1], Yashwantsinh Jadeja[1], Madhavi Patel[1], Hetal Jebaliya[1], Denish Karia[2] and Anamik Shah[1]

[1]*Department of Chemistry, Saurashtra University, Rajkot-360 005, Gujarat*
[2]*Arts Commerce and Science College, Borsad, Anand, Gujarat*
E-mail : batukdabhi@gmail.com; anamik_shah@hotmail.com

A simple precise accurate HPLC method has been developed and validated for quantitative analysis of dronedarone hydrochloride in tablets. An isocratic separation was achieved using Waters symmetry C_8 (100 × 4.6mm) i.d., 5µm particle size columns with flow rate of 1 ml/min and using a UV detector to monitor the elute at 290 nm. The mobile phase consisted of buffer: methanol (40:60 v/v) (Buffer: 50 mM KH_2PO_4 + 1 ml tri ethyl amine in 1 liter water, pH=2.5 adjust with Ortho phosphoric acid). The method was validated for specificity, linearity, precision, accuracy, robustness and solution stability. The specificity of the method was determined by assessing interference from the placebo and by stress testing of the drug (force degradation). The method was linear over the concentration range 20-80 µg/ml ($r^2 = 0.999$) with a limit of detection (LOD) and limit of quantitation (LOQ) of 0.1 and 0.3 µg/ml respectively. Intraday and interday system and method precision were determined and accuracy was between 99.22-100.54 %. The method was found to be robust and suitable for quantitative analysis of dronedarone hydrochloride in a tablet formulation. Degradation products resulting from the stress studies did not interfere with the detection of dronedarone hydrochloride and the assay is thus stability indicating.

AP-CYSA-09 : RP-UPLC Method Development and Validation of Linezolid by Photodiode Array Detector

Hetal Jebaliya*, Madhavi Patel, Batuk Dabhi, Yashwantsinh Jadeja and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : hetal_jebaliya@yahoo.com, anamik_shah@hotmail.com

A simple, precise, reliable and sensitive isocratic RP-UPLC assay method of linezolid in bulk drug has been developed and validated for reducing analysis time and maintaining good efficiency. An isocratic separation of Linezolid was achieved on Waters Acquity BEH C18 (50 × 2.1 mm i.d., 1.7 µm particle size) column with a flow rate of 0.25 ml/ min and using photodiode array detector to monitor the eluent at 245 nm. Mobile phase consisting of methanol : water (50:50 v/v) is utilised to achieve good resolution and retention. The detector linearity was established by concentrations range of 20-80 µg/ml (r^2=0.999) with a limit of detection and quantification of 0.4 and 1.5 µg/ml respectively. Recovery of drug was achieved between 99 to 101%.

AP-CYSA-10 : 2,4-Dihydroxy-5-Bromo-α-phenyl-Aetophenone Thiosemicarbazone [DHB-α-PAT] as an Analytical Reagent : Studies on Fe(III) Chelate

Nitinkumar B. Patel and Yahpal J. Solanki

Shree Jayendrapuri Arts & Science College, Bharuch-392002
E-mail : solanki20002@yahoo.co.in

2,4-Dihydroxy-5-bromo-α-phenylaetophenone thiosemicarbazone [DHB-α-PAT] has been used for the spectrophotometric determination of Fe(III) at pH = 4.0. Job's method of continuous variation and Yoe and Jones Mole ratio method show metal: ligand ratio in the complex to be 1:1.The molar absorptivity of complex at 380 nm was found to be 6.90 $\times 10^3$ lit $mol^{-1}cm^{-1}$ and Sandell's sensitivity was found to be 0.00809 µg/cm^2. The stability constant determined spectro-photometrically is found to be 1.13×10^6 and Gibb's free energy change for complex formation reaction is calculated to be -8.308 k cal /mole. The Beer law is obeyed up to 5.58 ppm of Fe(III) ion at 380nm. From TG studies, the energy of activation for the decomposition step has been calculated and was found to be 8.33 k cal/mole. The reagent has been successfully applied for the determination of Fe(III) in pharmaceutical sample.

AP-CYSA-11 : Particle Size and Its Potential Health Risk of Exposure in Domestic Homes Located in Different Micro-environments

Poorti Varshney, Laxmi Singh and Ajay Taneja

Department of Chemistry, Dr. B. R. Ambedkar University, Agra-282002
E-mail : poorti.varshney@gmail.com

Indoor air quality refers to the air quality within and around buildings and structures in indoor environments that are highly complex and exposed to a variety of contaminants in the form of solids, liquids and gases particles. The high levels of indoor air pollutants in developing countries and the apparent scale of its impact on the global burden of disease underline the importance of particulate matter and its chemical constituents. As an environmental health risk and the consequence of exposure to airborne particulate matter resulted in the deposition of millions of particle in the lung, need for monitoring them particularly in indoor microenvironment. In addition to this the trace elements, especially those associated with airborne fine particulate matter may play an important role in adverse health effects. Therefore, the present study is carried out to perceive the current scenario of indoor air quality in different micro-environments in Agra region. The samples of $PM_{2.5}$ were collected on PTFE filter paper with the help of Fine Particulate Sampler (APM 550-Envirotech, New Delhi) during the monsoon season of 2012. They were also characterized for elements for their toxicity.

AP-CYSA-12 : Carbons and Trace Elements in Urban Soil of Raipur City, Chhattisgarh

Madhavi Rajak

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur-492010 (C.G.)
E-mail: m.rajak27@gmail.com

The urban soil quality is changing due to enormous anthropogenic activities in Asian countries. In the central India, several metal industries and coal based thermal power plants are running. In the present investigation, sources of black carbon (BC), organic carbon (OC), carbonate carbon (CC), Al, K, Ca, Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Sr, Ba and Pb are apportioned using cluster and factor analysis in the urban soil of the most industrilized city, Raipur, Chhattisgarh, India (21° 8' 24" N and 81° 22' 48" E). The surface soil (0-10 cm) samples were collected in March, 2010 from 17 sketches of Raipur city. The samples were crushed, dried and seived out of particles of mesh size ≤ 0.1 mm. The content of carbons and elements were analyzed by the thermal and TXRF methods, respectively. Significantly high contents of BC, Al, K, Ca, Ti and Fe were detected. Their contents are well correlated with the BC content. Their spatial variations, enrichment and sources are discussed.

AP-CYSA-13 : A Facile Spectrophotometric Method for the Determination of Hydrazine with Methyl Orange

Kishore K. Tiwari*, Vandana Agrawal[1] and S. K. Chattarjee

**Government Nagarjun P. G. College of Science, Raipur-492010*

A simple, precise, sensitive and accurate method was developed for the determination of hydrazine at microgram level. The method is based on oxidation of hydrazine to nitrogen with a known excess of bromine. Bromine in acidic media bleaches the dye methyl orange. A known excess of bromine, when treated with hydrazine is reduced to bromide and the unreacted bromine is determined using methyl orange. The absorbance of the methyl orange after the reaction was monitored spectrophotometrically at 530 nm. Actually as a result of the reaction the absorbance decreased, depending on the concentration of hydrazine. Beer's law was obeyed over the concentration range of 0.9 – 10 µg hydrazine in an overall aqueous volume of 25 ml of water. The molar absorptivity and Sandell's sensitivity of the method were found to be 7.2×10^4 l mol^{-1} cm^{-1}, and 0.0031-µg cm^{-2} respectively. The variables including reagents concentration, and effect of foreign species, were studied in order to optimize the reaction conditions. The proposed method has been successfully applied for the determination of hydrazine in water and biological samples. The results obtained in the described method compare well with reported method and the recovery studies of added hydrazine.

AP-CYSA-14 : Photocatalytic Degradation of Rose Bengal in the Presence of Tantalum Pentoxide

Shikha Panchal, Rakshit Ameta and Ritu Vyas

Department of Chemistry, Pacific College of Basic & Applied Sciences
PAHER University, Debari, Udaipur-313024 (Raj.)

The photocatalytic degradation of rose bengal was carried out in the presence of semiconductor tantalum pentoxide and the progress of the reaction was observed spectrophotometrically at 540 nm. Visible light was used as the source of energy. The effect of various operating variables like pH, concentration of dye, amount of semiconductor and light intensity on the rate of degradation was observed and the optimum conditions were obtained as pH = 7.0, [rose bengal] = 1.0×10^{-5} M, tantalum pentoxide = 0.1 g, light intensity = 50 $mWcm^{-2}$,

where the rate constant [k] was observed as 6.39×10^{-5} sec^{-1}. A tentative mechanism has been proposed for the photocatalytic degradation of dye, involving hydroxyl radical as an active oxidizing species.

AP-CYSA-15 : Heterogeneous Photo-Fenton Degradation of the Rose Bengal Dye Over Pillared Bentonite Containing Iron

Sangeeta Kalal, Rajeshwari Arora, and Vinod K. Sharma

Photochemistry Laboratory, Department of Chemistry, Mohan Lal Sukhadia University, Udaipur (Raj.)
E-mail : sangeeta.vardar@yahoo.in

Degradation of rose Bengal dye by heterogeneous photo-Fenton oxidation has been investigated over pillared bentonite containing iron. The heterogeneous conditions for the degradation offers many advantages like recyclability of catalyst, wider range of pH, no secondary pollution etc. over homogeneous conditions. Effect of various parameters like solution pH, amount of H_2O_2, dye concentration, amount of pillared clay (catalyst) was observed on the efficiency of the reaction. It has been observed that degradation follows pseudo first order kinetics. A tentative mechanism has been proposed for this photocatalytic degradation of rose Bengal.

AP-01 : 2, 4 Dihydroxy-5-Bromo [2'-Methyl] Propiophenone Oxime [DHBMPO] as an Analytical Reagent: Studies on Pd(II) Chelate

Nitinkumar B. Patel and Nirav H. Parekh

Shree Jayendrapuri Arts and Science College, Bharuch-392002
E-mail : parekhnh_85@yahoo.in

2, 4 Dihydroxy-5-bromo [2'-methyl] propiophenone oxime has been used as an analytical reagent for gravimetric and spectrophotometric determination of Pd(II) at pH 2.0. The Beer law is obeyed upto 12.77 ppm of Pd(II) ion at 440nm. The molar absorptivity and Sandell's sensitivity of the complex were also been calculated. Job's method of continuous variation and Yoe and Jones moles ratio method had reveal the M:L ratio of the complex to be 1:2. Stability constant determined spectrophotometrically and Gibb's free energy change for complex formation reaction were also calculated. From TGA studies, the energy of activation for the decomposition step has been calculated using Broido method. The reagent has been characterized on the basis of Elemental, IR, UV and NMR spectral studies. The reagent has been successfully applied for the determination of Pd(II) in the sample of Palladised carbon.

AP-02 : Determination of Methyl Parathion by an Indirect Spectrophotometric Method Using Potassium Permanganate

Sunita Kurup and Ajai Kumar Pillai

Department of Chemistry, Govt. V. Y. T. P. G. Auto College, Durg (C. G.)
E-mail : sunik09@gmail.com

A simple sensitive spectrophotometric method has been developed for the trace determination of methyl parathion using rhodamine B as chromogenic reagent. The proposed method is based on the reaction of methyl parathion with slight excess of potassium permanganate in acid medium and the unconsumed potassium permanganate is determined with rhodamine B. The dye shows maximum absorption at 495 nm. The reaction between methyl parathion and potassium permanganate is accelerated by irradiating the mixture with microwave energy for 50s at 970 W. Beer's law is obeyed in the concentration range 0.004-0.04 µg mL^{-1} for methyl parathion. The molar absorptivity and Sandell's sensitivity were found to be 2.25×10^5 L mol^{-1} cm^{-1} and 0.0012 µg cm^{-2} respectively. The limit of detection and quantification were 0.0012 and 0.0035 µg mL^{-1}, respectively. The tolerance limits of interfering ions are discussed. All variables were studied in order to optimize the reaction conditions. The validity of the method was checked by its simultaneous determination in formulation and vegetable samples and the results were statistically compared with those of a reference method by applying the Student's t-test and f-test.

AP-03 : Stability Indicating Validated HPLC Method for Simultaneous Determination of Paracetamol, Guiphenisin, Ambroxol, Phenylephrine HCl and Chloropheniramine Maleate in Commercial Dosage Form

Surekha Kolhal, Rama Lokhande, Rajiv Sutar, Sandip Surve, Sanjay Pednekar and Sanket Gudekar

Department of Chemistry, Jaipur National University, Jaipur, Rajasthan

A simple, precise and rapid stability indicating HPLC method was developed for the simultaneous quantitative determination of Paracetamol, Guiphenisin, Ambroxol, Phenylephrine HCl, and Chropheniramine maleate in a commercial dosage form. The separation was achieved with a 250 mm x 4.6mm, 5µm C18 column, by using a simple linear gradient. The method was validated as per ICH & FDA guidelines. The mobile phase A was 0.01M sodium perchlorate, monohydrate, pH 3.0 and mobile phase B was Acetonitrile. The flow rate was 1.5 ml/min and column temperature was maintained at

25^0C. The gradient program was set, with shorter runtime. The gradient separation was achieved within 15 mins. The described method was validated with respect to system suitability, specificity, linearity, precision and accuracy. The precision of the assay method was evaluated by carrying out six independent assays of paracetamol, guiphenisin, ambroxol, phenylephrine HCl, and chropheniramine maleate. The accuracy of the method was evaluated in triplicate at three concentration level i.e. 50%, 100% and 150% of target test concentration. The described method was linear over the range of 50 to 150%. The method is simple, rapid and accurate and can be used for routine analysis of these drugs in commercial dosage form.

AP-04 : Simultaneous RP-HPLC Determination of Three Main Ingredients in Finished Dosage Form Aceclofenac, Thiocolchicoside and Paracetamol Tablet as Active Ingredients

Sanjay Pednekar, Rama Lokhande, Rajiv Sutar, Sandip Surve, Surekha Kolhal and Sanket Gudekar

Department Of Chemistry, Jaipur National University, Jaipur, Rajasthan

A novel and single RP-HPLC method was developed for the determination of four active ingredients (acelofenac thiocolchicoside and paracetamol) in pharmaceutical dosage form, and validated the method as per ICH and FDA guidelines. The separation was achieved on Thermo Hypersil CPS column, 25 cm × 4.6 mm, 5 µ in the simple isocratic mode using buffer containing potassium dihydrogen phosphate and methanol. Mobile phase prepared contained the mixture of buffer: Methanol (80:20) with flow rate of 0.5 mL per min. Column oven temperature maintained at 25°C and performed the analysis on UV detector using 220 nm. The method was validated by determining its sensitivity, linearity, accuracy and precision. The proposed method is single, shorter runtime, accurate and reproducible. This method can be applied for routine analysis of all three active ingredients quantification in pharmaceutical dosage form. The method is simple, rapid and accurate and can be used for routine analysis of these drugs in solid dosage form.

AP-05 : Nanotechnology in Medicine

Jeeru Sravan Kumar Reddy* and Shaik Basher Dada

Department of Biotechnology, GITAM University, Visakhapatnam-530045
E-mail : sravan.kumar.reddy.94@gmail.com

Nanotechnology is expected to open some new aspects to fight and prevent diseases using atomic scale tailoring of materials. The ability to uncover the structure and function of biosystems at the nanoscale, stimulates research leading to improvement in biology, biotechnology, medicine and healthcare. The size of nanomaterials is similar to that of most biological molecules and structures; therefore, nanomaterials can be useful for both in vivo and in vitro biomedical research and applications. The integration of nanomaterials with biology has led to the development of diagnostic devices, contrast agents, analytical tools, physical therapy applications, and drug delivery vehicles. In all the nanomaterials with antibacterial properties, metallic nanoparticles are the best. Nanoparticles increase chemical activity due to crystallographic surface structure with their large surface to volume ratio. The importance of bactericidal nanomaterials study is because of the increase in new resistant strains of bacteria against most potent antibiotics.

AP-06 : Stability Indicating HPLC Method Development and Validation of Chlorhexidine Gluconate and Lidocaine Hydrochloride in Throat Spray

Vijay R. Ram[a]*, Kapil L. Dubal[b], Govind J. Kher[c] and Hitendra S. Joshi[b]

[a]Department of Chemistry, KSKV Kachchh University, Bhuj-370 001, Gujarat
[b]Department of Chemistry, Saurashtra University, Rajkot-360 005, Gujarat,
[c]Department of Chemistry, Tolani college of Arts and Science, Adipur-370205, Gujarat
E-mail : drhsjoshi49@gmail.com

The objective of the current study was to develop simple, precise and accurate gradient reversed-phase stability indicating HPLC assay method and validate for determination of chlorhexidine gluconate and lidocaine hydrochloride in throat spray. Isocratic RP-HPLC separation was achieved on a SGE make SS Wakosil II 5C8RS column (150mm x 4.6mm i.d., 5 µm particle size) using mobile phase of acetonitrile – 50mM sodium hydrogen phosphate monobasic dihydrate buffer pH 3.0. At a flow rate of 1.0 ml/min and the detection was carried out at 215 nm by using photo-diode array detector. The drug was subjected to oxidation, hydrolysis, photolysis and heat to apply stress condition. The method was validated for specificity, linearity, precision, accuracy, robustness and solution stability. The method was linear in the drug for chlorhexidine gluconate, concentration range of 40-160 µg/ml with a correlation coefficient 0.9983 and for lidocaine hydrochloride concentration range of 16-64 µg/ml with a correlation coefficient 0.9998. The mean recovery for chlorhexidine gluconate was 100.74-102.60 % and 99.07-101.11 % for lidocaine hydrochloride. Degradation products produced as a result of stress studies did not interfere with detection of chlorhexidine gluconate and lidocaine hydrochloride and the assay can thus be considered stability indicating.

AP-07 : Limnochemical Studies Using Voltammetric Probe and Spetrophotometry

M. Sallam, G. P. Sahu and S. C. Lavale*

Chemical Research Laboratory, J. H. Govt. P. G. College, Betul 460001 (M.P.)

Limnochemist has rarely to deal with single water sampling. Internationalchemical year – 2011 motivated to study some plants, animal and water samples of distinct region of Betul belt district. Sallam et.al. has undertaken Advanced voltammetric method viz. polarography, NPP, DPP and amperometry have been successfully used to analyses multicomponenet material and the samples collected from the district places. A survey of district river of Betul district revealed important information and scope of studies from the Chemical view points. Analysis of plant material after soxhhet extretion, determination of various data in different water sample after proper sampling and discussion from biodiversity view point have been summerised in the present paper. The data computed shell be fruitful from the view point of Bio-analytical, limnochemical aspect. pH, conductance, TDS, salinity, alkalinity, MPN, colliform and bacterial parameter have been tabulated.

AP-08 : Isonitroso-4-methyl-2-pentanone Impregnated Amberlite XAD-4 Resin as a Novel Extractant Impregnated Resin for Th(IV) Enrichment from Different Real Samples

Sandesh R. Tetgure, Dipak J. Garole, Amulrao U. Borse and Arun D. Sawant

School of Chemical Sciences, North Maharashtra University, Jalgaon (M.S.)
E-mail : amulborse@gmail.com

A method based upon impregnation of Amberlite XAD-4 with extractant Isonitroso-4-methyl-2-pentanone (HIMP) was presented for Th(IV) enrichment and spectrophotometric determination in a variety of samples. Prepared novel Extractant Impregnated Resin (EIR) sorbent was characterised by FTIR and SEM analysis. The sorbent packed in a column was studied for various parameters such as pH, eluent, sample and eluent flow rates to optimize sorption desorption condition for Th(IV). Th(IV) was quantitatively sorbed at pH 3.0 and was recovered with 4.0 M HCl. The influence of other ions on Th(IV) sorption investigated and facilitated its determination in synthetic mixtures, monazite sand, sediments, spiked water samples. The method for Th(IV) determination had a limit of detection 0.24 µg L^{-1}, limit of quantification 0.81 µg L^{-1}, a preconcentration factor of 150 and a relative standard deviation (RSD) ≤ 1.5 %.

AP-09 : Synthesis and Characterization of Mannich Polyols by using Epoxides From Low-Cost Natural Oil

Tejas S. Gandhi[1], Mayank R. Patel[2] and Bharat Kumar Z. Dholakiya[1*]

[1]Department of Applied Chemistry, Sardar Vallabhbhai National Institute of Technology (SVNIT),Surat-395007, Gujarat
[2]Chemical Sciences Dept., N. V. Patel College of Pure & Applied Sciences, Vallabh Vidyanagar-388120, Gujarat
E-mail : tejsvnit.ac.in@gmail.com, tejasgandhi1401@gmail.com

Cashew nut shell liquid (CNSL) is natural aromatic organic oil consisting of phenolic interesting structures. Extraction of CNSL was carried out by using Soxhlet extraction method. The major component of CNSL is anacardic acid (90%) which is easily de-carboxylated to cardanol (10%) by using conventional method. This paper work described the synthesizes of mannich polyols for rigid foams and different types of mannich polyols based on epoxides from natural oil by three steps synthesizes process. Synthesized polyols were characterized by spectrometry methods (FTIR and ^{1}H-NMR) and thin layer chromatography.

AP-10 : Extractive Spectrophotometric Determination of Iron (II) With [N - (O -Methoxy Benzaldehyde)- 2 – Amino Phenol]

Ritika M. Makhijani and V. D. Barhate[*]

V.E.S. College of Arts, Science and Commerce, Sindhi Society, Chembur, Mumbai - 400071
E-mail : vasantbarhate@yahoo.co.in

A simple, rapid and sensitive spectrophotometric method has been developed for the determination of Fe (II) by using N - (o - methoxy benzaldehyde) 2 - aminophenol (NOMBAP) as an analytical reagent. NOMBAP has been synthesized and characterized by elemental and spectral analysis. NOMBAP extracts Fe (II) quantitatively (99.67%) into ethyl acetate from an aqueous solution of pH range 5.6 - 6.8. The ethyl acetate extract shows an intense peak at 470 nm (λ_{max}). Beer's law is obeyed over the Fe (II) concentration range of 1 - 7 µg/ml. The sandell's sensitivity and molar absorptivity for Fe - NOMBAP system is 0.0176 $\mu g cm^{-2}$ and 3166 L $mole^{-1} cm^{-1}$ respectively. The composition of extracted species is found to be 1:2 (Fe:NOMBAP) by Job's Continuous Variation and Mole Ratio Method. The average of 10 determination of 50 µg of Fe (II) in 10cm^3 of solution is 49.85 µg which is varied between 49.61 µg and 50.09 µg at 95% confidence limit and standard deviation is ±0.337. Interference by various ions has been studied. The proposed method has been successfully applied for determination of Fe (II) in Pharmaceutical samples.

AP-11 : Liquid-liquid Extraction of Chromium (VI) from Mineral Acid Solutions by TOAO

A.V.L.N.S.H. Hari Haran* and D. Murali Krishna

**Department of Chemistry, Gitam Institute of Technology, Gitam University, Visakhapatnam - 530 045*
E-mail : ahharan@gmail.com

Electroplating effluents containing chromium(III), chromates or dichromate are suitable for chrome-plating and for etching and passivation of metallic details. Moreover chromium (III) is less toxic than chromium(VI). In view of this the separation and determination of chromium has been receiving considerable attention. The extraction of chromium (VI) from tri-n-octyl amine oxide (TOAO) in benzene has been studied. The optimum conditions for extraction were established from the study of the effect of several variables like concentration of extractant, metal ion, acidity etc. The extractions are nearly quantitative hydrochloric and sulphuric acid & are partial from nitric acid systems. The extracted species are identified. The method has been applied for the recovery and determination of chromium in alloys as well as electroplating effluents.

AP-12 : N, N'-O-phenylene (Acetylacetoneimine) as a New Analytical Reagent for the Extractive Spectrophotometric Determination of Nickel

Sonali S. Patil[1] , Rama. S. Lokhande[2], S.B. Dharap[3], Poonam P. Shevde[4] and Jayashree S. Patil[5]

[1]Department of Chemistry, JSM college, Alibag, Raigad, Maharashtra, 402201
[2]School of Basic Sciences, Department of Chemistry, Jaipur National University, Jaipur
[3]Bhausaheb college of Arts, Science and Commerce, Pen, Raigad, Maharashtra
[4]Department of Chemistry, University of Mumbai, Vidyanagari, Santacruz (E) Mumbai, Maharashtra
[5]Department of Chemistry, JSM college, Alibag, Raigad, Maharashtra, 402201

N, N'-O-Phenylene (acetylacetoneimine) was synthesized subjected to FTIR, NMR, elemental analysis and Mass Spectroscopy for characterization. The synthesized reagent was then applied for liquid – liquid extraction and spectrophotometric determination of Ni (II). Nickel metal forms pinkish brown coloured complex, which can be extracted in chloroform at pH 3.8, having absorption maxima at 450 nm. The Molar absorptivity and Sandell's sensitivity was calculated on the basis of total nickel (II) taken. The developed method is highly sensitive, selective, simple, rapid, accurate, and has been satisfactorily applied for the determination of nickel in the synthetic mixtures.

AP-13 : Study of IR X-ray Diffraction and Thermo Gravimetric Analysis on Sr(II) and Zn(II) Ions Exchanged and Adsorbed Derivatives of Natural Zeolite-Na

P. P. Talware* and P. M. Yeole[1]

**Department of Chemistry, K.A.M. Patil Arts, Commerce and Science College, Pimpalner, (Dhule) 424306*

[1]Center for P.G. Research in Chemistry, R.L. College, Parola-425111 (Jalgaon)

In the present work natural zeolite is exchanged with Sr(II) and Zn(II) ions. The compositional analysis of the natural zeolite and the exchanged derivative has been carried out using inductive Coupled Plasma - Atomic Emission Spectroscopy (ICP- AES). The structural changes are studied by IR – Spectroscopy. The X-Ray Diffraction technique is used to determine the unit cell structure. Thermal studies of the natural zeolite, its exchanged derivatives and the adsorbed derivatives are carried out using Thermo Gravimetric Analysis, (TGA).

AP-14 : Fluorescence Studies on Solubilization of 4-Hydroxyacetanilide in Various Micellar Solutions

Seema Acharya and Komal S. Sengar

Department of Chemistry, JNV University, Jodhpur-342005

4-Hydroxyacetanilide (4-HA), paracetamol is a widely used analgesic and antipyretic drug. The study of interaction of 4-HA, a medicinally important molecule, with the micelles of nonionic and ionic surfactants is of great importance in pharmaceutical chemistry. The studies have been conducted by fluorescence and absorption spectral techniques at room temperature. The influence of surfactant structure, concentration and working experimental conditions on the solubilization of 4-HA is thoroughly evaluated and discussed. 4-HA shows fluorescence excitation peak at 290 nm and emission peak at 390 nm. The fluorescence intensity of 4-HA is significantly enhanced in micellar media of nonionic, anionic and cationic surfactants, accompanied by a large blue shift of 40-45 nm in emission peak position except TX-100 and CPC. TX-100 and CPC showed exceptional effects of quenching the fluorescence of 4-HA. To supplement the solubilizing action of the surfactants, theortical calculations of some spectral parameters like molar extinction coefficient, fluorescence quantum yield, empirical fluorescence coefficient and Stokes' shift values have been determined in these micellar media at their different concentrations. The data were found to be in good agreement with the experimental results. The results have been attributed to micellization of the surfactant followed by solubilization of the solubilizate. This gives a better view of interplay of different favorable and unfavorable forces guiding micellization.

AP-15 : Spectrophotometric Determination of Micro Amounts of Uranium (VI) using Bromocresol Purple as an Analytical Reagent

Aparna Bhardwaj

Department of Chemistry, B.N. Bandodkar College, Thane, Mumbai
E-mail : dr.aparna73@rediffmail.com

Bromocresol Purple dye is used as a reagent for the spectrophotometric determination of uranium (VI). The reagent forms a strawberry red coloured complex with uranium (VI) instantaneously at pH 5.0 - 6.0. A six fold molar concentration of the reagent is necessary for the full development of the colour intensity. Beer's law is valid over the concentration range 0.2380 -2.142 μgml^{-1} . The complex has absorption maximum at 498 nm with molar absorptivity 2.1×10^5 $Lmol^{-1}cm^{-1}$ and sensitivity is 4.76 ng ml^{-1} respectively. The standard deviation has been found to be 0.00063.

AP-16 : Alcohol Production from Cellulose by *Zymomonas* Bacteria

P. K. Jain[*] and Amrita Verma

[*]*Physical Chemistry Division, National Sugar Institute, Kanpur-208017*
E-mail : drjainnsi@gmail.com

The alcohol production is generally carried out with yeasts; however some bacterial strains such as *Zymomonas mobilis* and *Zymomonas anaerobia* have also been used. Bacterial fermentation is more advantageous than yeast fermentation in certain respects viz. fast rate of growth, low biomass formation etc. In the present study the bagasse cellulose hydrolysate has been subjected to fermentation by *Z. mobilis* and *Z. anaerobia*, sugar concentration ranging from 1-5%. For the study the bacterial cultures were attenuated on the hydrolysate for a period of six days by adding traces of nutrients in the form of ammonium sulfate, phosphoric acid and yeast extract. The fermented wash was analyzed for residual sugar and alcohol % based on which fermentation efficiency values were calculated. The results show that all the sugars were consumed when initial concentration of sugar was 1%. The data obtained from the fermentation of cellulose hydrolysate with *Z. anaerobia* shows the same pattern of fermentation parameter as obtained with *Z. mobilis* but in this case the values of residual sugars were lower than those obtained with *Z. mobilis.* Thus both the strains could carry out effective

fermentation of bagasse cellulose hydrolysate but at lower initial sugar concentration.

AP-17 : Physico-chemical Study of Ground Water of Different Locations of Agra City

Amit K. Agarwal* **and Sandhya Agarwal**

Department of Chemistry, Agra College, Agra-282002 (U.P.)
B. R. Ambedkar University, Agra
E-mail : agarwal.chem@yahoo.co.in

In today's world the demand of water is continuously increasing due to massive increase in population and human activities. For the present study, different samples of groundwater have been collected from the different locations of Agra city. The results of this study were compared with the water quality standards of WHO and ISI. In this study physico-chemical parameters like turbidity, temperature, odour, color, conductance, pH, chemical oxygen demand (COD), total dissolved solids (TDS), total alkalinity and concentrations of ions like 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 odour, quality characteristics.

AP-18 : Use of 2,4-Dihydroxy-5-BromoButyrophenone Oxime [DHBBO] as an Analytical Reagent for Cu(II)

Amish B. Patel*[a] and Nitinkumar B. Patel*[b]

[a]Faculty of Engineering Technology and Research, Bardoli-394 620
*[*b] Shree Jayendrapuri Arts and Science College, Bharuch-392 002*
E-mail : amishrofel@yahoo.com, abp.fetr@gmail.com.

2,4-Dihydroxy-5-bromobutyrophenone oxime [DHBBO] has been used as an analytical reagent for the gravimetric and spectrophotometric determination of Cu(II) ion. The reagent gives buff precipitate with Cu(II) in the pH range 2.0 to 10.0. Job's method of continuous variation and Yoe and Jones mole ratio method show metal:ligand ratio in the complex to be 1:2. Beer's law is obeyed up to 20.33 ppm of Cu(II). The molar absorptivity of complex was found to be 1.444×10^3 lit. mol^{-1} cm^{-1}. and Sandell's sensitivity was found to be 0.044 µg of Cu(II)/cm^2. The stability constant of the complex is found to be 5.875×10^9. The reagent and its complex have been characterized by elemental analysis and IR spectra. The complex was subjected to thermogravimetric analysis to study its decomposition pattern. The reagent has been used for the analysis of brass.

AP-19 : XRD and SEM Analysis of Tapti River Sediments

B.H. Patil and V.S. Shrivastava

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar - 425412

For this study the sediment samples were collected from Tapti basin near Chopra district Jalgaon, Maharashtra, India. The samples were sedimented and concentrated by centrifuge method for extraction of clay. X-ray Diffaction (XRD) and scan electron microscopy (SEM) analysis have been carried out for the samples. The analysis indicate the clay samples contain Quartz(Silica) and Kaolinite minerals while smectie was found in traces. Beside the above analysis the same samples have also been analysed for Physico Chemical and metallic Status.

AP-20 : Degradation of Indigo Caramine Dye by Sol Gel Deposited Nanocrystaline Cadmium Sulphide Thin Film

Yogesh V. Marathe, Swapnil Padvi, Prafulla Patil and V. S. Shrivastava*

Nano Chemistry Research Laboratory, G.T.P. College, Nandurbar-425412, (M.S.)
E-mail : drvinod_shrivastava@yahoo.com, yogeshmarathegtpc@gmail.com

The photo catalytic degradation of azo dye indigo caramine was investigated using CdS thin film in aqueous solution under irradiation of mercury lamp. CdS nanocrystaline thin film was prepared by using sol gel dip coating method. The surface characterization, morphology and size of crystals were examined by SEM and XRD technique. The size of nano particle found 45 nm. SEM revealed that film is uniform and without any cracks. Optical characterization of thin film was performed by UV Visible spectroscopy. CdS film shows high transmittance i.e. more than 60% and increases with increase in wavelength. Absorption band edge found in the wavelength ranges 350-450 nm. The optical band gap of sol gel deposited thin film is found to be 2.84 eV. The obtained nanocrystaline thin film was employed in experiment of photo catalytic oxidation of water soluble indigo caramine azo dye. The effect of operational parameters i.e. pH of the solution, dye concentration, irradiation time, solar irradiation and reusability of photo catalyst on degradation rate of azo dye in aqueous solution was examined. The best conditions for maximum photo catalytic degradation of indigo caramine were found acidic pH, solar irradiation and 40 ppm initial dye concentration. The mineralization of indigo caramine dye was examined by TOC.

AP-21 : Investigations on Polycyclic Aromatic Hydrocarbons and Poly Chlorinated Biphenyls Yearly Based Concentration in Waste Oil-sludge at Mathura-Agra Region

Mitali Sharma*, **M. K. Rawat and S. C. Goyal**

Department of Chemistry, Agra College, Agra-282002
E-mail : m.sharma333@yahoo.com

Methodology for the determination of Polycyclic Aromatic Hydrocarbons (PAHs) and Poly Chlorinated Biphenyls (PCBs) was used to investigate yearly based Concentration in Waste Oil-sludge at Mathura-Agra Region. The average concentration of total PAHs and PCBs in all samples was 11.14 µg g^{-1}, 6.76 µg g^{-1} and 13.44 µg g^{-1}, 20.38 µg kg^{-1}, 12.91 µg kg^{-1} and 29.19 µg kg^{-1}. The maximum concentration of PAHs and PCBs were found to be in winter season.

AP-22 : Accumulation of Heavy Metals through Industrialisation

B. H. Patil and V. S. Shrivastava

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar-425412

The accumulation of metals (viz. Cu, Zn, Cd , Pb, Ni, Cr, As, Hg) have been studied in water, soil, sediment, aquatic sediment, and plant samples. The concentration of these metals was determine by inductively coupled plasma atomic emission spectrometry. In river water sample, only Cu and Zn were detected. In aquatic sediment, Ni, and As were not found, whereas in soil samples, As and Hg have not been detected. For accumulation of the metals by plants, chilli, jawar, cotton, rice, sugarcane, groundnut and maize plants were selected and analysed. This concentration of metals is due to industrialistion.

AP-23 : Heavy Metals in Cultivated Soils and River Sediments and their Correlation Study

B. H. Patil and V. S. Shrivastava

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar-425412

The soil samples were collected from surface of the soil from different agriculture fields in the Khandesh region where cotton, sugarcane, chilli, banana, jawar crops were cultivated. Tapti river aquatic sediments samples were also collected from the five different stations which were 10 – 15 kms away from each other for the similar study. The concentration of heavy metals like Cu, Zn, Cd, Pb, As, Hg, Cr and Fe was estimated by ICP-AES. Beside the metal analysis the physiochemical characteristics of samples have also been evaluated.

AP-24 : Metallic and some Physico –Chemical Studies of Soil and Aquatic Sediments

B. H. Patil and V. S. Shrivastava

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar-425412

The soil samples were collected from surface of the soil from different agricultural fields in the Khandesh region where wheat, Jowar, cotton, sugarcane and groundnuts crops were cultivated. The tapti river sediments samples were also collected from five different stations which were 7-8 km away from each other. The concentrations of heavy metals such as Cu, Zn, Cd, Pb, Hg, As, Ni and Cr have been determined by ICP-AES. Physico chemical characteristic like pH, EC, TA, WES,Cl and HCO_3 – have been detected by following standard methods.

AP-25 : Deposition of Macro and Micro Nutrients in Soil and Sediments of River Tapti Because of Industrial Developement

B. H. Patil and V. S. Shrivastava

Centre for P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar-425412
E-mail : clayminerals@rediffmail,com

In the present study soil and sediment samples were collected from the bank of Tapti river from Taloda to Kukurmunda for their physico chemical and metallilc characteristics. These samples showed two fold increased level of studied parameters in comparison with relatively non polluted values. The stastical evaluations were made by following standard methods. Also, metal analyses by ICP-AES were included in the statistics. Further the results of correlation coefficient and t-test values indicate positive correlation in deposition and significant at 5 % level of confidence. The higher contents of concentration of parameters of physico – chemical characteristics and metals in soil and sediments are attributed to surrounding industrial activity.

AP-26 : Adsorption Kinetics for the Removal of Hexavalent Chromium from Aqueous and Mixed Aqueous-organic Solvents on Weak base Anion Exchanger

Prasanna S. Koujalagi, Sanjaykumar V. Divekar and
Raviraj M. Kulkarni

Department of Chemistry, Gogte Institute of Technology, Udyambag, Belgaum 590 008
E-mail : pskoujalagi@git.edu

Removal of Cr(VI) from aqueous and aqueous-organic solvent mixed media was investigated using Tulsion A-2X (MP). The efficiency of this resin was studied under various experimental conditions, such as initial metal ion concentration, temperature, pH and dielectric constant of the medium. Percentage of adsorption of Cr(VI) was found to decrease with increase in temperature at varying concentrations of solvent medium. Under the optimum experimental conditions 70% of Cr(VI) was removed in 15 minutes with an initial feed concentration of 0.0011M. Kinetic experiment revealed that the adsorption equilibrium was attained within 225 minutes. Removal of Cr(VI) was maximum (95.91%) on weak base resin in the pH range of 5 to 6. The negative values of ΔG indicated the feasibility and spontaneous nature of adsorption. Freundlich and Langmuir adsorption isotherms were studied and discussed for the Cr(VI) removal. Separation factor for adsorption of Cr(VI) was between 0 and 1, which indicated the adsorption was favorable. Chromium adsorption follows the first order kinetics. The resin Tulsion A-2X(MP) can be used in the treatment of chromium contaminated water effectively.

AP-27 : Determination of Physico-chemical Parameters of Untreated Waste Water Samples, Bhopal (India)

Ram Kumar Kushwah[1], Suman Malik[1], Avinash Bajpai[2] and Raj Kumar[3]

[1]Department of Chemistry, Sadhu Vaswani College, Bhopal
[2]Makhanlal Chaturvedi University, Bhopal
[3]Sagar Institute of Science and Technology (SISTec), Bhopal
E-mail : ramkumarkushwah@yahoo.com

The investigation was conducted to monitor the physico-chemical parameters of untreated waste water at sewage treatment plant, Bhopal. The result revealed that the untreated waste water has high inorganic and organic pollution load. The treatment plant received the waste water from various sewage pumping houses. In the present study, some physico-chemical parametes like turbidity, chloride, alkanity, phosphate and total hardness was analyzed using standard methods. The results of analysis of waste water indicates that it's highly polluted. Therefore it's recommended for treatment and management of waste water for reuse.

AP-28 : Synthesis and Characterization of Activated Carbon Prepared from Bio-waste Materials

Chubaakum Pongener, K. S. Rao and Dipak Sinha

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

Activated carbons have been prepared from *Mucuna purine plant* waste materials by heat treatment and subsequent oxidation with

Nitric acid. The activated carbon prepared is characterized in terms of its ash content, moisture content, volatile matter, acid-soluble matter, water soluble matter, pH, elemental analysis, surface area, pores size etc. From SEM analysis It is found that the prepared activated carbon contains different pore sizes ranging from around 50 nm to few microns. The EDX studies confirms the presence of Nitrogen, Oxygen, Sodium, Calcium, Sulphur and elements. IR studies reveal the presence different functional groups like Hydroxyl, Carbonyl, amines etc. Presence of different functional groups on the surface of the activated carbon and also formation of different pore sizes can make this prepared activated carbon a candidate for different applications such as purification of water samples and removal of fluoride from water samples.

AP-29 : Flyash in Concrete : Economic and Ecological Benefits

Rashmi Mohan Mathur and Anuradha Varshney

Department of Chemistry, Dayanand Girl's P.G. College, Kanpur (U.P.)

Fly-ash(FA) a residue of coal combustion in thermal power plants is an environmental hazard all over the world. FA management is a great concern for environmentalists. FA is a cementacious material which improves workability, reduces segregation and bleeding by providing greater fine volume and lower water content for a given workability of fresh and hardened concrete. The increased fineness usually increases the water demand; the spherical particle shape of FA lowers particle friction and offsets such effects. Concrete with relatively high FA content requires less water than non FA concrete of equal slump and hence to maintain w/c ratio, less cement is required. Compressive strengths of ready-mix concrete (RMC) with FA and cement obtained from 150mm cubes following IS 519:1999 were compared with the RMC without FA. Various types of super-plasticizers were used with different w/c ratio to find best combination to make concrete more economic and environment friendly.

AP-30 : New Approach in Utilization of Photocatalysts in Removing Heavy Metals from Industrial Waste Water

K. M. Joshi*and V.S. Shrivastava

Nanochemistry Research Laboratory, G.T.P. College, Nandurbar 425412
E-mail : kmjoshi35@gmail.com, drvinod_shrivastava@yahoo.com

Strong contenders as environmentally harmonious catalysts are photocatalysts that operate at room temperature and in a clean manner, while applications of such safe photocatalytic systems are urgently desired for the purification of waste water. Innovative process for treating industrial wastewater containing heavy metals often involved technologies for reduction of toxicity in order to meet photoctalysis technology. It is recent developments and technical applicability of various treatments for the removal of heavy metals from industrial wastewater. A particular focus is given to innovative removal process for continuous photocatalysis by thin film. Their advantages and limitations in applications are evaluated. The main operating conditions such as pH, dosage of photocatalysis are presented. In the near future, the most promising method to treat on metal complex will be nano photocatalytic compounds. To address such enormous tasks, photocatalytic systems that are able to operate effectively and efficiently not only under UV light but also under the most environmentally ideal energy source, sunlight.

AP-31 : An Eco-friendly Synthesis, Characterization Morphology and Electrical Properties of a Copolymer Resin

Charulata S. Makde[a], Mudrika Ahamed[a] and W. B. Gurnule[b*]

[a]*Department of Chemistry, Priyadarshni College of Engineering, Nagpur 440019, Maharashtra*
[b]*Department of Chemistry, Kamla Nehru Mahavidyalaya, Sakkardara, Nagpur 440010, Maharashtra*
E-mail : wbgurnule@yahoo.co.in

A 2,4-dihydroxyacetophenone-Adipamide-Formaldehyde (2,4-DHAAF) terpolymer resin was synthesized by an eco-friendly technique using hydrochloric acid as a reaction medium. The 2,4-DHAAF terpolymer was characterized on the basis of elemental analysis, ultraviolet-visible, FTIR, ^{13}C NMR, ^{1}H NMR, viscosity and average molecular weight. The physicochemical parameters have been evaluated for the copolymer resin. The kinetic parameters such as energy of activation and the order of reaction have also been evaluated on the basis of the thermogravimetric data using Freeman-Carroll method. The surface morphology of the copolymer resin was examined by scanning electron microscopy and it established the transition state between crystalline and amorphous nature. The colour of the copolymer resin was confirmed by optical photograph. The electrical property of the copolymer resin showed an appreciable change in the conductivity of the resin at various concentration and temperature.

AP-32 : Adsorption of Fluoride from Aqueous Solution by Azadirachta Indica (Neem) Leaf Powder

R. S. Dave* and M. T. Machhar[1]

**Dept. of Chemistry, Arts, Commerce, & Science College, Pilvai (North Gujarat)*
[1]Department of Chemistry, J & J Science College, Nadiad (Gujarat)
**E-mail : rajendradave_63@yahoo.com*

In this study, powder of bioadsorbent was prepared from the neem (Azadirachta indica) tree leaves by crushing the dry leaves and the prepared powder of bioadsorbent was used to remove fluoride from aqueous solutions. Adsorption was carried out in batch process with several different concentrations of fluoride by varying amount of adsorbent, pH, agitation time and temperature. The uptake of the fluoride ions was very fast initially, but gradually slowed down indicating penetration into the interior of the adsorbent particles. Both first order and second order kinetics were tested and it was found that the latter gave a better explanation. The experimental data closely followed both Langmuir and freundlich isotherms. The adsorbent had a considerably high Langmuir monolayer capacity of 200 mg/L. A small amount of adsorbent (1 gm/ L) could remove as much as 90 % of fluoride in 300 min from solution of concentration of 100 mg/L at 300 K. The adsorption continuously increased in the pH range 2.0-7.0, beyond which the adsorption could not be carried out due to the precipitation of the fluoride ions.

AP-33 : Synthesis and Characterisation Of Process Related Impurity in Bosentan Monohydrate.

Sanket Gudekar , Rama Lokhande, Rajiv Sutar, Sanjay Pednekar, Sandip Surve and Surekha Kolhal

Department of Chemistry, Jaipur National University, Jaipur, Rajasthan

One of the known impurity in Bosentan monohydrate is N,N'-(ethane-1,2diyl{oxy[5-(2-methoxy)-2,2'-bipyrimidine-6,4-diyl]})bis(4-tert-butylbenzenesulphonamide.(Dimer impurity in Bosentan monohydrate) is synthesized by novel method and characterised.

Dimer impurity in Bosentan Monohydrate is synthesized using Bosentan monohydrate and 4-(1,1-dimethylethyl)-*N*-[6-chloro-5-(2-methoxyphenoxy)[2,2'-bipyrimidin]-4-yl]-benzenesulfonamide using sodium tertiary butoxideas a reagent and dimethyl formamide as a solvent. Reaction is carried out at ambient temperature. Resultant oil is then stirred with mixture of methanol and ethyl acetate to yield crude dimer solid,which is then purified by using column chromatographic technique to give pure Bosentan Dimer solid. It is then characterized with the help of NMR ,IR and Mass.

AP-34 : Study of Photochemical Reaction Involving Nitrosyl Pentacyanoferrate(II) : Dimethyl Urea System

Mayank R. Mehta[1]**, Tarun J. Patel**[2] **and Vipul P. Prajapati**[2]

[1,2]Shri P.H.G. Muni. Arts and Science College, Kalol-382721 (Gujarat)
[3]Sheth M.N. Science College, Patan-384 265 (Gujarat)
E-mail : vipul_hely@yahoo.com

Sodium nitroprusside contains cyanide ligands that cannot be so easily replaced chemically. An effort has been made to substitute this ligand by another ligand like dimethyl urea. The progress of this photochemical reaction has been observed spectrophotometrically and the product was isolated and characterized. The effect of different parameters like pH, intensity of light concentration of sodium nitroprusside and ligand, concentration on the yield of this substitution reaction have been studied. A tentative mechanism for this reaction has been proposed.

AP-35 : Observation of Photochemical Ligand-substitution Reaction Involving Nitrocy Pentacyano Ferrate(II) and Mixed Ligand Like Sulphite and Dithionate

Mayank R. Mehta[1] **and Vipul P. Prajapati**[2]

[1]Shri P.H.G.Muni. Arts and Science College, Kalol-382721 (Gujarat)
[2]Sheth M.N.Science College, Patan-384 265 (Gujarat)
E-mail : vipul_hely@yahoo.com

Nitrosyl pentacyanoferrate(II) contains cyanide ligands that cannot be so easily replaced chemically. An effort has been made to substitute CN- ligand by another mixed anionic ligand like sulphite and dithionate. The progress of this photochemical reaction has been observed spectrophotometrically and the product was isolated and characterized. The effect of different parameters like pH, intensity of light concentration of sodium nitroprusside and ligand, concentration on the yield of this substitution reaction have been studied. A tentative mechanism for this reaction has been proposed.

AP-36 : Drinking Water Quality in Agra District, India with Special Reference to Heavy Metals

Durgesh Raj Mohan and M. K. Rawat[*]

Department of Chemistry, Agra College, Agra
E-mail : mkrawat_chem.@yahoo.co.in

Contamination of drinking water by arsenic and other heavy metals and their related toxicology is a serious concern now-a-days. Millions

of individual world-wide are suffering from the arsenic and other heavy metal related diseases due to consumption of contaminated groundwater. 40 water samples from different localities of Agra district were collected to study the potability of water for drinking purpose. The water samples collected from sources like hand pumps and jet pumps were analysed for arsenic, heavy metals like manganese, zinc, iron, lead, cadmium, copper etc. with pH, total hardness, total dissolved solids, total alkalinity, calcium, magnesium, chloride, fluoride and sulphate. The results were compared with the values stipulated by WHO and BIS and found that the groundwater of most of the localities of Agra district is not fit for direct human consumption with respect to total dissolved solids, total hardness, fluoride, chloride and most of the heavy metals. The study reveals that the water quality of most of the localities of Agra district is not suitable for drinking purpose which recommends the use of indigenous technologies to make water fit for drinking purpose.

AP-37 : Groundwater Quality in Amalner Town, Maharashtra, India

V. T. Patil* **and P. R. Patil**

**Department of Chemistry, Z.B. Patil College, Dhule-424002*
School of Environmental and Earth Sciences, North Maharashtra University, Jalgaon-425 001, Maharashtra
E-mail : vijaypatil14@rediffmail.com

Groundwater samples from five different locations in Amalner town were collected during July2008-October2008 and subjected to comprehensive physicochemical analysis. Fourteen physicochemical parameters were analyzed and the results were compared with water quality standards prescribed by WHO and IS 10500-91. In the present study, groundwater from sites Shirud Naka and Cotton market showed high EC, TDS, TA, TH values indicating poor water quality. The sampling sites Shivaji Nagar, Dheku road and Weekly Market showed physicochemical parameters within the water quality standards reflecting good water quality. The correlation coefficients were calculated. The significance of the results is further discussed.

AP-38 : Extract of *Catharanthus roseus L*Flower: Natural Acid-base Indicator

Mayur C. Shah

Science Wing, Gujarat Vidyapeeth, Sadra (Dist.-Gandhinagar),Gujarat-382 320
E-mail : mayurchemistry@yahoo.co.in

Highly coloured fruit or vegetable or flower petal has potential for use as an acid-base indicator. Pink coloured flower of *Catharanthus* *roseus L* contains anthocyanine derivative pigment. 10%w/v extract of *Catharanthus roseus L*flower was prepared by boiling in water. It behaves as an acid-base indicator. The results show that this indicator is more suitable for as an acid-base indicator in HCl→NaOH; and NH_4OH → HCl titrations due to its different colour change at different pH intervals(0-2.52: pink, 2.53-3.04: light pink, 3.05-4.30: colour less, 4.31-5.86: light green above 5.86: dark green). This indicator shows end point as same as phenolphthalein and methyl orange for above titrations, respectively.

AP-39 : Influence of Photo Catalytically Treated Dyed Water on the Growth of Different Microbes

Tarun J. Patel[1], M.R.Mehta[1] and Vipul P. Prajapati[2]

[1]*Shri P.H.G. Muni. Arts and Science College, Kalol-382721 (Gujarat)*
[2]*Sheth M. N. Science College, Patan (Gujarat)*
E-mail : vipul_hely@yahoo.com, maku_mehta@yahoo.com

Toxic effluents containing dyes are discharged from various industries and they adversely affect water resources, soil fertility, aquatic organisms and ecosystem integrity. They pose toxicity (lethal effect, genotoxicity, mutagenicity and carcinogenicity) to aquatic organisms (fish, fungi, algae, bacteria, etc.) as well as animals. They are not readily degradable under natural conditions and are typically not removed from waste water by conventional waste water treatment systems. Aqueous solutions of various dye; both acidic and basic were treated photo catalytically using ZnO as semi conductor. Various parameters like pH, concentration of ZnO and concentration of dyes were standardized in terms of minimum time required for bleaching of coloured solutions. Influence of bleached water on growth of common soil fungi and bacteria like *Aspergillus niger, Enterobacter aerogens, Bacillus cereus, Micrococcus luteus, Pseudomonas aeruginosa* etc were studied.

AP-40 : Physicochemical Analysis of Some Industrial Effluents from Thane District, Maharashtra

Sanjay Shukla, Nivruti S. Nirgude and A.Venkatachalam*

Department of Chemistry, Bhavan's College, Andheri(West), Mumbai-58
E-mail : avenkat54@yahoo.co.in

Physico-chemical characteristics of some industrial effluents collected from various industries in and around Thane district were studied for the effect of pollution from these sources. A total of 17 parameters were studied. Colour, pH, electrical conductivity, odour, TDS, TSS, BOD, COD, Cl, SO_4, Ca, Mg, Na, K, etc are studied. The industrial effluents collected from these industries are deeply coloured,

with a high BOD and COD and low dissolved oxygen levels. They are suitably diluted to take readings from colorimeter, flame photometer, conductivity meter pH meter. The pH values are in the range 5-9 for the samples collected. This is in accordance with the ISI permissible limits. Depending on the nature of the contents, the pH changes from acidic to basic. Electrical conductivity values are found to be very high and the corresponding increase in the total solids was observed. Total hardness, TDS, chlorides, sulphates was also found to be very high on the samples suggesting high pollution levels. For chlorides estimation, Mohr's method was used, and for sulphate estimation gravimetric method using precipitation of $BaSO_4$was used. The overall results indicate that the pollution levels from these industries are alarming.

AP-40 : Novel PVC Membrane Selective Electrode for the Determination of Cadmium(II) Ion in Chocolate Samples

Sulekh Chandra[*a], Deepshikha[a,b] and Anjana Sarkar[b]

[a]*Department of Chemistry, Zakir Husain Delhi College, University of Delhi, New Delhi, 110002*
[b]*School of Applied Sciences, Netaji Subhas Institute of Technology, University of Delhi, New Delhi, 110002*
[*]*E-mail : schandra_00@yahoo.com, deepshikha.research@gmail.com*

Benzilbis(carbohydrazone) (BBC) has been prepared and explored as new N-N Schiff's base which plays the role of an excellent ion carrier in the construction of a Cd(II) ion membrane sensor. The best performance was obtained with a membrane composition of 30% poly (vinyl chloride), 65% TEHP, 3.5% BBC and 1.5% Tetradodecylammoniumtetrakis(4-chlorophenyl) borate (ETH 500). This sensor shows very good selectivity and sensitivity towards cadmium ion over a wide variety of cations, including alkali, alkaline earth, transition and heavy metal ions. The effect of membrane composition, selectivity, pH and influence of additive on the response properties of electrode were investigated. The response mechanism was discussed in the view of UV-spectroscopy. The electrode exhibits a Nernstian behavior (with slope of 29.7 mV per decade) over a very wide concentration range 1.0×10^{-1} to 1.0×10^{-8}M with a detection limit of 3.2×10^{-8}M. It shows relatively fast response time, in whole concentration range (<8 s), and can be used for at least 10 weeks in the pH range of 2.0–9.0. The proposed sensor was successfully used for the determination of cadmium in different chocolate samples and as indicator electrode in titration with EDTA.

AP-41 : Physico-chemical Analysis of Groundwater of Bhopal City, M.P.

Suman Malik, Bharti Jain[*] and Jyoti Jotwani

Department of Chemistry, Sadhu Vaswani College Bairagarh, Bhopal-462030
[*]Department of Chemistry, SNGGPG Autonomous College, Bhopal-462003
E-mail : drsumanmalik@gmail.com, bhartikjain@yahoo.com

Water is one of the basic indispensable sources on the living planet, Earth. Human beings depend on the natural resource of water for drinking, irrigation, washing and industrial purposes. The growth of human population along-with industrialization, urbanization have started exerting pressure on natural resources. The surface water resources are not acceptable directly for drinking purposes due to deterioration in quality. The suitability of groundwater for drinking purpose depends on the physico-chemical properties. Present paper deals with the physico-chemical analysis of groundwater of Bhopal city in winter season. Groundwater samples were collected from fifteen different locations of Bhopal during Nov-Dec 2010 and were analyzed for pH, electrical conductivity, TDS, TSS, total hardness, calcium hardness, magnesium hardness and chloride. Most of the physico-chemical parameters were within the permissible limits of WHO, IS: 10500 and ICMR Standards for drinking water. Thus ground water from most of the locations may be used directly for domestic purpose but should be properly treated before using for drinking purpose.

AP-42 : Sorptive Removal of Cu(II) and Ni(II) from Wastewater by Synthesized Zeolitic Materials : Equilibrium, Kinetics and Column Dynamics

Bhavna A. Shah[a*], Chirag B. Mistry[a] and Ajay V. Shah[b]

[a]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat,
[b]Science and Humanities Department, Vidyabharti Polytechnic trust, Umrakh, Bardoli-394345, Surat, Gujarat
E-mail : bhavna606@gmail.com

The use of low cost zeolitic materials (CZBFA and ECZBFA) derived from bagasse fly ash (BFA), has been investigated as a substitute of expensive methods for the amputation of Cu(II) and Ni(II). The sorbents BFA and zeolitic materials were well characterized by XRF, FTIR, PXRD, and SEM instrumental techniques, which proves the chemical constituents, functional groups and morphology of the sorbents. The sorption studies were carried out by varying the different operational parameters such as: pH, contact time, dosage, initial metal ions concentration, and temperature. The metal sorption capacities of synthesized zeolitic and native material were determined by batch

and column methods. The equilibrium data are in a superior way fitted by Langmuir isotherm. Kinetic studies have been performed to understand the mechanism of sorption and pseudo-second-order kinetic model better fitted to the equilibrium data. The breakthrough capacities found for Cu(II) and Ni(II) sorbates are 43.15 mg g^{-1} and 49.10 mg g^{-1} respectively on ECZBFA during column operation.

AP-43 : Studies on Soil and Ground Water Quality Around Parola Region, Jalgaon District (Maharastra)

P. M. Yeole

Centre for P. G. Research in Chemistry, R. L. College, Parola-425111(M.S.)
E-mail : pmy_chem@rocketmail.com

In the present study an attempt has been made to find the quality of soil and ground water, around parola region. The water quality parameters such as pH, EC, TDS, DO, total alkalinity, total acidity, total hardness etc. and physico chemical parameters of soil samples are organic matter, Cl, nitrogen etc.were studied.The result shows that ground water from some sampling sites are within permissible limit according to WHO and hence safe for domestic irrigation purposes. The soil quality was determine with respect to a large number of physico chemical properties.

AP-44 : Crosslink Density of Hydroxyl Terminated Polybutadiene Based Polyurethane Elastomers from Stress-Strain Profile : An Eco-friendly Method

Abhay K. Mahanta and Devendra D. Pathak*

Defence Research & Development Organization, SF Complex, Jagdalpur-494001, Chhattisgarh
**Department of Applied Chemistry, Indian School of Mines, Dhanbad-826004, Jharkhand*
E-mail : mahanta_ak@yahoo.co.in

The polyurethane (PU) elastomers based on hydroxyl terminated polybutadiene is widely used in solid composite propellant (CSP) as a binder matrix to hold the solid filler particles together. The tensile properties of the CSP entirely depends upon the tensile properties of the binder matrix. Crosslink density (CD) is one of the most important structural parameters used to characterize the crosslinked PU. The magnitude of CD significantly affects the physical and mechanical properties of the PU elastomers.

Polyurethane elastomers based on HTPB were synthesized with different stoichiometry, i.e. NCO/OH values and cured at 60 °C for 3 days. The tensile properties of cured PUs were evaluated by Instron

Universal Testing Machine (UTM) using dumb-bell shaped specimens. From the stress-strain profile, the crosslink densities of the cured PUs were determined as per the theory of rubber elasticity. The CD values were also determined by Flory-Rhener equation based on the swelling data of the cured PUs. The calculation of input parameters required in Flory-Rhener equation, i.e. polymer solvent interaction parameter and solubility parameter of the cured PUs were elaborated. The values of CD determined from stress-strain profile were compared with those obtained by swelling method and empirical correlation was developed. The method of calculation of CD based on tensile properties has the advantage of being eco-friendly as it obviates use of hazardous solvents or chemicals.

AP-45 : Removal of Arsenic from Ground Water Using Low Cost Adsorbent

Kalpna Kumari
Department of Chemistry, B.P.S. College, Desari (Vaishali)
B.R.A. Bihar University, Muzaffarpur, Bihar
E-mail : kalpna.chemistry@rediffmail.com

Higher Concentration of arsenic in drinking water are hazardous to the health of the people. It causes many diseases like melanosis (skin cancer), hepato-megaly (lever enlargement), dyspnoea (bronchilasthma), digestive problem, urinary cancer, kidney and intestinal problem, hyperkeratosis of palm and soles, black foot-disease (Dry Gangrene). Arsenic leaching in ground water is due to waste water discharge, plating industry, emission from pesticide, pigment dyes, textile operation, coal fired power generator, metal mines. Removal process is ultimately dependent upon technology being validated and sustainable. Biological process is eco-friendly low cost, less side effect. Implement this principle present research is based on sorption of As(III) ions in aqueous solution on citrus sinensis skin acts as a good bio-sorbet for As. In this study the sorption capacity of citrus sinensis skin (mausmi) in removing As(III) for aqueous solution was investigated with different parameters, Such as pH, temperature and initial metal ion concentrations in a batch adsorption system. The arsenic removal from ground water was estimated over a wide range of initial concentration 1-20mg/l, contact time:-20min, sorbent dose-1-10g/L pH6-7 of a temperature 25°C and rpm 120. The sorption increased with increasing contact time but equilibrium was attained in 8 hrs. The sorption followed Freundlich as well as Langmuir isotherms.

Ap-46 : A New Approach to Berthelot Reaction for Determination of Ammonia in Natural Waters and Milk

Archana Jain

Department of Chemistry, Rani Durgavati University, Jabalpur 482001, Madhya Pradesh

New generation of fibre optic-based micro-spectrophotometers are equipped to accommodate sample volumes as small as 1 µL for absorbance measurement with high accuracy and reproducibility. Utilizing the principle of surface tension, it holds the test solution in place between the two ends of optical fibres giving a sample path length of 0.1 and 1 mm. However, the decreased path length used in this cuvetteless spectrophotometric measurement diminishes the sensitivity and it has a bearing on the concentration effect when the sample solution is dilute. The present work addresses this problem and investigates the potential of analyte enrichment by solvent micro-extraction for fibre optic-based micro-spectrophotometry.

It is essential to determine ammonium ion because this is one of the important micronutrients in the water ecosystem. Since phenol and nitroprusside that are used in the determination of ammonia by the Berthelot reaction are highly toxic, it would be desirable to develop a method that could substitute these reagents or minimize their amounts in the analysis. Micro-extraction and fibre optic-based spectrophotometry contributed to the miniaturization of the method, and to realize additional strengths of the Berthelot reaction for ammonium ion. The method developed utilized single-drop extraction by headspace and direct immersion mode. In the first method, the sample solution was rendered alkaline in a closed vial and ammonia liberated in the headspace was extracted into a single-drop of phosphoric acid. The extract was reacted in an insert tube in sequence with micro-litres volumes of phenol reagent and hypochlorite, and the indophenol blue formed was measured. In the second method, it was possible to further modify the method by a direct reaction of

sample solution of ammonia with the reagents, and to extract and pre-concentrate the red form of indophenol into octanol-isooctane mixture after acidification, or to re-extract into aqueous alkali as blue form of the dye. The colour was measured by micro-spectrophotometry. The limit of detection was found to be 0.39 µg L^{-1} of ammonia. The method has been applied to determine ammonia in environmental waters, and to real samples of milk and its products.

AP-47 : Sample Clean-up and Preconcentration for the Determination of Parabens in Cosmetics by High-Performance Liquid Chromatography-diode Array Detection

Krishna K. Verma

Department of Chemistry, Rani Durgavati University, Jabalpur 482001, Madhya Pradesh

Parabens, esters of 4-hydroxybenzoic acid, are antimicrobial agents that are used as preservatives for cosmetics, pharmaceuticals and food. Methyl- and propylparabens are most frequently used together owing to their synergistic preservative effects. Parabens can cause allergic reactions at high concentrations, and are carcinogens. As personal care products these compounds constitute a new class of contaminants. The use of parabens in cosmetics is restricted to 0.4% (w/w) for individual compounds and to 0.8% (w/w) for total of them, expressed as 4-hydroxybenzoic acid.

To deal with the stubborn problem arising from oily and waxy matrix of cosmetics in the chromatographic analysis of parabens, an efficient, rapid and economic sample preparation method is proposed that involving (i) sample clean-up by salt-assisted homogeneous liquid-phase microextraction by 2-propanol in the presence of sodium hydroxide, and (ii) selective preconcentration of parabens from the aqueous extract by liquid-liquid-liquid microextraction using isooctane/ 1-octanol (1: 1, v/v) as organic solvent and 5 µL of sodium hydroxide as acceptor drop. Using the optimized procedure, the method gave a rectilinear graph for 0.01-8 mg/L of parabens with correlation coefficient (r^2) in the range 0.9982-0.9990, and limit of detection in the range 1.7-4.3 µg/L. Intra-day (and inter-day) RSD at 0.01 and 5 mg/L spiked levels of parabens were found as 7.7% (9.2%) and 4.7% (5.6%), respectively. The method has been applied to a number of commercially available cosmetic samples. Average relative recovery of spiked amounts of parabens to cosmetics was 98.9% with an average RSD of 6.1%. A distinct superiority of the present method was evident over literature HPLC and CE. methods which use UV detection, and some others where mass spectrometric detection is used, and it was primarily due to the adequate clean-up and pre-concentration attained by the method.

INORGANIC CHEMISTRY SECTION

Sectional President's Address

IIL-01 : Chemistry of Some Group 15 Metal Complexes with Mixed Sulphur Donor Ligands

H. P. S. Chauhan

School of Chemical Sciences, Devi Ahilya University, Takshashila Campus,
Khandwa Road, Indore – 452001 (M.P.)
E-mail : hpsc@rediffmail.com

In view of different possible structural features and various types of applications, I am going to present here the synthesis of a number of mixed sulphur donor ligand nano complexes of group 15 elements [(As(III), Sb(III) and Bi(III)] by various suitable procedures. All these soluble compounds have been characterized by melting point, molecular weight determinations, elemental analysis and spectroscopic [UV, IR and NMR (^{1}H, ^{13}C and ^{31}P)] studies as well as single crystal X-ray structural analysis of few of the complexes provide us full structural details. FAB$^+$ Mass indicates the molecular weight, decomposition pattern and thermal stability of the ligands. SEM and powder XRD studies of the compounds indicate the morphology structural parameters and nano particle size of these complexes Thermal (TGA, DTA and DSC) studies of some of the compounds have also been carried out in an inert atmosphere and the final decomposition product was found to be pure M_2S_3 which may be used in a number of ways. Some of these compounds have also been screened for their antimicrobial activities using the well diffusion method. In addition to the metal complexes, free ligands as well as their metal precursors were also tested *in-vitro* against bacterial strains two gram positive and two gram negative and also against fungi.

Prof. T.N. Srivastava Memorial Lecture

IIL-02 : Chemistry of Multimetal Multiligand Equilibria and Synthetic Models of Copper(II) Complexes and their Biological Properties

R. N. Patel

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

The copper containing enzymes and proteins constitute an important class of biologically active compounds. The biological function of copper proteins/enzymes include electron transfer, dioxygen transport, oxygenation, oxidation, reduction and disproportionation. Mixed ligand mixed metal complexes involving more than one metal ion of the same, or, of different metals way prove as better models, for multimetal multiligand equilibria occurring in the biological system. Such species are of importance in the study of biofluids, particularly when hyperaccumulated metal ions are present for physiological or pathological regions. Also the mixed metal mixed ligand equilibria are very common in the various enzymatic process. Complexes of peptides and imidazoles with metal ions have aroused increasing interest in recent years because the imidazole group of histidine plays a fundamental role in several metal protein and metal enzyme reactions of living organisms, where mixed metal mixed ligand equilibria are very common. Systematic studies with relatively simple molecules of known structure often yield valuable information, that gives idea to the roles of the metal ions in biological systems. Synthetic binuclear transition metal complexes provide models for metalloproteins sites and lend insight towards the design of new catalysts. Binuclear complexes have been subject of extensive investigation owing to their industrial and biological applications. The biochemical relevance will be discussed by using superoxide dismutase (SOD) and particular emphasis will be given to the identification of oxidation states using electronic spectroscopy, electron paramagntic resonance (epr) and X-ray data analysis.

The emphasis in the present lecture is therefore mainly laid on the brief review of interesting aspects of the chemistry of multimetal multiligand equilibria and synthetic models of copper(II) complexes and their biochemical relevance.

IIL-03 : Biomedicinal Aspects of Metal Chelates: Studies on Silver and Vanadium Complexes

A.P. Mishra

Synthetic Inorganic & Coordination Chemistry Laboratories, Department of Chemistry, Dr. H.S. Gour Central University, Sagar (M.P.)-470 003
E-mail : apm19@rediffmail.com

Medicinal inorganic chemistry as discipline has only existed for about last forty years, since the discovery of the antitumour activity of cis-platin (Rosenberg,1964). Biocoordination chemistry have been used in medical sciences in a number of ways. Chelates can be used in the treatment, management or diagnosis of diseases.Ehrlich, the founder of chemotherapy dreamed about the drugs which injure an invading organism without injury to the host; thus a concept of 'magic bullet' in drug targeting emerged out. The idea to bind therapeutic drug molecules or toxin molecules onto the surface of metal-nanoparticles (nano-biotechnology) and the use of magnetic 'tag and drag' to improve drug treatment efficacy along with reducing the amount of administered doses; are the challenges before molecular biologists and chemists.

Although the "war on cancer" is now in its fourth decade and despite much progress has been made in categorizing the environmental causes and cellular/molecular biological basis for this dreaded disease, we still do not have a precise understanding of the differences between a cancer cell and its normal counterpart. The completion of the human genome sequence and its subsequent improvements in the sequence data are important steps to fully comprehend cancer cell biology. We have synthesized and studied some new water soluble Ag(I) mixed ligand complexes containing nitrogen and sulfur donors.

Diabetes is a group of metabolic diseases characterized by hyperglycemia resulting from defects in insulin secretion, insulin action, or both.. During the past 25 years,Vanadium compounds have been reported to exhibit insulin like effects. It mimics most of the physiological effects of insulin, such as stimulation of the glucose uptake and metabolism in the fat cells, the enhancement of glycogenesis in the muscles and the liver, inhibition of the reformation of glucose (gluconeogenesis) from proteins, or the stimulation of fatty acid formation in the adiposities.The main advantage of these vanadium compounds relative to insulin is that they may be administered orally. Accordingly, the aim of research in this field is to make vanadium compounds which can reach the target cells with high efficacy. In this study, we are taken a targeted approach to synthesize and study some novel active Vanadium complexes with low molecular mass and optimal absorptivity as antidiabetics.

Metal chelated multidrug therapy (Combination therapy and Synergistic action) and metal ion-mediated delivery and distribution of pharmaceuticals/ nutriceuticals may come up as a part solution of the problems like drug resistance in 21st century; where principles of biocoordination chemistry may be applicable to medical sciences for questions , hitherto unanswered.

IIL-04 : Synthesis and Optoelectronic Characterization of the Green Nano Phosphor

Devender Singh

Department of Chemistry, Maharshi Dayanand University, Rohtak, Haryana
E-mail : devjakhar@gmail.com

Phosphors are technological very important materials for the display panels. $SrAl_2O_4:Eu^{2+}$ material was synthesized by the rapid combustion method. The combustion technique has emerged as an alternative technique for the nano materials. The prepared phosphor was treated at 600 ^{0}C temperatures to study the luminescence and surface crystallinity of the materials. The phosphor materials gave green luminescence under UV lamp at 540 nm. The green luminescence was due to the $4f^65d^1 \rightarrow 4f^7$ transition. The materials obtained through this technique were also characterized by using the Scanning electron microscopy (SEM), X-ray diffraction (XRD) and photoluminescence spectra (PL). The particle size of the material was found to be in the average range of 35-80 nm.

IIL-05 : Synthesis, Spectroscopic and Antibacterial Studies of Transition Metal Complexes with Schiff Bases

R.K. Dubey

Synthetic Inorganic and Metallo-organic Research Laboratory, Department of Chemistry,University of Allahabad, Allahabad- 211002
E-mail : rajalkoxy@yahoo.com

The interactions of sodium salts of Schiff bases; salicylidene-2-methyl-1-aminobenzene (smab**H**), salicylidene-2-aminopyridine (sap**H**), salicylidene-thiosemicarbazone (stsc**H**) with metal salts [titanium(IV) chloride, zirconium(IV) chloride and vanadyl chloride] in THF-C_6H_6 mixture produced complexes of the type; $[Cl_3M(sb)]$ and $[Cl_2M(sb)_2]$ (where M = Ti(IV), Zr(IV) & VO(V), sb= Schiff bases) in 1:1 and 1:2 molar ratio(s) respectively. All the complexes were found to be coloured solid and were soluble in DMSO, DMF, ethanol and methanol. These complexes have been characterised by elemental analysis, spectral

[IR, NMR (^1H, ^{13}C & ^{51}V)] and thermogravimetric and PXRD investigations. Structural composition of the complexes has been tentatively proposed by mass spectrometric data. Titanium(IV) and vanadium(V) complexes were found to be dimeric in association whereas zirconium(IV) complexes are monomeric in structure. Based on these studies structure of the complexes have been tentatively suggested. In addition to the above studies, antibacterial activity of some synthesized complexes has also been investigated. In the present lecture, some newer trends in the field of coordination chemistry have been found to be very important as novel material will also be discussed.

IIL-06 : Macrocyclic Compounds as Potential Anti-Infective Therapeutics

C. P. Bhasin

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

Novel therapeutic strategies are in the rapid progress for the treatment of serious diseases caused by viral, bacterial and parasitic infections, because currently used drugs are facing the problem of rapidly emerging resistance. There is also an urgent need for agents that act on novel pathogen-specific targets, in order to expand the repertoire of possible therapies. The high throughput screening of diverse small molecule compound libraries has provided only a limited number of new lead series, and the number of compounds acting on novel targets is even smaller. Natural product screening has traditionally been very successful in the anti-infective area. Several successful drugs on the market as well as other compounds in clinical development are derived from natural products. Amongst these, many are ***macrocyclic*** compounds in the 1-2 kDa size range. This review will describe recent advances and novel drug discovery approaches in the antiinfective area, focusing on synthetic and natural macrocyclic compounds for which *in vivo* proof of concept has been established. The review will also highlight the Protein Epitope Mimetics (PEM) technology as a novel tool in the drug discovery process. Here the structures of naturally occurring antimicrobial and antiviral peptides and proteins are used as starting points to generate novel macrocyclic mimetics, which can be produced and optimized efficiently by combinatorial synthetic methods. Several recent examples highlight the great potential of the PEM approach in the discovery of new anti-infective agents.

IIL-07 : Supramolecular Chemistry : An Interdisciplinary Subject Encompassing Biology and Chemistry

S. Jagannatha Swamy

Department of Chemistry, Kakatiya University,Warangal - 506009,(AP)
E-mail : sj_swamy@yahoo.com

Supramolecular Chemistry, also known as Host-Guest Chemistry is relatively young branch of chemistry, even though the first mention in literature dates back to 1893 – Alfred Werner's concept of secondary (neben) valency; Emil Fischer's lock-and-key model (1894) and introduction of the word "Übermolekül" (supramolecule) by Wolf (1937) to describe the intermolecular interactions between coordinatively saturated dimers of carboxylic acids. The subject has received its identity only after the three chemists; D. J. Cram, C. J. Pederson and J. M. Lehn have extensively reported the novel ligands: the crown ethers, the cryptands and their complexes. The supramolecular interactions play an important role in biomolecules and biochemical processes like – DNA double helical structure, protein folding, hydrophobic interactions etc. The lecture discusses the different types of supramolecular (non-covalent) interactions in biology and chemistry. Further, the role of anions in biology and their interactions are also discussed. The methods of developing anion specific ligands and structures of some of the complexes of anions reported from our laboratory are covered in the lecture.

IIL-08 : Role of Metal Oxides in Chemical Evolution

Kamaluddin

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee-247 667
E-mail : kamalfcy@iitr.ernet.in

Steps of chemical evolution have been designated as formation of biomonomers followed by their polymerization and subsequent modification in an organized structure leading to the formation of the first living cell. Formation of small molecules like amino acids, organic bases, sugar etc. could have occurred in the reducing atmosphere of the primitive Earth. Polymerization of these small molecules could have required some catalyst. In addition to clay, the role of metal ions and metal complexes as prebiotic catalyst in the synthesis and polymerization of biomonomers cannot be ruled out. Metal oxides are important constituents of Earth's crust and that of other planets. These oxides might have adsorbed organic molecules and catalyzed the condensation processes, which may have led to the formation of the first living cell. Different studies were performed in order to investigate the role of metal oxides (especially oxides of iron and manganese) in chemical evolution. Iron oxides (goethite, akaganeite and hematite) as well as manganese oxides (MnO, Mn_2O_3, Mn_3O_4 and MnO_2) were synthesized and their characterization was done using IR, powder XRD, FE-SEM and TEM. Role of the above oxides in the adsorption of ribose nucleotides, formation of nucleobases from formamide and oligomerization of amino acids was studied. Above oxides of iron and manganese were found to have good adsorption affinity towards ribose nucleotides, high catalytic activity in the formation of several nucleobases from formamide and oligomerization of glycine and alanine. Characterization of products was performed using UV, IR, HPLC and ESI-MS techniques. Presence of hematite-water system on Mars has been suggested to be a positive indicator in the chemical evolution on Mars.

IO-CYSA-01 : Synthesis, Structural, Antibacterial and Antidiabetic Studies of Some Oxovanadium - Schiff Base Complexes

A.P. Mishra*, B.S. Kusmariya, M. Soni and S. Shukla

Department of Chemistry, Dr.H.S.Gour Central University, Sagar-470003 (M.P.)
E-mail : apm19@rediffmail.com, kusmariya@gmail.com

The design and synthesis of multidentate Schiff bases as ligands have received attention due to their biomimetic fascinations. Biochemicals and therapeutic potential of such ligands can be tailored by chelating them with life essential metals ions. The oxovanadium complexes of Schiff bases *viz.* 2-furfurylidine-3,4-dichloroaniline; 2-hydroxyacetophenone isoniazide; methyl isobutyl ketone-2-amino-4-chloro phenol; 2-pyridine carboxylidine-4-aminobenzoic acid; 1-(-4-aminophenyl)ethanaledine-4-thiobiuret and 1-(naphthyl) ethanaledine-4-thiobiuret have been synthesized (M:L ratio 1:2). Characterization of the compounds have been done by elemental analysis, FT-IR, Uv-vis, FAB –MASS, conductance, esr, magnetic, thermal studies etc. The geometrical structures have been found to be square pyramidal/trigonal bipyramidal. FAB-MASS and thermal studies show the degradation pattern of compounds. Some complexes have also been screened for their antibacterial activity against *E.coli*, *S.aureus*, *S.fecalis* and exhibited appreciable activity. Some complexes have been tested on male wistar rats as possible antihyperglycemic agents. Such studies reflect biomedicinal potential of metal-chelates.

IO-CYSA-02 : Ag/Cu/TiO_2 : A Visible Light Active Photocatalyst for the Solar Generation of Hydrogen from Water Splitting

Jakkidi Krishna Reddy, Mandari Kotesh Kumar and Akula Venugopal*

Inorganic and Physical Chemistry Division, Indian Institute of Chemical Technology, Hyderabad-500607
E-mail : akula@iict.res.in; krishnareddyiict@gmail.com

Visible light active Ag/Cu/TiO_2 photocatalysts with varying amounts of Cu and Ag were prepared by incipient wet impregnation method. Photo catalytic activity of these catalysts was evaluated for the decomposition of water under solar irradiation. The amount of Cu and Ag species over TiO_2 were optimized to achieve the maximum photocatalytic activity for H_2 production. Prepared catalysts are characterized by the techniques such as X-ray diffraction (XRD), X-ray photoelectron spectra (XPS), transmission electron spectroscopy (TEM) and UV-Vis Diffuse reflectance spectra (UV-Vis DRS). The characterisation results shows that Cu and Ag particles are highly dispersed and in interacted with TiO_2 thus leading to the redshift in the DRS band. The measured band gaps of these catalysts are found to be in the range of 2.5 to 2.9 eV. Among the series of catalysts the $Ag_{1.0}/Cu_{5.0}/TiO_2$ showed good photocatalytic activity with a production rate of 316.5μmol/h/g of H_2.

Reaction conditions : 0.05 g catalyst, 45 ml H_2O and 5 mL methanol in a quartz reactor and solar irradiation as a source of light.

IO-CYSA-03 : Photocatalytic Degradation of Rose Bengal in Presence of Copper Hexacyanoferrate(II)

Paras Tak* and Pinki B. Punjabi

Photochemistry Laboratory, Department of Chemistry, University College of Science M.L. Sukhadia University, Udaipur - 313002 (Raj.)
**Department of Chemistry, Pacific College of Basic & Applied Sciences, PAHER University, Debari, Udaipur - 313024 (Raj.)*
E-mail : parastak2011@gmail.com

Photolabile property of ferrocyanide ion is well known. The electron generated by ferrocyanide ion on exposure to light may be utilized for the photocatalytic degradation of rose Bengal. Copper Hexacyanoferrate (II) was prepared as chocolate brown powder by precipitation. The main advantage of using it was its insoluble nature and capability to absorb in visible light. Effect of different parameters like pH, concentration of dye, light intensity etc. was observed on the rate of reaction. A suitable mechanism for the phototcatalytic degradation of rose Bengal dye has been proposed.

IO-CYSA-04 : Synthesis, Characterization, Antimicrobial Studies and Liquid Crystalline Properties of Metallomesogenes Derived from Mesogens Containing Coumarin and Quinoline Moieties

Pulin Nath and S.D. Dhumwad

Department of Chemistry, Karnatak University's, Karnatak Science College, Dharwad, Karnataka
E-mail : dhumwadsd@gmail.com

New liquid crystalline mesogens containing the six-membered heterocyclic derivatives of Coumarin and quinoline and their corresponding metallomesogenes of Co(II), Ni(II), Cu(II) and Zn(II) were synthesized and characterized by C, H, N analyzer, Magnetic moments, spectral analysis like UV, IR, NMR, Mass, ESR, Thermal analysis, etc. From the above studies it is concluded that, these mesogens are monobasic, tridentate in nature and all the metallomesogenes exhibit octahedral geometry with slight distortion in case of Cu (II) complexes. The transition temperatures and textures of the mesophases were characterized using polarized optical microscope. The mesogenes showes nematic and smectic C phases, while the metallomesogenes show nematic(N), smectic-C(Sm_C), and smectic-A(Sm_A) mesophases. The synthesized mesogens and the metallomesogenes were screened for the antimicrobial activities in comparison with the standard drugs. Form the antimicrobial studies; it is found that the metallomesogenes possess higher activity than the mesogenes.

IO-CYSA-05 : Investigation of Novel Tripodal Chelators Based on 8-Hydroxyquinoline: Synthesis, Complexation and In-Silico Studies

Rifat Akbar[1]*, Minati Baral[2] and B K Kanungo[1]

[1] Department of Chemistry, Sant Longowal Institute of Engineering & Technology, Longowal-148106
[2] Department of Chemistry, National Institute of Technology Kurukhestra, Haryana
E-mail : rifatslietphd@gmail.com

The chemistry of 3-fold symmetrical tripodal ligands has received new impetus in recent years due to stabilization of early transition metal and main group metal. 8-Hydroxyquinoline is a long-known molecule which due to its metal-complexation ability frequently is used for analysis or metal-precipitation. Due largely to the importance of metals in biological systems, there has been growing interest towards modeling metal-binding sites in biomimitic chelators. In this present study two novel multidentate tripodal chelators 5-[[[3-[(8-hydroxy-5 quinolyl)methylamino]2[[(8hydroxy5quinolyl) methylamino]

methyl] 2methylpropyl] amino] methyl]quinolin-8ol(TAM5M8HQ,L1) and5-[[2-[[3-amino-4-hydroxy-2-[(Z)-prop-1-enyl] phenyl] methoxymethyl]-3-[(8-hydroxy-5-quinolyl)methoxy]-2-methyl-propoxy] methyl] quinolin-8-ol(TMO5M8HQ,L2) have been designed and synthesised. The ligands were characterized through elemental analysis, melting point, ^{1}HNMR, C^{13}NMR, infrared, electronic and mass spectral data. The binding properties of the ligands for iron(III) were investigated by Potentiometric as well as Spectrophotometric method in water at 0.1N ionic strength and 298 K. The molecular modeling of the ligand as well as its complexes with some trivalent bioactive metals were carried by molecular mechanics using MM$^+$ force-field and semi-empirical method using PM6 parameters. The bonding properties, coordination behaviours, electronic spectra, infrared spectra, thermodynamic properties and the HOMO- LUMO energies have been determined by semi-empirical method using PM6 parameters. The DFT calculations of the optimized molecules were done using B3LYP method through the 6-31G** basis set.

IO-CYSA-06 : Synthesis, Characterization *in vitro* DNA Binding and Cleavage Properties of Zn(II) Complexes of Pro–Gly and Pro–Leu Dipeptides

Shazia Parveen and Farukh Arjmand*

Department of Chemistry, Aligarh Muslim University, Aligarh–202002
**E-mail : farukh_arjmand@yahoo.co.in*

Zinc(II) complexes **1** and **2** derived from dipeptide ligands Pro–Gly and Pro–Leu, were synthesized and thoroughly characterized by various spectroscopic techniques (*viz.,* IR, ^{1}H NMR, ESI–MS), elemental analysis and molar conductance measurements. The i*n vitro* DNA binding studies of complexes **1** and **2** were carried out employing various biophysical techniques (viz., UV–vis, fluorescence and circular dichroism) which revealed the groove binding nature of these complexes to the CT DNA. Zn(II) Pro–Gly complex showed greater binding affinity to CT DNA as compared to the Zn(II) Pro–Leu complex due to steric constraints in the latter. The speciûc mode of binding was examined by carrying out the interaction of complexes were with mononucleotides of interest, viz., 5' –GMP and 5' –TMP by using absorption and NMR (^{1}H, ^{31}P) spectroscopy. The supercoiled pBR322 DNA cleavage activity of complexes **1** and **2** was ascertained by gel electrophoresis demonstrating that both the complexes are efficient cleavage agents cleaving the DNA via hydrolytic pathway. Both these complexes specifically bind to the minor groove of DNA.

IO-CYSA-07 : Carbonylative Synthesis of *N*-substituted Phthalimides using Pd/C as an Efficient, Heterogeneous and Reusable Catalyst

Mayur V. Khedkar and Bhalchandra M. Bhanage*

Department of Chemistry, Institute of Chemical Technology, Matunga, Mumbai 400019
E-mail : mayurkhedkar02@gmail.com, bm.bhanage@ictmumbai.edu.in

Phthalimides constitutes a key component of the various natural products and biologically important compounds. They also have vital contribution in medicinal chemistry due to its application in the treatment of acquired immune deûciency syndrome (AIDS), leprosy and other diseases. In context, Perry *et al.* reported palladium catalyzed formation of phthalimide from *o*-halo aryls using carbon monoxide (CO). Few more homogeneous palladium based catalytic systems have been developed, however reported methods suffer from one or more drawbacks. In this regards for the first time carbonylative cyclization of *o*-halo aryls with variety of primary amines under carbon monoxide was investigated by using 10% Pd/C. The catalytic system represents efficient, heterogeneous and phosphine-free approach for the synthesis of wide variety of *N*-substituted phthalimides furnishing good to excellent yield of desired products. Present methodology circumvents the use of the phosphine ligands and also solves the basic problem of palladium catalyst recovery and reuse. The catalyst exhibited remarkable activity and was effectively recycled for eight consecutive cycles.

IO-CYSA-08 : Synthesis and Characterization of Some Vanadium Complexes used as a Insulinomimetic Agent

A. P. Mishra and Shraddha Shukla

Bio-coordination Laboratories, Department of Chemistry, Dr. H.S. Gour University Sagar -470 003
E-mail : apm19@rediffinail.com, shuklashraddha25@gmail.com

Metallodrugs are nowadays, inviting much attention of biochemists and physiologist. A few research reports are available on insulinomimetic effect of vanadium ions on cells and diabetic model animal (1980). Vanadium ions and their complexes exert various insulinmimetic and antidiabetic effects involving the enhancement of glucose transport and metabolism in isolated adipocytes and hepatocytes, skeletal muscle, stimulation of glycogen synthesis and lipogenesis, inhibition of lipolysis. Since inorganic Vanadium ion are less absorbed by the digestive tract (low bioavailability), the complexation of vanadium ions with organic ligands may be a useful method for reducing toxicity and improving bioavailability and tissue uptake of ions. The coordination complexes of VO (II) with the Schiff base derived from 4 aminoacetophenone, 1-acetonaphthone, 4-methoxybenzaldehyde with 2-imino,4-thiobiuret; 3 acetoxypyridine with 2-amino, 4-benzathiazol and 5-chloro aniline with salicyldehyde have been synthesized and characterized by micro analytical data, molar conductance, magnetic susceptibility, FTIR, UV-Vis. and ESR, FAB mass spectral studies. FAB mass and thermal data show degradation of complexes. The Schiff base ligands behave as bidentatedltridenated. The stoichiometry of the complexes are in 1:2 of 1:1 (M:L) ratio. The Schiff base and their Oxovanadium metal complexes shows a good antidiabetic activity comparatively to standard drug *Glibenclamide*. The synthesized vanadium complex are used for the treatment of Diabetes. We tasted diabetes of synthesized compound are Male Wister rates (230-250 g) and selected Alloxan Induced diabetes model. Animals were allowed to freshly prepare aqueous solution of Alloxan monohydrate in a dose of 120mg/kg animal weight (intraperitoneal). Blood glucose was measured after 20 hrs. of alloxination and they were maintained in diabetic state over a period of 30 days. Rates showing fasting blood glucose levels around 300mg/dl were selected for study. Animals blood glucose levels checked by Glucometer.

IO-01 : Role of Metal Ion Incorporation in ZnO for the Enhancement of Oxygen Vacancies and their Solar Photocatalytic Activity

A.B. Patil and S.K. Pardeshi*

Department of Chemistry, University of Pune, Ganeshkhind, Pune-411007
**E-mail : skpar@chem.unipune.ernet.in*

Metal doped zinc oxide crystallites were synthesized by two steps, solution free-mechanochemical method. These photocatalysts are then characterized by XRD, XPS, SEM, EDX, FT-IR, PL and UV-Visible spectrophotometer. The XRD data of metal doped ZnO matches to that of JCPDS card No. 36-1451 and incorporation of Cu, Cd and Sr in to ZnO was supported by broadening and lower Bragg angle shift in XRD pattern of these samples as compare to that of undoped ZnO. The XPS study supports incorporation of Cu^+ in Cu-doped ZnO, Cd^{2+} in Cd-doped ZnO and Sr^{2+} in Sr-doped ZnO. The characteristic XPS peak of Cu^{2+}species is usually positioned at 933 eV (Cu $2p_{3/2}$) together with the shake-up feature at 942 eV, while slightly lower binding energy (932.6 eV) and the absence of shake-up peaks is indication of Cu^+. UV-visible spectra imply lowering of band gap energy of metal doped ZnO as compare to bare ZnO. The order of λ_{max} was found to be: undoped ZnO < Sr–doped ZnO < Cd –doped ZnO < Cu –doped ZnO.

The PL spectra suggest that the more number of oxygen vacancies exist in metal doped ZnO as compare to that in pure ZnO. Solar PCD efficiency bisphenol A was found to be in the order of Cu-doped ZnO > Cd-doped ZnO > Pure ZnO > Sr-doped ZnO. Thus, metal ion impurity of variable oxidation states contributes efficiently in solar photocatalysis. Photocatalytic degradation of bisphenol A follows first order reaction kinetics.

IO-02 : DNA-binding, Cytotoxicity, Photocleavage, Antimicrobial and Docking Studies of Ru(II) Polypyridyl Complexes

A. Srishailam, G. Srinivas and S. Satyanarayan*

**Department of Chemistry, Osmania University, Hyderabad-500007 Andhra Pradesh*
E-mail : ssnsirasani@gmail.com

The three Ruthenium(II) polypyridyl complexes, $[Ru(phen)_2PTIP]^{+2}$(1), $[Ru(bpy)_2PTIP]^{+2}$(2) and $[Ru(dmb)_2PTIP]^{+2}$(3), phen= 1,10-phenanthroline, bpy= 2,2'-bipyridine, dmb= 4,4'-dimethyl-2,2'-bipyridine, PTIP= (2-(5-phenylhtiophen-2-yl),4-H-imidazo[4,5-f][1,10]-phenanthroline), have been synthesized and characterized by elemental analysis, IR, UV-VIS, ^{1}HNMR, ^{13}CNMR and mass spectra. The DNA-binding properties of the Ruthenium (II) complexes were investigated by spectrophotometric methods, viscosity measurements, thermal denaturation and docking studies. DNA binding constant (K_b) of these complexes in the order of 10^5. The result reveals that these complexes bind to calf thymus DNA through intercalation. Photo activated cleavage studies with pBR-322 and antimicrobial studies were done with these complexes. The cytotoxicity studies have been evaluated with MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide) method. The apoptosis-inducing activity was assessed by acridine orange/ethidium bromide staining assay.

IO-03 : Preparation and Characterization of Transition Metal Complexes Supported by NO-bidentate Schiff-Base Ligand

Anita Sharma and M.K. Shah*

Chemical Research Laboratory, Department of Chemistry
Saurashtra University, Rajkot-360005, Gujarat
E-mail : drmks2000@hotmail.com

In present paper, transition metal complexes derived from substituted 2-((3-(4-substituted)-1phenyl-1H-pyrazol-4-yl) methyl-eneamino) phenol were synthesized. The general composition of the complexes is $[M(L)_2 \cdot nH_2O]$, where M= Cu(II), Co(II), Ni(II). The ligand act as bidentate ligand. The ligand was Characterized by Mass, IR,

^{1}H NMR and ^{13}C NMR spectral studies. Complexes are characterized on the basis of elemental analysis, molar conductance measurements, magnetic susceptibility measurements, Mass, ^{1}HNMR, IR, electronic spectral techniques and TGA studies.

IO-04 : Use of Well-Dawson Polyoxometalate as Photocatalyst for Degradation of Organic Pollutant

Daksha Sharma[a], Mamta Ordia[b] and Rakshit Ameta*[c]

[a] Department of Chemistry, Vidya Bhawan Rural Institute, Udaipur (Raj.) India
[b] Central Academy School, Sardarpura, Udaipur (Raj.)
[c] Department of Chemistry, Pacific College of Basic & Applied Sciences, Paher University, Udaipur (Raj.)
E-mail : sha09daks@yahoo.co.in

The sunlight mediated photocatalytic degradation of Azure-B (AB) was studied using Well-Dawson Polyoxometalate. The photocatalytic behaviour of the prepared Iron containing Well-Dawson Polyoxometalate was tested through the degradation of AB. The disappearance of organic molecules follows pseudo-first order kinetics. The effect of operational parameters such as dye concentration, photocatalyst amount, pH of the solution and light intensity on the degradation rate of aqueous solution of AB has been examined. Results revealed that the use of photocatalyst was efficient and the selection of optimal operational parameters lead to complete decolorization of the dye solutions.

IO-05 : Combustion Synthesis and Photoluminescence Characteristics Sm^{3+} doped $BaLa_2O_4$ Nanoparticles

Dimple, S. P. Khatkar, V.B. Taxak*-- and Sonika

Maharshi Dayanand University, Rohtak-124001
E-mail : v_taxak@yahoo.com

An orange red light emitting Sm^{3+} doped $BaLa_2O_4$ nanophosphor was synthesized by combustion synthesis using an organic fuel. The paste is kept in a preheated furnace maintained at 500^0C. The combustion process utilizes the enthalpy of combustion for the formation and the solid obtained was again fired at 700 °C, 900 °C for 3hrs to increase the brightness and crystallinity. Comparing with traditional material processing techniques, combustion method is a relatively simple method. The advantages of short time reaction and low temperature solution based process have been exploited to produce Sm^{3+} doped $BaLa_2O_4$ nanoparticles. The nanocrystals obtained through combustion method were characterized by using scanning electron microscopy (SEM), X-ray diffractions (XRD) and photoluminescence (PL) spectra. The average particle size of the synthesized nanophosphor was around 30-80 nm. The photoluminescence (PL) spectra show predominant orange red color of the nanocrystals prepared under an UV source that was attributed to transitions $^4G_{5/2} \rightarrow {}^6H_{7/2}$ peak at 609 nm.

IO-06 : Synthesis and Characterization of Complexes of Chromium(III), Manganese(II), Iron(III) & Cobalt(III) Metals with Schiff's base β – Hydroxy Naphthyl Methanal Thiosemicarbazone Ligand

Prem Mohan Mishra

Dept. of Chemistry, MLSM College, Darbhanga – 846004
E-mail : mishrapm6@gmail.com

Schiff's bases are organic compounds having an azomethine group (>C=N). Various studies have shown that >C=N group has considerable biological importance. Schiff base can be considered as useful chelating agents when a suitable functional group such as – OH, - SH, - NH_2 etc are present sufficiently close to azomethine group Metal complexes with Schiff bases have occupied an important place in the development of coordination chemistry due to its interesting structural features and important applications.

In this paper we report the synthesis, properties, elemental analysis magnetic susceptibility, electrical conductivity, electronic measurements and IR spectral studies of the ligand β-hydroxy naphthyl methanal thiosemicarbazone and its complexes with chromium (III), manganese (II), iron (III) and cobalt (III). On the basis of these observations, probable structures of all the metal complexes have been assigned.

IO-07 : Thermo Analytical Studies of Cu(ll) Complex of 5-Anilino-1,2,3,4-Thiatrizole

Upendra Nath Verma[*] and Birendra Kumar

University Department of Chemistry, Magadh University,
Bodhgaya Magahi Lok, Tootbari Gaya - 823001
E-mail : unverma.mu@gmail.com

The Cu(ll) Complex of 5-1,2,3,4-thiatriazole was prepared by mixing 45ml of ligand (0.02M) in ethanol and 45ml copper formate (0.01M) in ethanol. Bluish green color precipitate was filtered, dried over anhydrous $CaCl_2$ in desiccators. The recorded thermo gram exhibits four stage of decomposition. First stage decomposition shows the loss of moisture while second stage shows the loss of two formate ions. Third stage decomposition shows the loss of whole ligand moiety and fourth stage shows formation of CuO. Second stage of transformation was selected to study the kinetic parameters like the order of reaction, activation energy, entropy of activation and frequency factor using Freeman and Carroll method and compared the values obtained by Doyle's method as modified by Zsako.

The values of order of reaction and activation energy were found one and 18.97 kcal/mol respectively. The apparent activation entropy and apparent frequency factor were calculated-151.08961 e.u. and 1.52808X105 sec-1 respectively. These values are in good agreement with each other and hence may be utilized in the study of solid state reaction mechanism.

IO-08 : Complexes of Nickel(II) and Cobalt(II) with Furildihydrazone

Sushma Sinha

Department of Chemistry, M.S.K.B.College, Muzaffarpur - 842001
E-mail : ssinha52@gmail.com

A number of furildihydrazone complexes of the type $[M(FDH)_2 X_2]$, where M = Ni(II), Co(II), X = Cl^-, Br^-, I^-, SCN^-, NO_3^-, BF_4^- and FDH^- furildihydrazone have been isolated in good yield by metal ion-catalysed template synthesis. The complex posses characteristic colours and are not hygroscopic, springly soluble in water and can be stored for long periods without decomposition. The infrared spectra show considerable metal to ligand π-electron interaction which are manifested by the shift of $n_{c=N}$ band to a higher frequency region. The complexes are found to be spin-free paramagnetic with nearly octahedral arrangement of ligand atoms about the central metal ion.

IO-09 : Synthesis, Characterization and Luminescent Properties of an Imidazole based Zinc Complex

Ishwar Singh[1*], Partap S. Kadyan[1], Vandna Nishal[1] and Ritu Srivastava[2]

[1] Department of Chemistry, Maharshi Dayanand University, Rohtak, Haryana - 124001
[2] Center for Organic Electronics, OLED Lab, National Physical Laboratory, New Delhi 110012
E-mail : ishsingh@rediffmail.com

Zinc(II) complex i.e. 2-(2-pyridyl)benzimidazolato)2-methyl-8-hydroxyquinolinato zinc(II) [(Meq)(PBI)Zn] has been synthesized and characterized by NMR, FTIR and CHN analysis techniques. The luminescent properties of the metal complex are investigated by UV-VIS spectroscopy and photoluminescence spectroscopy. The multilayered electronic device ITO/α-NPD/Zinc-complex/BCP/Alq_3/LiF/Al has been fabricated. The device exhibited bright blue-green emission with peak at 535 nm. The device showed maximum luminescence of 2639 cd/m^2 at 16 V. The metal complex has shown high thermal stability (>350 ^{0}C). The current-voltage characteristics of the device have also been studied. The results showed that the complex has been suitable for optoelectronic application.

IO-10 : Minerals as Anticancer Drugs with Different Vitamins and Amino Acid

K. M. Fulzele[a], S. M. Vhankate[a], N. S. Dhawale[a] and V. B. Tadke[a]*
[a]Department of Chemistry, Fergusson College, Pune – 411004
E-mail : vijaytadke@gmail.com

Minerals and vitamins are most studied supplement for cancer treatment. Epidemiology study has shown that minerals along with vitamins intake is closely correlated with reducing the risk of cancer.

Minerals and vitamins are antioxidants with free radical fighting skills. Antioxidants protest the body from oxidative damage which is considered a major factor in cancer development. In our study we have used *N-Acetyl Cystein, Selenium Epican Forty* and different amino acid which are prescribed to cancer patients. *Epican Forty* is a combination of different minerals and amino acids. Here we have investigated the effect of graded concentration and synergistic effect of minerals and nutrients on cancer cell lines.

IO-11 : Synthesis, Characterization, Crystal Structure, DNA Binding, Protein Binding and Anticancer activity of Novel ternary Cu(II) complex Derived From 4-Propionyl Pyrazolone and 2, 2' Bipyridyl Ligands

Komal M. Vyas and R. N. Jadeja
Department of Chemistry, Faculty of Science, M. S. University of Baroda, Vadodara - 390 002
E-mail : rajendra_jadeja@yahoo.com, komalvyas_26@yahoo.in

With the aim of exploring the anticancer properties of coordination compounds with bioactive ligands such as pyrazolone derivatives and polypyridyls, for the first time here we report the new synthesis of a novel ternary complex [Cu(PPMP)(Bipy)NCS] (where, PPMP; 3-methyl-1-phenyl-4-propionyl-1H-pyrazol-5(4H)-one and Bipy; 2, 2' bipyridyl). The ligand was in detailed characterized by different techniques. The complex was characterized by elemental analysis, Cu-estimation, molar conductance, FT-IR, magnetic measurement and single-crystal X-ray crystallography. The structure of the complex, based on the trigonality index *tau*, suggests an intermediate square pyramidal (SP) geometry. The Cu(II) ion in the complex exhibited square pyramidal geometry with the 4-propionyl pyrazolone acting as a bidentate chelating agent coordinating a Cu(II) ion *via* two O atoms, bipyridyl coordinating *via* two N atoms and the fifth coordination position around Cu(II) is occupied by an N-bonded thiocyanate ligand. The interaction of the ligands as well as complex with calf thymus DNA (CT-DNA) has been explored, which revealed that the complex could interact with DNA through intercalation. Corresponding binding constants suggested that the complex can bind more effectively than the ligands. To explore the potential medicinal value of the new complex, the protein binding ability has been monitored by quenching of tryptophan emission in the presence of ligands and complex using bovine serum albumin (BSA) as model protein. The complex showed dynamic quenching behavior, revealing their affinity for this protein with relatively high value of binding constant compared to ligands. Further, the anticancer activity of the complex on A549 (human lung cancer) cell line has been studied and it induced effective cell death and no significant effect on normal cells.

IO-12 : Second Harmonic Generation Studies on Bisthiourea Zinc Succinate and Bisthiourea Cadmium Succinate : A Novel Non-Linear Optical Materials

Malhari N. Raste and Satish K. Pardeshi*

Department of Chemistry, University of Pune, Ganeshkhind, Pune, Maharashtra-411007
E-mail : skpar@chem.unipune.ac.in

A novel class of semiorganic nonlinear optical materials such as bisthiourea zinc succinate (BTZnS) and bisthiourea cadmium succinate (BTCdS) have been synthesized by solvent free mechanochemical method. The synthesized materials are well characterized by various techniques. The chemical composition of synthesized material was confirmed by CHNS analysis and chemical analysis. FT-IR studies confirmed the presence of various functional groups and coordination of metal ions to thiourea through sulphur atom. Thermal behaviour of materials has been investigated by using TG, DTA and DSC. The data of X-ray diffractogram suggest that the synthesized compounds are polycrystalline in nature. Crystallite size of BTZnS and BTCdS are 47nm and 68nm respectively. Transmittance spectra reveal that BTZnS has lower cut-off wavelength at 334nm and that of BTCdS has 290nm. The wide transmission range in the entire visible region is essential requirement for NLO materials, which enables it to be a potential candidate for optoelectronic applications such as electric

eyes, optical fiber communications, etc. The Second harmonic generation (SHG) conversion efficiency measured by Kurtz-Powder technique using Nd: YAG laser was found to be comparable for BTZnS and 0.448 times lower for BTCdS than that of KDP as reference which confirmed the nonlinear optical nature of materials.

IO-13 : DNA Binding and Cytotoxicity Properties of Co(III) Complexes with 2-(4'-chloro-phenol) imidazo[4,5-f][1,10]phenanthroline, Ligand

Nazar M. Gabra[a,b], V. Satheesh[a] and S. Satyanarayana*

[a]*Department of Chemistry, Osmania University, Hyderabad-500007, (A.P.)*
[b]*Department of Chemistry,Red Sea University, Portsudan, Sudan, P.O. Box:24*
E-mail : ssnsirasani@gmail.com

Three complexes of the type [Co(phen)$_2$PIP-Cl](**1**) [Co(bpy)$_2$PIP-Cl] (**2**) and [Co(dmp)$_2$PIP-Cl](**3**) (phen = 1,10-phenanthroline; bpy = 2,2'-bipyridine; dmb = 4,4-Dimethyl-(2,2')bipyridine), PIP-Cl = 2-(4'-chloro-phenol) imidazo[4,5-f] [1,10]phenanthroline) have been synthesized and characterized by UV–VIS, IR and ^{1}H-NMR,^{13}C-NMR spectral methods. Absorption spectroscopy, emission spectroscopy, viscosity measurements and DNA melting techniques have been used to investigate the binding of these Co(III) complexes with calf thymus DNA and photocleavage studies have been used to investigate the binding of these complexes with plasmid DNA. The spectroscopic studies together with viscosity measurements and DNA melting studies support that Co(III) complexes bind to CT DNA(calf thymus DNA) by an intercalation mode via PIP-Cl into the base pairs of DNA. Upon irradiation, this novel Co(III) complex can cleave the plasmid pBR 322 DNA from the supercoiled form I to the open circular form II.

IO-14 : Synthesis of 3-Acetyl-4-[(1,3-benzothiazole - 2-yl) imino]-6-methyl-3, 4-dehydro-2H-pyran-2-one and its Cu(II) Complex; Theoretical, Experimental and Microbial Studies

Mohmed Jaheer[a], Palreddy Ranjithreddy[a] and Ch. Sarala Devi[b]*

[a]*Department of Chemistry, University College of Science, Osmania University, Hyderabad*
[b]*Department of Chemistry, University College of Science, Osmania University, Hyderabad*
**E-mail : dr_saraladevich@yahoo.com*

In all benzoheterocycles, benzothiazole has considerable place in research area especially in synthetic as well as in pharmaceutical chemistry because of its potent and significant pharmacological activity. A novel 3-acetyl-4-[(1,3-benzothiazole -2-yl)imino]-6-methyl-3,4-dehydro-

2H-pyran-2-one was synthesized. The purity of the synthesized compound was judged by C, H and N analysis, and the chemical structure was analyzed on the basis of IR, ^{1}H NMR and Mass spectral data. The title compound when treated with sulfate of Cu (II) yielded its complex. The metal complex was characterized by elemental analysis, molar conductivity, IR, UV, ESR, SEM, magnetic susceptibility measurements and thermal studies. The HyperChem 7.5 software was used for quantum mechanical calculations. The geometry optimization was carried out using abinitio method. Employing semiempirical single point PM3 method, theoretical data for IR and NMR are generated. The experimental spectral data was compared with the data computed. QSAR properties like surface area, volume, hydration energy, log P, refractivity, polarisability, mass, total energy and the frontier molecular orbital energies [E_{homo} & E_{lumo}] were computed. The title compound and its copper complex were screened for antimicrobial activity.

IO-15 : Effects of Feed Additives on Body Weights at Different Ages in Rabbit

R. R. Jha

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

The rabbit farming is emerging pattern of body weight gain was observed in the rabbit of different groups. The overall feed conversion ratio during 6 – 12th week of age in the rabbits of G_3 (3.87) group was observed to be better than the rabbits of G_2 (4.50) and G_1 (5.28) groups. At the end of experiment (i.e. 6 – 13 week of age), the overall feed conversion ratio in the rabbits of G_3 (4.35) group was observed to be better than G_2 (4.91) and G_1 (6.01) groups. The above findings indicated that the as an important enterprise in many countries of the world. In addition to better nutritional status of rabbit meat, it has no racial and religious restriction for consumption. Cholesterol creates several health problems in human being. In view of this now a days people avoid to take more cholesterol rich content food like red meat and prefer white meat. Rabbit meat has high biological value, high in protein (21%), good quality white meat with low % of cholesterol and sodium (Chakrabarti *et al.* 1995). Probiotic that contain yeast, live bacteria or bacterial spores can also prevent enteric diseases of rabbits. Instead of growth promoters with antibiotics that kill some of the rabbit's own gastrointestinal flora, Probiotic promote gut colonization and stabilize eubiosis by competitive growth against harmful microorganisms, reducing the intestinal pH with production of lactic acid and encouraging digestion by producing enzymes and vitamins.

IO-16 : Studies on Some Biopotential Complexes of Lanthanides(III) Derived from Thiosemicarbazone and Heterocyclic Base

Ram K. Agarwal

Departmentof Chemistry, Lajpat Rai Postgraduate University (C.C.S.University) Sahibabad-201005 (Ghaziabad)
E-mail : ram_agarwal54@yahoo.com

Heterocyclic compounds are widely distributed in nature and are essential to life. They play a vital role in the metabolism of all living cells. The chemistry of heterocycles will continue to grow for the creation of new drugs, agrochemicals, novel materials etc. Pyridine and its derivatives possess significant importance. In present studies some mixed ligand complexes of lanthanides (III) salts derived from 4[N(2'-hydroxy-1'-naphthalidene) amino] antipyrinethiosemicarbazone (HNAAPTS) and quinoline (Qn) with the general composition LnX_3.n(HNAAPTS).Qn (Ln = La, Pr,Nd, Sm, Gd, Tb, Dy or Ho; X = NO_3^-. n = 1; X = NCS^- or ClO_4^- , n = 2 are reported. All the synthesized complexes were characterized through various physico-chemical studies. The coordinated HNAAPTS behaves as neutral tridentate (N,N,S-donor) while quinoline acts as unidentate N-donor. The ligand and the corresponding Ln(III) complexes were simultaneously screened for their antibacterial and antifungal activities. Depending on the nature of the anionic ligands, the coordination number of lanthanide (III) in case of nitrate or thiocyanate complexes was ten, while it was seven in case of perchlorate complexes.

IO-17 : Modification of Silica Surface using Silatrane with Schiff base Moiety

Ruchi Mutneja[a], Varinder Kaur[a] and Raghubir Singh[b]

[a]Department of Chemistry, Panjab University, Chandigarh-160014
[b]Department of Chemistry, Bhojia Institute of Life Sciences, Baddi-173205
E-mail : chem.ruchimutneja@gmail.com

A Schiff base moiety is introduced into the axial chain of silatrane by the condensation of the 2-acetylphenol with 3-aminopropylsilatrane in the presence of anhydrous sodium sulphate. It was characterized by elemental analysis, spectroscopic techniques and X-ray diffraction analysis. As the Schiff base moieties are capable of coordinating with metal ions, so the synthesized silatrane was immobilized on to the silica surface. The use of silatrane to modify the silica surface was not known previously. In the present work, it is found that use of silatranes in modification of silica is advantageous over their alkoxy analogues because these can be separated in pure solid form whereas their analogues are oily in nature. The modified silica surface can be further used as heterogeneous catalyst and in metal analysis and its application is in progress.

IO-18 : Mn(III) Complexes with Porphyrins ligand and 1,3-diaminopropane

Shashi Lata Bharati and Sudha Yadava*

**Department of Chemistry, DDU Gorakhpur University, Gorakhpur-273009 (U.P.)*
E-mail : dr_sudhayadava@yahoo.co.in

A series of some novel Mn(III) complexes with 5,10,15,20-tetra(p-tolylporphine) and 1,3-diaminopropane have been synthesized. These complexes have been characterized by U.V.-visible, IR, *ESI-mass spectra*, elemental analyses, conductivity and magnetic susceptibility measurements. These Mn(III) porphyrins exhibited a red-shift in Soret band in comparison to the non-metallated porphyrins. The molar conductance values of these complexes show their non-electrolytic nature in ethanol. The tentative structures have also been proposed.

IO-19 : Synthesis and Characterization of Tetra 2,9,16,23 – naphtho[2,1-b]furan substituted Metal (II) Phthalocyanines through 1,3,4 - Oxadiazole Bridge

Shoukat Ali R.A, J.Keshavayya* and Rajesha T.

Department of Chemistry, School of Chemical Sciences, Jnana Sahyadri,
Kuvempu University, Shankaraghatta - 577 451, Shimoga, Karnataka
**E-mail : jkeshavayya@gmail.com.*

The present investigation describes about the synthesis of 1,3,4-oxadiazole bridgednaphtho[2,1-b]furan substituted metal(II) phthalocyanines by the condensation of 2,9,16,23 - tetra carboxy metal(II) phthalocyanine with ethyl naphtho[2,1-b]furan-2-carbohydrazide in the presence of suitable condensing and dehydrating agent. The newly synthesized complexes are dark green in colour and are characterized by the various techniques like Elemental analysis, UV-Visible, IR spectroscopic and thermal methods.

IO-20 : Synthesis and Reactivity of Metal-Alkenyl Complexes

Sadhana Venkatesh, Chinduluri Sravani, Wrickban Mazumdar, Dhrubajyoti Das, and Akella Sivaramakrishna*

Department of Chemistry, School of Advanced Sciences, VIT University,
Vellore 632 014, Tamil Nadu
E-mail : asrkrishna@vit.ac.in

Metal-alkenyls are a well known class of compounds and are key intermediates in catalytic reactions including ethylene oligomerization[1,2]. A variety of metal-alkenyls complexes (M = Pt, Pd, Ir and Rh) were prepared by the reaction of 1-alkenyl Grignard reagent with L_2PtCl_2 and characterized by various spectroscopic techniques. We have recently reported a novel synthetic route for the preparation of platinacycloalkanes with different ring sizes[3] by the ring closing metathesis reactions of the corresponding bis(alkenyl)platinum(II) complexes with Grubbs' catalysts.

Thermal decomposition studies of these compounds indicated the formation of corresponding 1-alkene, 2-alkene and dienes depending on the experimental conditions. The present work describes the investigations pertaining to the factors affecting the stability of these metal-alkenyl complexes.

IO-21 : Facile Synthesis of Caulophyllumine B and Pinidine Alkaloids via Pd(II) N-heterocyclic Carbene Catalyzed Heck and Negishi Cross-coupling Reactions

Shravankumar Kankala[a], Ravinder Vadde*[a] and
Chandra Sekhar Vasam*[b]
[a]*Department of Chemistry, Kakatiya University, Warangal-506009*
[b]*Department of Chemistry, Satavahana University, Karimnagar-505001*
**E-mail : ravichemku@yahoo.co, csvasamsa@gmail.com*

A direct and convenient synthetic methodology for two natural piperidine alkene-alkaloids, namely (+)-Caulophyllumine B and (+)-Pinidine, has been developed by two different routes involving Heck and Negishi cross-coupling as key steps catalyzed by simple *in situ* formed Pd-*N*-Heterocyclic carbenes (Pd-NHCs). Our approach could be an efficient alternative to the reported synthetic methodologies of both the alkaloids, depending on the availability of starting materials. The added PTC has accelerated the Pd-NHC catalyst to form high yields of (*E*)-olefin intermediate and also responsible for Pd(0) nanoparticles formed *in situ*. The cross-coupling methodology will allow attaching many other organic moieties to the *N*-Boc-piperidine to produce the analogues of these two alkaloids.

IO-22 : Microwave Assisted Combustion Synthesis of $BaLa_2O_4:Tb^{3+}$ Nanoparticles

Sonika, V.B. Taxak--*, S. P. Khatkar and Mukesh Kumar
Maharshi Dayanand University, Rohtak-124001
E-mail : v_taxak@yahoo.com

A novel green light emitting Tb^{3+} doped $BaLa_2O_4$ nanophosphor was synthesized by microwave assisted combustion synthesis using an organic fuel. The synthesized powder was further treated at different temperatures for 3 hrs to increase luminescence intensity and crystallinity of the materials. The microwave assisted combustion synthesis provides an interesting alternative over other elaborated techniques because it offers several attractive advantages such as simplicity of experimental set-up, surprisingly short time between the preparation of reactants and the availability of the final product and being cheap due to energy saving. The crystalline structure of prepared materials, morphology of particles and their photoluminescence properties are characterized by X- ray diffraction (XRD), scanning electron microscopy (SEM) and photoluminescence spectra (PL) under an UV source for excitation. The particle size of nanophosphor was found to have an average range of 25-80 nm size. The photoluminescence was maximum for sample prepared with 2 mole % of terbium ions. The predominant green color from magnetic dipole transition $^5D_4 \rightarrow {}^7F_5$ of Tb^{3+} was located at 544 nm.

IO-23 : Synthesis and Characterization of Some Novel Schiff Base Complexes

L. N. Sharada,* V.Balakrishna and B. Sammaiah,

Department of Chemistry, Osmania University, Hyderabad-500007
**E-mail: lnsharada@gmail.com*

New coordination complexes of oxovanadium (IV), manganese (II), Iron (II) and nickel(II) have been synthesized and characterized on the basis of elemental analysis, electrical conductance, infra-red electronic spectra and magnetic susceptibility measurements with the Schiff base NN' ethylene bis(2 amino benzamide with dehydroacetic acid .The donor ligand is coordinating through four nitrogen atoms and two oxygen atoms .It acts as dibasic donor ligand coordinating through N N'N"N"'and deprotonated phenolic oxygen. All the complexes have been assigned octahedral stereochemistry.

IO-24 : Studies on Synthesis, Spectral, Magnetic, Analytical and Biological Properties of Some Transition Metal Complexes of 1,5-Benzodiazepines

Suresh

**Department of Chemistry, Ballatri Institute of Technology & Management, Bellary, Karnataka*
E-mail : drsuresh61@yahoo.com

Copper(II), cobalt(II), nickel(II), zinc(II), cadmium(II) and mercury(II) complexes of substituted 2,3-dihydro-2-phenyl-4-(2'-hydroxy phenyl)-1H-1,5-benzodiazepine have been synthesized. Elemental analysis of the complexes indicate that copper(II), zinc(II), cadmium(II) and mercury(II) forms the complexes of the stoichiometry of the type LMCl and cobalt(II), nickel(II) forms complexes of the stoichiometry of the type ML_2. IR, PMR, ESR, X-ray and electronic spectral studies indicate involvement of NH, C=N and phenolic –OH groups in coordination with metal ions. Molar conductance values in DMF at 10^{-3}M fall in the range of 10.21 to 20.00 moh cm mol^{-1} suggesting non-electrolytic behavior of these complexes in DMF. Copper(II) complexes shows magnetic moments in the range 1.71-2.12.B.M., nickel(II) complexes shows magnetic moments in the range 3.56 – 4.16 B.M. and cobalt(II) **c**omplexes exhibit in the range of 4.20 – 4.70 B.M. attributable to tetrahedral geometry. X- Ray spectral analysis indicates these forms cubic crystalline nature.

IO-25 : Synthesis, Characterization, Cytotoxic Activities and Single Crystal Studies of Ternary Copper(II) Complexes of Isoxazole Schiff Base with Heterocyclic Bases

Vijay Kumar Chityala, Sathish Kumar K. and Shivaraj[*]

Department of Chemistry, Osmania University, Hyderabad-500 007 Andhra Pradesh
**E-mail : shivaraj_sunny@yahoo.co.in*

New ternary copper(II) complexes $[Cu(L)B^1]ClO_4$, $[Cu(L)B^2]ClO_4$, $[Cu(L)B^3]$, $[Cu(L)B^4]$ where L is the N O donor Schiff base derived from the condensation of 5-amino-3,4-dimethyl isoxazole with 2-hydroxy naphthaldehyde and 1,10 phenanthroline (phen)(B^1) / 2,2^1 bipyridyl (bipy) (B^2) / 8-hydroxy quinoline (oxine) (B^3) / 5-chloro-8-hydroxy quinoline (5-chloro oxine) (B^4) are synthesized and characterized by IR, UV, TGA, ESR, Elemental analysis and magnetic studies. The $[Cu(L)B^1]ClO_4$ is structurally characterized by single crystal analysis. Based on the spectral data $[Cu(L)B^1]ClO_4$, $[Cu(L)B^2]ClO_4$ complexes exhibit distorted square pyramidal geometry whereas $[Cu(L)B^3]$, $[Cu(L)B^4]$ complexes exhibit square planar geometry. Biological studies of these complexes have been studied against gram +ve, gram -ve, Rhizopus oryzae and Aspergillus niger. These complexes have been evaluated for their cytotoxic activities towards Human Cervical Carcinoma Cells (HeLa) by MTT assay.

IO-26 : Optoelectronic Characterization of the Nano Blue Phosphor

Vijeta Tanwar, Ishwar Singh, Pratap Singh Kadyan and Devender Singh

Department of Chemistry, Maharshi Dayanand University, Rohtak, Haryana
E-mail : devjakhar@gmail.com

$BaMgAl_{10}O_{17}$:Eu blue phosphor was synthesized by the rapid combustion method. The combustion method has emerged as an alternative technique because it is a simple, rapid and energy saving.

The prepared phosphor was treated at 600 ^{0}C temperatures to study the effect on luminescence and surface crystallinity of the materials. The phosphor materials gave blue luminescence under UV lamp at 420 nm. The blue photoluminescence was due to the transition $4f^6 5d^1 \rightarrow 4f^7$. The particle size of the material was found to be in the range of 40-70 nm. The luminescent materials obtained through combustion technique were also characterized by using the Scanning electron microscopy (SEM), X-ray diffraction (XRD) and photoluminescence spectra (PL).

IO-27 : Designing, Structural Elucidation, DNA Cleavage, Antibacterial and Antioxidant Activity of Binuclear Metal Complexes Containing Tetradentate Schiff Base

E. Akila, M. Usharani and R. Rajavel*

Department of Chemistry, Periyar University, Periyar Palkalai Nagar, Salem-II, Tamil Nadu
Email : drrajavel@rediffmail.com

A novel binuclear Cu(II), Ni(II) and YO(II) complexes have been synthesized by the simple Schiff base condensation of 3, 3'-dihydroxybenzidine, 2,3-pentadione and 2-aminophenol in the molar' ratio of 1:2:2. The ligand and its metal complexes have been characterized by physico-chemical methods including elemental analysis, Eleotrochemical, Magnetic, Thermal and Spectral studies. All the complexes are non-electrolyte in DMF due to their low molar conductance value. The IR spectral data suggest the involvement of azomethine nitrogen and phenolic oxygen in co-ordination to the central metal ion. Electronic spectral data proposed the square planar geometry for Cu(II), Ni(II) and square pyramidal for YO(II) complexes under investigations. By using YSM, the magnetic moment value indicates no interaction between two metal centres in binuclear complexes. The electrochemical properties of the Schiff base metal complexes were studied; the observed redox transitions were assigned to specific redox-active sites of the molecule. The ESR spectral data also shows the evidence for the geometry of the metal complexes. The nucleolytic cleavage activities of the ligand and their complexes were assayed on pUC18 plasmid DNA using gel electrophoresis in the presence and absence of H_2O_2. Streptomycin was used as standard in disc diffusion method. The complexes and free ligands show significant activity against the bacteria like *Staphylococcus aureus, Escherichia coli, Bacillus subtilis* and *Klebsilla pneumonia* but lesser than standard. The in vitro antioxidant properties of the Schiff base ligand were evaluated by (DPPH·) free radical scavenging assay.

IO-28 : 2, 2'- Biphenyl Dicarboxylates of Lanthanides

Kamini Sharma* **and A. M. Bhandari**

**Department of Chemistry, JIET School of Engineering and Technology for Girls, Mogra, Jodhpur-Rajasthan*
Department of Chemistry, J.N.V. University, Jodhpur-Rajasthan
**E-mail : kaminisharma206@gmail.com*

Light coloured, water- insoluble lanthanide (III) 2,2'- biphenyl dicarboxylates of the composition, $Ln_2(O_2\ C.A.CO_2)_3.10H_2O$ where $A(CO_2H)_2$ stands for 2,2'- biphenyl dicarboxyllic acid and Ln stands for lanthanum, praseodymium and neodymium, get precipitated on treating sodium salt of the acid with an aqueous solution of lanthanide chloride. The infrared spectral separations (Δv) of the two OCO ir bands which are equal for praseodymium and neodymium dicarboxylates possibly favour bidentate chelating type of carboxylates bonding in these derivatives. Thermal degradation of these dicarboxylates seems to involve species such as Ln_2X_3.3(or 4) H_2O, Ln_2X_3, and certain oxy species as partially stable intermediates where XH_2 stands for 2,2'-biphenyl dicarboxyllic acid.

IP-CYSA-01 : Application of Magnetic Nanoadsorbent Fe_2O_3 for Removal of Hazardous Ponceau-S Dye from Aqueous Solution

Bharat N. Patil and V. S. Shrivastava

Nanochemistry Research Laboratory, G.T.P. College, Nandurbar -425412,(M.S.)
E-mail : drvinod-_shrivastava@yahoo.com, bharatchemy@gmail.com

The photodegradation of Ponceau-S dye was investigated using UV radiation in presence of nanosized Fe_2O_3. Removal efficiency of Ponceau-S was sensitive to the operational parameters such as dye concentration, catalyst dose, pH, contact time, TOC and COD. The photocatalytic treatment of red colored Ponceau-S dye by magnetic nano semiconductor (Fe_2O_3) is an effective, economic and faster mode. The kinetics and isotherm studies were carried out. A simple kinetics model is proposed which confirms pseudo second order reaction. Langmuir isotherm was fit with this study. The optimum conditions for the degradation of the dye were initial concentration 50 mgL^{-1}, pH 8, contact time 20 minutes and catalyst dose 5 gL^{-1} of Fe_2O_3 .

The semiconductor photocatalyst was also carried out for SEM and XRD analysis which confirms the utilized semiconductor was nanosized.

IP-CYSA-02 : Design, Synthesis and Characterization of 2–amino–2–methylpropane–1,3–diol Derived Organotin(IV) Schiff Base Complexes of o–Vanillin: *in vitro* DNA Binding and Cleavage Studies

Shipra Yadav and Sartaj Tabassum*
Department of Chemistry, Aligarh Muslim University, Aligarh–202002
E-mail : tsartaj62@yahoo.com

The biological activity of the organotin complexes is due to the presence of easily hydrolysable groups resulting in the intermediates which bind with DNA. Furthermore, there has been a considerable interest in the development of complexes suitable for cleaving DNA hydrolytically or modeling phosphoester hydrolysis promoted by metal center. In this prospect, we have synthesized new heterobimetallic complexes **1–6** of composition, $[M–Sn_2(en)_2(L)_2]$ (M = Cu(II): **1**; Ni(II): **2**) and $[M–Sn_2(R)_4(en)_2(L)_2]$ (M = Cu(II), R = Me: **3**) (M = Ni(II), R = Me: **4**) (M = Cu(II), R = Ph: **5**) (M = Ni(II), R = Ph: **6**). Interaction of the heterobimetallic Cu-Sn complexes **1**, **3** and **5** with CT DNA was investigated using spectroscopic techniques, viscosity measurements and gel electrophoresis which revealed strong electrostatic binding to CT DNA *via* phosphate backbone of DNA helix, in addition to H–bonding. The K_b values were calculated and the results suggested pronounced binding of complex **5** with DNA double helix. Further to evaluate the molecular recognition at target site, interaction studies of **3** and **5** with 5'–GMP were carried out by UV–vis titration and by NMR studies. The supercoiled pBR322 plasmid DNA nuclease activity of the complex **5** demonstrated an ability to cleave DNA *via* hydrolytic pathway mechanism.

IP-CYSA-03 : Synthesis, Characterization and Antimicrobial Activity of 1,3-Dithia-2-arsa(III) Cyclopentane Derivatives with Oxygen and Sulphur Donor Ligands

Sumit Bhatiya and H. P. S. Chauhan*
School of Chemical Sciences, Takshashila Campus, Khandwa Road,
Devi Ahilya University, Indore-452001
E-mail : hpsc@rediffmail.com; sumit.bhatiya@gmail.com

Replacement reaction of 1,3-dithia-2-arsa(III)cyclopentane chloride and oxygen or sulphur donor ligands like benzoic acid, thiobenzoic acid, acetic acid, thioacetic acid, phenol, thiophenol, sodium salicylate and thio glycolic acid in 1:1 molar ratio in refluxing anhydrous benzene (~5h) yielded 1,3-dithia-2-arsa(III)cyclopentane mono

carboxylic or phenolic derivatives of general formula SCH_2CH_2SAsR {R = $OOCC_6H_5$, $SOCC_6H_5$, $OOCCH_3$, $SOCCH_3$, OC_6H_5, SC_6H_5, $OOCC_6H_4(OH)$, SCH_2COOH}. These newly synthesized derivatives are white/ pale yellow solid/ liquid and soluble in common organic solvents like benzene, chloroform, dichloromethane, DMF, DMSO etc. These derivatives have been characterized by melting point determination, molecular weight determination, elemental analysis (C, H, S and As) and spectral {UV, IR and NMR (^1H and ^{13}C)} and SEM studies. These complexes have been screened for their antimicrobial activities using the disc diffusion method. All the complexes have shown good activity as antibacterial and antifungal agents on some selected bacterial and fungal strains, which increased on increasing the concentration.

IP-CYSA-04 : Synthesis, Characterization of Ruthenium(II) Polypyridyl Complexes and DNA Binding, Photocleavage, Cytotoxicity Studies

Yata Praveen Kumar, P. Venkat Reddy and S. Satyanarayana*

Department of Chemistry, Osmania University, Hyderabad
E-mail : ssnsirasani@gmail.com

The new ligands 6-HEPIP (2-ethoxy-6-(1H imadazo[4,5-f][1,10]phenathroline-2-yl)phenol)) and 4-HEPIP (2-ethoxy-4-(1H imadazo[4,5-f][1,10]phenathroline-2-yl)phenol)) its two Ruthenium (II) complexes $[Ru(phen)_2(6\text{-}HEPIP)](ClO_4)_2$ (1) and $[Ru(phen)_2(4\text{-}EHPIP)](ClO4)_2$ (2) have been synthesized and characterized. These complexes have been shown to act as promising calf thymus DNA intercalates and a new class of DNA light switches, as evidenced by UV-visible and luminescence titrations with Co^{2+} and EDTA, steady-state emission quenching by $[Fe(CN)_6]^{4-}$, DNA competitive binding with ethidium bromide, viscosity measurements, DNA and photo activated cleavage. The results suggest that these complexes interact with DNA through intercalative mode. Further, these two complexes were screened for their antimicrobial activity. Cell viability experiments indicated that the Ru(II) complexes showed significant dose dependent cytotoxicity to Four human tumor cell lines like human cervical cancer HeLa, A549, DU145 and HEPG cells. The cytotoxicity of these two complexes was evaluated by the MTT method. Ru(II) complexes 1 and 2 exhibited promising growth inhibitory effects.

IP-01 : Equilibrium and Thermodynamic Study of the Aqueous Complexation of 5-Amino Salicylic Acid with d^{10}-Metal Cations

A. S. Prajapati[a] **and J. J. Vora**[b]

[a]*M. N. College, Visnagar, Dist.Mehasana, Gujarat*
[b]*Department of Chemistry, Hemchandracharya North Gujarat University, Patan, Gujarat*
E-mail : arvindprajapati10@gmail.com

Chemical equilibrium studies on d^{10} metal complexes with 5- Amino salicylic acid have been investigated pH metrically. Three different temperatures were selected for the study. The formation characteristics in solution state have been characterized along with important thermodynamic parameters. The Irving and Rossotti technique has been adopted to determine the formation constants corresponding to the various complexation equilibria.

IP-02 : Synthesis and Characterization of Some Transition Metal Complexes with Schiff Base Ligands

M. R. Anil Kumar*, S. Shanmukhappa* and B. E. Rangaswamy[Ø]

[Ø]*Department of Biotechnology, Bapuji Institute of Engineering and Technology,*
**Department of Chemistry, Bapuji Institute of Engineering and Technology*
Post Box – 325, Shamanur Road, Davangere – 577004, Karnataka
**E-mail : drsschemical@gmail.com*

The synthesis of new Schiff base ligands and their metal complexes were carried out. The ligands were characterized by using various physical and chemical methods. The spectral data suggest the formation of immine group in the ligands containing N and O donor atoms. Coordination metal complexes were synthesized by reacting these Schiff base ligands with metal ions such as Cu(II), Zn(II), Mn(II), Co(II), Ni(II) and Cd(II). The metal complexes have been characterized by elemental analysis, UV-Visible, IR, ^1H NMR, molar conductance and magnetic susceptibility measurements. The spectral data suggest that the immine group in the ligand is involved in the coordination with the metal ion. Based on the above studies octahedral geometry is tentatively proposed for the new complexes.

IP-03 : Self Compacting Concrete : Concrete of the Future

Anuradha Varshney and Nalini Jain

Department of Chemistry, Dayanand Girl's PG College, Kanpur
E-mail : anurmc@gmail.com

Self Compacting concrete is the greatest advancement and most revolutionary development in concrete technology over last 30 years. Self compacting concrete is the concrete which flows under its own weight without any segregation and maintaining its homogeneity through all shapes and obstructions, without any need of vibrations. Self compacting Concrete requires low yield stress and high resistance to segregation (high viscosity). Addition of water decreases the yield stress but lowers the viscosity. Superplasticizers also lowers the yield stress, but slightly. Viscosity of the mix can be improved by taking a proper mix design. Addition of viscosity modifier, when added, increases yield stress of the paste. An attempt has been made to use modern superplaticizers (based on carbolxylic ethers) which promotes good workability due to electrostatic repulsion in combination with steric hindrance. Increased quantity of polymer admixture and use of flyash gives Self Compacting Concrete with higher slump. Various testing methods used are:Slump flow Test, L Box Test and Fill box Test.

IP-04 : Spectral Charaterization of the Product of $[Np(OH)_2]_3$ and Adipic Acid

Atul Gupta and S. P. S. Jadon*

Department of Chemistry, S.V. College, Aligarh (UP), 202001, India
E-mail : sps_jadon@yahoo.co.in

$[Np(OH)_2]_3$ was heated with adipic acid in presence of conc. H_2SO_4 (1ml) dissolved in alcohol. The product, obtained, was estimated qualitatively, quantitatively, Mass, IR and ^{1}HNMR spectrometrically. The molecular weight of the product, found, gravimetrically as 493gmol^{-1} is supported by prominent mass line m/z 492, observed, in its mass spectrum, assigning it as $[P_3N_3(OH)_4](CH_2)_8(COO)_2(COOH)_2$. The formation of the adduct is also confirmed by the vibration, 678.6, 1068.6, 1689.8 and 2800.9 cm^{-1} subsequently for $P-N$, $P-O-CH_2$, $=C=O$ and CH_2–COOH bands in its IR spectrum and Chemical shifts for different groups in its ^{1}HNMR spectrum.

IP-05 : Speciation of Ternary Complexes of Ca(II), Zn(II) and Mn(II) with L-proline and L-valine in Acetonitrile-water Mixtures

B. Veeraswami[$], G. Nageswara Rao[§,*] and U. Viplavaprasad[§]

[$]Gitam Institute of Technology, Gitam University, Visakhapatnam-530045
[§]School of Chemistry, Andhra University, Visakhapatnam-530003
**E-mail : gollapallinr@yahoo.com*

Chemical speciation of ternary complexes of Ca(II), Zn(II) and Mn(II) with L-proline and L-valine was studied in various concentrations (0-60% v/v) of acetonitrile-water mixtures maintaining an ionic strength of 0.16 mol L^{-1} (NaCl) at 303.0 K. Alkalimetric titrations were carried out in different relative concentrations (M: L: X = 1:2.5:2.5, 1:2.5:5.0, 1:5.0:2.5) of metal (M) to L-proline (L) to L-valine (X) with sodium hydroxide as titrant. Stability constants of ternary complexes were calculated and various models were refined with MINIQUAD75. The trend of the variation in the stability constants with changing dielectric constant of the medium was explained based on the electrostatic interactions of the ligands, charge neutralization, chelate effect, stacking interactions and hydrogen bonding. Distribution diagrams with pH at different compositions of aqua-organic mixtures and structures of plausible ternary complexes were also presented.

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

Ashwini Kumar[1] and Anamika[2]

[1]Department of Chemistry, S.N.S.College, Muzaffarpur.
[2]Department of Chemistry P.G. Mahila College, Chaibasa, Jharkhand.
E-mail : ashwinikumar.chem@gmail.com

Two new dioxomolybdenum(VI) complexes [MoO_2(acac)LL'] (I) and [$MoO_2L_2L_2$"] (II)[L=OC(CH_3)$CHCOCH_3$, L' =$NH_2C_6H_4NH_2$, L" = $NH_2C_6H_3CH_3NH_2$] 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. ^{1}H, ^{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.

IP-07 : Co(II) and Cu(II) Complexes of N_2O_2 and N_2O_4 Schiff Base Ligands : Their Catalytic and Antibacterial Studies

E. Ravikrishna, V. Srinivas, M. Chandrashekar, B.Ramesh and V. Ravinder*

Department of Chemistry, Kakatiya University, Warangal-506 009
**E-mail : ravichemku@yahoo.co.in*

A series of new heterodentate N, O-donor ligands derived by condensing *o*-phthalaldehyde (OPA) with hydroxy benzoic hydrazides (HBHs) and some substituted aromatic amines (AAs) were used to afford new mononuclear Co(II) and Cu(II) coordination compounds. All the complexes were characterized by IR, ^{1}H NMR, ^{13}C NMR, mass, ESR,electronic spectra, conductance,magnetic, thermal studies and their structures have been proposed. While the ligands derived from OPA and HBHs displayed hexadentate coordiantion around the metal ion, the ligands derived from OPA and AAs displayed tetradentate coordination as suggested by spectral studies. These mononuclear complexes were investigated as catalysts in the hydrogenation of substituted aromatic nitrates. The reduced products of hydrogenation were further treated with nitrous acid followed by β-napthol to develop the colored products (azodyes), which were determined spectrophotometrically. The Schiff base Co(II) compounds were further screened for antibacterial activity against Gram +ve and Gram-ve bacteria and the results were compared with standard drugs streptomycin and ampicillin.

IP-08 : Synthesis, Thermolysis and Coordination Behaviour of Aminophosphine Oxides

E. Veerashekhar Goud, B.B. Pavankumar, Arjita Paul, Yacham Shruthi and Akella Sivaramakrishna*

Department of Chemistry, School of Advanced Sciences, VIT University,
Vellore 632 014, Tamil Nadu
E-mail : asrkrishna@vit.ac.in

The study of ligands containing either trivalent or pentavalent phosphorus atoms has been of great interest throughout inorganic and organic chemistry due to their wide range of applications as insecticides and antitumor agents and their involvement in a great number of catalytic reactions [1-3]. In this connection, some aminophosphine oxides (AmPOs) of the type $(R_1)(R_2)(R_3)P{=}O$ [$R_1 = R_2 = R_3 = HNCH_2CH{=}CH_2$ (**L_1**); $R_1 = R_2 = Ph$; $R_3 = HNCH_2CH{=}CH_2$ (**L_2**); $R_1 = R_2 = R_3 = HNNMe_2$ (**L_3**); $R_1 = R_2 = Ph$; $R_3 = HNNMe_2$ (**L_4**); $R_1 = R_2 = R_3 = NC_4H_8O$ (**L_5**); $R_1 = Ph$; $R_2 = R_3 = NC_4H_8O$ (**L_6**)] have been synthesized. The coordination chemistry of these AmPOs is studied with La(III), Th(IV) and U(VI) salts. The products obtained have been characterized by various analytical and spectroscopic techniques. The thermal properties of the ligands and their complexes are examined. The TGA data for these compounds shows the different decomposition temperatures, as well as the thermal stability of the metal complexes. Comparisons are made among different ligands on their selective complexing ability towards some chosen metal salts.

IP-09 : Hot Amperometric Titration of Rare Earth, Metals using Methyl Thymol Blue (MTB) as Reagent

E.N. Nirapure, G.P. Sahu and S.C. Lavale*

Chemical Research Laboratory, Jaywanty Haksar Lead Govt. College, Betul-460001 (M.P.)

Methyl thymol blue have been used as a reagent in verious spectrophotometric studies. Wosdorh & Cooper method have been used $\square_{max}$ and stoichiometry with rare metals have been computed. Parellel investigations using electrode probe was not fair upto certain extent hence reduction wave of methyl thymol blue have been obtained at 40°C, 50°C & 60°C. The hot amperometric titrations of Tb (III), Dy (III) and Nd (III) have been successfully perform. The complexes were also found to be reversible in nature. Rare metals could be successfully estimated up to 0.14 mg. with the standard deviation up to 0.00012, CV = 0.47 and confidence limit 99.5%. Study have been made in presence of various diverse ion viz Na^+, K^+, Li^+, Ca^{++}, Mg^{++}, Al^{+++}, Be^{++} most suitable platue potential for methyl thymol blue is found to be - 1.15 volt vs Hg - pool. The study have been done at pH 4.8 + 0.02. Ionic strength were kept constant during titrimetric process. The tolerance limit of the other ions which caused an error less than + 2.0% and a fairly large amount of anions like Cl^-, ClO_4^-, NO_3^-, CH_3COO^-, I^-, SO_4^{--} and PO_4^{---} do not hemper the titremetric process. The effect of various experimental factor have been discussed.

IP-10 : Quantum Chemical Vibrational Study, Molecular Property and HOMO-LUMO Gap Energies of Zirconium Chelate of 1, 2 Napthoquinone – 1, oxime

G. S. Jagtap, N. S. Suryawanshi, K. D. Jadhav and R. G. Sarawadekar*

Bharati Vidyapeeth Deemed University, Pune
Yashwantrao Mohite College, Pune - 411 038
E-mail : rgsarawadekar@yahoo.co.in

The vibrational frequencies of ZrO (NQO) 2 where NQO = 1, 2 napthoquinone–1, oxime, were calculated using Gaussian 09 software code, employing RHF / Lanl2DZ and DFT

(B3LYP) basis set to predict the molecular structure. The fundamental modes are assigned by using animation software. The calculated frequencies are in good agreement with the experimental values. The calculated geometrical parameters are also given. The study is extended to calculate the HOMO-LUMO energy gap, Ionization potential (I), Electron affinity (A), Global hardness (η), chemical potential (μ) and global electrophilicity (ω). The calculated HOMO-LUMO energies show the charge transfer occurs in the molecule.

IP-11 : Characterization of Complex of Co(II) with Se_4N_3Br: Mass and IR Spectra

Govind Gupta and S. P. S. Jadon*

Department of Chemistry, S.V. College, Aligarh - 202001 (UP)
E-mail : sps_ jadon@yahoo.co.in

Being donar, Se_4N_3Br was refluxed with CoCl2 in DMF for 6-8 h. The brownish black mass, formed, was separated and estimated gravimetrically as well as Mass spectrometrically. The analytical data and molecular weight 1562.8 g mol^{-1} , which is supported by prominent mass line at m/z 1562, observed, in its Mass spectrum, formulated it as $(Se_4N_3)_4.CoCl_2$. The coordination of $Se_4N_3^-$ ion to Co atom is supported by the vibrations, at 670.8 , 1079.4 ,1399.4 and 3405.1 cm^{-1} for the Se -N— Co bonds appeared in its IR spectrum, resulting hexadentated coordinated complex.

IP-12 : Template Directed Synthesis of a Supramolecule

H.C. Rai[1] and Ashwini Kumar[2]

[1]Department of Chemistry, Univ. Dept., B.R.A Bihar University, Muzaffarpur
[2]S.N.S.College, Muzaffarpur
E-mail : ashwinikumar.chem@gmail.com

Molecular recognition and self assembly may be used with reactive species in order to pre-organize a system for a chemical reaction. It may be considered a special case of supramolecular catalysis. Non covalent bonds between the reactants and the template hold the reactive sites of the reactants close together facilitating the desired chemistry. This technique is particularly useful for situations where the desired reaction conformation is thermodynamically or kinetically unlikely such as in the preparation of a large macrocycles. This pre-organization also serves purposes such as minimizing side reactions, lowering the activation energy of the reaction and producing desired stereochemistry. After the reaction has taken place the template may remain in place, be forcibly removed or may be automatically decomplexed on account of the different recognition properties of the reaction product. The template may be as simple as a single metal ion or may be extremely complex. A reaction between nikel (II) sulfate and glyoxal in aqueous solution yields blue crystals of $[Ni_6(H_2C_2O_2)_6(SO_4)_2(OH)_2(H_2O)_8]SO_4(H_2O)_{10}$. The complex cation in the compound has a remarkable structure with unusual diversity of bridging groups including glyoxal, sulfate ions and hydroxo groups. Glyoxal molecules bridge nickel (II) ion into trimer which are further linked into hexamer through bridging sulfates. The magnetic susceptibility study reveals antiterromagnetic interaction between nickel (II) ions in the polynuclear complex.

IP-13 : Synthesis, Structural Elucidation and Antimicrobial Studies of Some Transition Metal Complexes of Itopride Hydrochloride

J.K.Prasannakumar[*], S.Shanmukhappa[*], M.Revanasiddappa[@] and J.Thimmashetty[$]

[@]*Department of Chemsitry, PES Institute of Technology (South Campus), Bangalore*
[$]*Department of Pharmaceutics, Bapuji Pharmacy College, Davangere*
[*]*Department of Chemistry, Bapuji Institute of Engineering and Technology*
Post Box-325 Shamanur Road, Davangere-577004, Karnataka
**E-mail: drsschemical@gmail.com*

New transition metal complexes of Itopride hydrochloride with tertiary nitrogen were prepared. The metals used for the complex formation are Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II). The metal chelates were characterized by elemental analysis, IR, ^{1}HNMR, UV-Vis, Molar conductance and magnetic susceptibility measurements. The spectral data suggests that Mn(II), Co(II) & Ni(II) complexes shows octahedral geometry, Cu(II) complex shows distorted octahedral geometry and Zn(II), Cd(II) & Hg(II) complexes shows tetrahedral geometry. The solid state conductivity studies of the complexes vary from 6.92×10^{-8} mhos/cm +to 2.60×10^{-3} mhos/cm indicating that they are insulators at room temperature. All the compounds were tested for their antimicrobial activity against Escherichia coli, Pseudomonas and Staphylococcus aureus. The new metal complexes showed potent antimicrobial activity against tested organisms.

IP-14 : Unusual Reactivity Patterns of Hypervalent Silicon(IV) Complexes Bearing Hydrazide Ligands

Janardan Sannapaneni, Suman Pothini, Swapna Gullapalli, Jotsna Lata and Akella Sivaramakrishna*

Department of Chemistry, School of Advanced Sciences, VIT University,
Vellore 632 014, Tamil Nadu
E-mail : asrkrishna@vit.ac.in

Studies on hypervalent silicon(IV) complexes are one of the pioneer topics of modern silicon chemistry. Various eminent scientists like Richard Tacke, Daniel Kost, Robert West etc. have demonstrated the diverse reactivity patterns of various 5- and 6-coordinate silicon(IV) complexes in the past. We here report novel synthesis of five and six-coordinate silicon(IV) complexes derived from tran-silylation reactions of various hydrazide ligands with halosilanes. All the products were characterized by various spectroscopic and analytical techniques. These silicon complexes exhibit aldol-type rearrangement and methyl halide elimination reactions. Various factors including temperature, solvent, substituents on silicon and steric and electronic properties affecting the stability and reactivity of these complexes are discussed.

IP-15 : Synthesis and Structural Studies of 3-(N-methylamino)-2-Naphthalidine Thiosemicarbazone Complexes of Ni(II), Pd(II) and Cu(II)

K.M.Singh* and Bhartendu Prasad Rai**

**Post Graduate Centre of Chemistry, H.D. Jain College, Ara*
*** Purvottar Railway College, Sonpur, Bihar*

The present communication reports the synthesis and characterization of ligand 3-(N-methylamino)-2-naphthalidine thiosemicarbone for which firstly 10 g (0.05 mole) 3-nitro-2-naphthaldehyde was dissolved in 150 ml methanol and added with Conc. hydrochloric acid (5 ml), Raney Ni (2.5 g) was added carefully under nitrogen atmosphere at room temperature and put for hydrogenation at 40 psi for two hours. The content was filtered through a pad of celite and washed thoroughly. The solvent was evaporated to get a brown solid which on titration with petroleum ether afforded 3-(N-methylamino)-2-naphthaldehyde hydrochloride (yield 8.51 g, 82.5%). 5.0 g (0.024 mole) of this compound was dissolved in 25 ml dry dimethylformamide and cooled the content to 273-278K . 8.0 g (0.058 mole) anhydrous potassium carbonate , and 2.88 g (0.023 mole) dimethylsulphate were added one after another at an interval of 15 min. The reaction mixture was stirred at this temperature for half an hour and then at room temperature for an hour. The content was poured into ice-water, stirred and then extracted with ethylethanoate. The combined organic layer was washed with water, dried over anhydrous sodiumsulphate and solvent was evaporated under rotary evaporator under vacuum at 298 – 303K. The concentrated mass was titrated with minimum volume of petroleum ether to get a brown solid of 3-(N-methylamino)-2-naphthaldehyde (yield 3.5 g, 79%, m.p – 408 – 410K). The thiosemicarbazone was finally prepared by the reported method. The compound was characterised by elemental analysis and spectral studies. Ni(II), Pd(II) and Cu(II) complexes with 3-(N-methylamino)-2--naphthaldine thiosemicarbazone of the type [MLX], (where L = titled legand and X = H_2O or NH_3) have been synthesized. IR spectral data suggest the coordination of ligand through of -$NHCH_3$, sulphur of the SH group and N of the C ≡ N group. The coordination of H_2O

or NH_3 is indicated by ir and nmr spectral studies. Magnetic properties and electronic spectradata suggest them to have a square planar structure.

IP-16 : Synthesis, Characterization and Catalytic Applications of Ru(II) Organometallic Compounds Containing Schiff Base Ligands Derived from Salicylaldehyde and Amino Acids

M. Sarangapani, G. Hanmanthu, T.N.Swamy and V. Ravinder

Department of Chemistry, Kakatiya University, Warangal - 506009 (A.P.)
E-mail : ravichemku@yahoo.co.in

The precursor [η^6-*p*-cymene)$RuCl_2]_2$ reacts with schiffbase ligands derived from salicylaldehyde treated with different types of aminoacids to give monemeric complexes with the formula [(η^6-*p*-cymene)RuL)]. The probable geometries of all the complexes have been established on the basis of elemental analysis, molar conductance, IR, ^1H, ^{13}C, ^{31}P NMR, Mass and electronic spectral data and octahedral geometry has been tentatively proposed for all the complexes. Further these compounds were used as catalysts in the organic transformations like Heck coupling and dimerization of phenyl acetylenes.

IP-17 : Synthesis, Sharacterization and Biological Activity of Some Mixed Metal Dicarboxylates

M.A. Betallu[a], S.M. Vhankate[a], B.T. Hake[a], V.B. Tadke[a] and M.B. Ubale[*]

[a]Department of Chemistry, Ferguson College, Pune-4
[*]Dept. of Chemistry, Vasantrao Naik College, Aurangabad
E-mail : mbubale@yahoo.com

Metal complexes of general molecular formula M $Ca(C_4H_4O_6)_3$ X H_2O, M = Mn, Fe, Co have been synthesized. The synthesized metal complexes were characterized by various techniques like elemental analysis, XRD, AAS, TGA as well as FTIR data. Based on these characterizations, the metal complexes of the transition metal and alkaline earth metal ions may be suggested 1:1:3 (M_1:M_2:L) stoichiometry, with polymeric octahedral arrangement. The metal complexes were formed by the coordination of two oxygen atoms of the ligand. These newly synthesized compounds have been tested for their antibacterial activity against Bacillus subfilis, staphylococcus Aureus and Escherichia coli. Compounds shown significant activity against these bacteria.

IP-18 : Synthesis, Characterization and Biological studies of Binary Cu(II) Complexes of Novel 4-amino 3,5-dimethyl Isoxazole Schiff Bases

Marri Pradeep Kumar, Sathish Kumar K, Aveli Rambabu and Shivaraj*

Department of Chemistry, Osmania University, Hyderabad-500007,(A.P), India.
E-mail : shivaraj_sunny@yahoo.co.in

Two novel Schiff bases, [(2-methoxy-6-{[[3,5-dimethyl-4-isoxazolyl]imino]methyl}phenol] (L^1) and [2-{[[3,5-dimethyl-4-isoxazolyl]imino]methyl}naphthol] (L^2) are derived by the condensation of 4-amino-3,5-dimethyl isoxazole with 3-methoxy salicylaldehyde and 2-hydroxy naphthaldehyde respectively. Binary Cu(II) complexes with general stoichiometry [ML_2] where M= Cu(II), L= L^1 / L^2 are synthesized and characterized by elemental analysis, magnetic susceptibility measurements, IR, ^{1}H NMR, ^{13}C NMR, Mass, TGA and ESR data. The ligands and their complexes have been screened for their antifungal and antibacterial activities. Isoxazoles themselves show more activity, which is enhanced further to their Schiff bases and their metal complexes. The ligands and their metal complexes have been evaluated for their cytotoxic activities towards Human Cervical Carcinoma Cells (HeLa) by MTT assay.

IP-19 : Studies on Some Transition Metal Complexes of Monodentate *N*-((3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazol-4-yl)methylidene)-4-bromobenzenamine Schiff Base

S. Maru Minaxi, N. Sharma Anita and K. Shah Manish*

Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot - 360005, Gujarat
E-mail : minaxi.maru777@gmail.com

A monodentate Schiff base *N*-((3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazol-4-yl)methylidene)-4-bromobenzenamine Schiff base ligand (HL) derived by the condensation of substituted pyrazole aldehyde and 4-bromobenzenamine, to synthesize four novel Cu(II), Ni(II), Co(II) and Zn(II) complexes, which, have been synthesized by monodentate Schiff base ligand (HL) and metal(II) chloride salt (where, metal = Cu(II), Ni(II), Co(II) and Zn(II) ions) in the appropriate 2:1 mole ration of ligand and metal respectively, in alcoholic media. *N*-((3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazol-4-yl)methylidene)-4-bromobenzenamine have been synthesized by the condensation of 4-bromobenzenamine and 3-(4-nitrophenyl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde in presence of glacial acetic acid. All newly synthesized Schiff base were characterized by

^{1}H NMR, Mass, IR and UV-Visible spectroscopy. All complexes were characterized by IR, UV-Visible spectroscopy, magnetic susceptibility, molar conductance and Thermogravimetric analysis.

IP-20 : Mn-peroxidase from *Musa paradisiaca* Stem Juice

Meera Yadav, Pratibha Yadav, Sudha Yadava and K.D.S.Yadav*

Department of Chemistry, DDU Gorakhpur University, Gorakhpur (U.P.)
E-mail : kds_chemistry@rediffmail.com

Mn-peroxidase has been purified to homogeneity from a plant source, *Musa paradisiaca* stem juice, using concentration by ultra filtration and anion exchange column chromatography on diethyl amino ethyl cellulose. The molecular weight of the purified enzyme has been found to be 43 kDa determined by sodium dodecyl sulphate polyacrylamide gel electrophoresis. The Km values using $MnSO_4$ and H_2O_2 as the variable substrates for the purified enzyme were 21.0 µM and 9.5 ìM respectively. The calculated k_{cat} value for the purified Mn-peroxidase using Mn(II) as the substrate in 50 mM lactate buffer *pH* 4.5 at 25^0C was $6.7s^{-1}$ giving a k_{cat}/Km value of 0.32 $\mu M^{-1}s^{-1}$. The *pH* and temperature optima of the purified enzyme were 4.5 and 25 ^{0}C respectively. The k_{cat} value for the Mn-peroxidase catalyzed reaction has been found to be dependent of the Mn(III) chelator molecules malonate, lactate and oxalate indicating that the enzyme oxidizes chelated Mn(II) to Mn(III) and not the free Mn(II) ion. The purified enzyme in combination with H_2O_2 liberates bromine and iodine respectively in presence of KBr and KI indicating that it can be used as a reagent in organic bromination reactions.

IP-21 : Synthesis, Spectral, Thermal and Antimicrobial Studies of Pd(II), Pt(II), Ru(III) and Ir(III) Complexes Derived from *N,N,N,N* – Tetradentate Macrocyclic Ligand

Monika Tyagi# and Sulekh Chandra*

Department of Chemistry, Zakir Husain College (University of Delhi) JLN-Marg, New Delhi - 110002
E-mail: schandra_00@yahoo.com, mnk02tyg@yahoo.co.in

Palladium(II), platinum(II), ruthenium(III) and iridium(III) complexes of general stoichiometry $[PdL]Cl_2$, $[PtL]Cl_2$, $[Ru(L)Cl_2]Cl$ and $[Ir(L)Cl_2]Cl$ were synthesized with a tetradentate macrocyclic ligand derived form dibenzoylmethane and urea. Ligand was characterized by elemental analyses, Mass, IR and ^{1}H NMR spectral studies. All the complexes were characterized by elemental analysis, molar conductance, magnetic susceptibility measurements, IR and electronic spectral studies. The value of magnetic moments indicates that all the complexes are diamagnetic except Ru(III)complex which shows magnetic moments corresponding its one unpaired electron. The molar conductivities show that Pd(II) and Pt(II) complexes are 1:2 electrolytes while Ru(III) and Ir(III) complexes are 1:1 electrolyte. Various ligand field parameters were calculated using energy - level diagrams. The macrocyclic ligand and its metal complexes were also evaluated *in vitro* against some plant pathogenic fungi to assess their biocidal properties.

IP-22 : Synthesis, Characterization, Antibacterial and Antifungal Studies of Some Transition-Alkaline Earth Metal Oxalato Complexes

N. D. Dhawale[a], S. M. Vhankate[a], S. S. Pawar[a], S. A. Dhanmane [a], V. B. Tadke [a*], G. R. Pathade[a], R. P. Pawar[b] and C. S. Patil[b]

[a]Department of Chemistry, Fergusson College, Pune
[b]Department of Chemistry, Deogiri College, Aurangabad
E-mail : vijaytadke@gmail.com

The neutral bidentate oxalato complexes of Ni(II), Cu(II) and Zn(II) complexes have been synthesized. Treatment of the oxalato ligand OX^- with metal salts like $NiSO_4.6H_2O$, $CuSO_4.5H_2O$, $ZnSO_4.7H_2O$ and $MgSO_4.7H_2O$ gave metallic complexes of the octahedral $[M_1M_2(OX)_3]$. xH_2O types [Where M = Ni(II), Cu(II), Zn(II) and M_2 = Mg(II), OX = Oxalato]. The ligand OX^- behaves as a bidentate and coordinated to the metal ion centers through two oxygen atoms. The ligand and metal complexes were characterized on the basis of elemental analysis, IR, AAS, XRD and thermal analysis (TGA/DTA). The analytical data were suggested 1:1:3 (M_1:M_2:L) stoichiometry for all the synthesized complexes. The ligands and their respective mixed metal complexes have been screened for their antimicrobial activities against the bacteria like *Bacillus subfilis, Staphylococcus aureus* and *Escherichia coli*.

IP-23 : Combustion Synthesis and Photoluminescence Characteristics of Eu^{3+}- Sm^{3+} Co-doped $BaGd_2O_4$ Nanoparticles

Mukesh Kumar, S. P. Khatkar*, V.B. Taxak^{--} and Sonika

Maharshi Dayanand University, Rohtak-124001
Email: s_khatkar@rediffmail.com

A red light emitting Eu^{3+}- Sm^{3+} co-doped $BaGd_2O_4$ nanophosphor was synthesized by combustion synthesis using an organic fuel. The paste is kept in a preheated furnace maintained at 500^0C. The combustion process utilizes the enthalpy of combustion for the formation and the solid obtained was again fired at 700 ºC, 900 ºC and 1100 ºC for 3hrs to increase the brightness and crystallinity. Comparing with traditional material processing techniques, combustion method is a relatively simple method. The advantages of short time reaction and low temperature solution based process have been exploited to produce Eu^{3+}- Sm^{3+} co-doped $BaGd_2O_4$ nanoparticles. The synthesis conditions such as calcinations temperature and dopant concentration were varied in order to determine the exact optimum conditions for synthesizing nanoparticles with superior optical properties and smaller particle size. The nanocrystals obtained through combustion method were characterized by using scanning electron microscopy (SEM), X-ray diffractions (XRD) and photoluminescence (PL) spectra. The average particle size of the synthesized nanophosphor was around 40-70 nm. The photoluminescence (PL) spectra exhibit predominant red color of the nanocrystals prepared under an UV source that was attributed to transitions $^5D_0$ - $^7F_2$ peak at 612 nm. The effect of the doping concentration of Sm^{3+} on the luminescence properties of the obtained products was investigated.

IP-24 : Synthesis, Characterization and Antimicrobial Activity of Bivalent Metal (Zn, Cd, Hg, Pb and Ag) Chelates of 1, 2 Naphthoquinone Dioxime

N. R. Gonewar, V. B. Jadhav, S.S. Sakure[1], K. D. Jadhav and R. G. Sarawadekar*

Bharati Vidyapeeth Deemed University, Pune
Yashwantrao Mohite College, Pune - 411 038
[1] S.B.B. alias Appasaheb Jedhe College, Shukrawar Peth, Pune - 411002.

Transition metal chelates of the type M [NQO] $_2$ where M = Hg, Cd, Zn, Pb: NQO = 1, 2 napthoquinone dioxime and Ag (NQO) have been synthesized. All chelates have been characterized by modern methods such as elemental analysis, FTIR and Electronic spectra. ^1H & ^{13}C NMR, Thermogravimetry, Differential scanning calorimetry and electron microscopy with EDAX analysis of chelates were carried out. Metal chelates of mercury, lead, zinc and cadmium are octahedral while silver chelate has been assigned square planer. These chelates are thermally stable up to 350^0C and all are crystalline in nature. Their particle sizes are in the range of 15-42 nm. The ligand and the metal chelates have been screened for antimicrobial activity on gram positive and gram negative bacteria and fungi and the results are compared with cisplatin as standard chemotherapy agent.

IP-25 : Synthesis and Characterization of Mixed Ligand Complexes of Transition Metals with Schiff Bases

P.R. Shirode[a], R.K. Agrawal[a], A.M. Jain[a] and P.M. Yeole[b]

[a]*Department of Chemistry, Pratap College, Amalner*
[b]*R.L.College, Parola North Maharashtra University. Jalgaon (MAHARASHTRA)*
E-mail : prshirodepca@gmail.com

The mixed ligand complexes of the type[ML_1L_2]Cl_2 where M=Cr(III), Mn(II), Co(II), Ni(II) and Cu(II), and L_1=Pyruvic acid semicarbazone L_2= benzaldehyde semicarbazone have been synthesized, by the reactions of metal chlorides with two different semicarbazones in 1:1:1 molar ratios.The resulting products have been characterized on the basis of elemental analysis, magnetic measurement, IR, electronic spectra, conductivity measurement, thermal analysis and antimicrobial activities. 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.

IP-26 : Synthesis, Characterization and Biological Studies of Metal Complexes of (4-oxo-2-phenyl-3,4-dihydroquinazolin-3-yl) Thiourea and (4-oxo-2-phenyl-3,4-dihydroquinazolin-3-yl) Urea

Palreddy Ranjith Reddy, P. Mamtha, Mohmed Jaheer and Ch. Sarala Devi *

Department of Chemistry, University College of Science, Osmania University, Hyderabad
**E-mail : dr_saraladevich@yahoo.com*

The substituted quinazolinones are considered as important therapeutic scaffolds. Quinazolinon-4(3H)-ones and its derivatives are versatile nitrogen heterocyclic compounds which have long been known as a promising class of biologically active compounds. As the interaction of these derivatives with metal ions is expected to yield the corresponding complexes which may have biological activity, in the present investigation the complexes of Cu (II), Ni(II), Co(II), Mn(II) and VO(II) involving (4-oxo-2-phenyl-3,4-dihydroquinazolin-3-yl)thiourea and (4-oxo-2-phenyl-3,4-dihydroquinazolin-3-yl) urea as chelating agents have been synthesized. The complexes were characterized by elemental analysis, magnetic susceptibility measurements, IR, Mass, TGA, ESR and SEM data. Computational studies were also carried out to know the energies and orientation of HOMO and LUMO frontier orbitals in order to understand mode of bonding in metal complexes. The compounds have been screened for their antifungal and antibacterial activities.

IP-27 : Effect of Chemical Composition of $Sr_xCa_{1-x}Fe_2O_4$ (x= 0, 0.2, 0.4, 0.6, 0.8 and 1.0) Catalyst Towards the Selective Epoxidation of Styrene

Ravindra Y. Pawar and Satish K. Pardeshi*

Department of Chemistry, University of Pune,Ganeshkhind, Pune, Maharashtra-411007
**E-mail : skpar@chem.unipune.ac.in*

The strontium substituted calcium (SSC) ferrite $Sr_xCa_{1-x}Fe_2O_4$ (x= 0, 0.2, 0.4, 0.6, 0.8 and 1.0) spinel type catalyst is synthesized by citrate gel combustion method. The precursors and oxides are well characterized by various techniques such as TG-DTA, FT-IR, X-ray diffraction, SEM, and EDS. The crystallization temperature of the spinel particle prepared by citrate gel is 600°C, which is lower than that of the ferrite prepared by other methods. $Sr_{0.2}Ca_{0.8}Fe_2O_4$ shows the better catalytic efficiency towards the epoxidation of styrene in presence of 30% H_2O_2 as oxidizing agent. GCMS analysis revealed that, during the course of reaction the insertion of oxygen takes place selectively than the oxidative cleavage of C=C bonds to give the epoxide as major product. The further isomerization of the styrene epoxide is suppressed by NaOH, the adsorption of substrate over the active sites of catalyst enhance desorption of product which prevent the ring opening in styrene epoxidation, thereby increasing the selectivity of epoxide remarkably. The optimization and the effect of various reaction conditions like reaction time, temperature, solvent, substrate to oxidant molar ratio, oxidizing agent and amount of catalyst on the conversion of styrene and their product distribution were also studied.

IP-28 : Synthesis and Characterization of Some Charge Transfer Complexes of Lanthanum (III) with Isomeric Juglones

R. B. Mhaske[1], Mrudula Wadekar[2], Pritam Shinde[2], Meera Deshmukh[2], Shivaji Takale[3] and Pratibha Jadhav[2]

[1]Huttatmma Rajguru College of Arts and Science, Rajgurunager, Pune
[2]Department of Chemistry, Y. M. College, Pune - 38
[3]Bharati Vidyapeeth, Technical Campus, College of Engineering, Lavale, Dist - Mulshi, Pune-412 115
E-mail : shivaji_takale@yahoo.co.in

Isomeric juglones are the hydroxy derivates of 1,4 naphthoquinone in which the hydroxyl group is situated adjacent to the carbonyl group. Isomeric lawsone i.e 2 hydroxy 1,4 naphthoquinone and juglone i.e 5 hydroxy 1,4 naphthoquinone are the parent member of the juglone series and the other members of this series are derived by replacing one or more hydrogens by various functional groups. Among these, isomeric lawsone-juglone, phthiocol plumbagin, 3-bromolawsone, 3-bromojuglone and 3-iodolawsone and 3-iodojuglone are the members of current interest. Lanthanum(III) chelates of these isomeric juglones have been synthesized by mixing equimolar solutions (concentration 10^{-3} M) of lanthanum tri-chloride in water and each juglone derivative in methanol in a 250 mL 3 necked flask provided with an electric heater and magnetic stirrer. After the addition of metal ligand solutions in the proportion of 1:3, the reaction mixtures were kept under stirring at 60^0C and pH 4-5, adjusted by 10 percent aqueous ammonia for about one hour. The precipitated chelates were then thoroughly washed with distilled water, methanol and acetone and dried completely under suction. These were present in vacuum desiccators. The chemical composition of all these chelates was established through elemental analysis and thermogravimety which corresponds to $ML_3.4H_2O$ where n = 2,3 or 4. All these isomeric chelates possess intense visible colours which are stable state in their solid state for very long period of several years. Their structural investigations are done with the help of XRD, TG/DTG, IR and UV spectroscopy with an object to explore the nature of origin of intense visible colour.

IP-29 : Effect of Ring Isomerism on the Antimicrobial Activity of Sn(II) and Pb(II) Phthiocolates and Plumbaginates

S. B. Jagtap[1], B. L. Khade[2], V. B. Jadhav[2], Mrudula Wadekar[2], M. G. Bodhankar[2] and V.V. Dhapte[2]

[1]*Annasheb Magar College, Hadpser, Pune*

[2]*Department of Chemistry, Bharati Vidyapeeth University, Y. M. College, Pune*
E-mail : shivaji_takale@yahoo.co.in

Ring isomerism is a new type of isomerism introduced by our research group in coordination chemistry since past four decades. This kind of isomerism which is caused exclusively due to difference in ring size is exhibited by the metal chelates of isomeric juglones. These juglones are the hydroxy derivatives of 1, 4 naphthoquinone in which the hydroxy group is situated adjacent to the carbonyl group. Isomeric phthiocol (3 methyl 2 hydroxy 1,4 naphthoquinone) and plumbagin (2 - methyl 5 - hydroxy 3 - methyl 1,4 naphthoquinone) are the most important members of the isomeric juglone series. Both phthiocol and plumbagin which possess natural occurrence exhibit significant antimicrobial activity against Gram positive, Gram negative and fungal microorganisms. This activity is expected to show remarkable alteration in their metal chelates. Since ring isomerism is a unique and characteristic property of isomeric metal juglonates, it will be interesting to examine the effect of ring isomerism on the antimicrobial activity against different microorganisms and this is the subject of our special interest. The present communication is a part of this subject. In this communication, we would like to report our recent work on the synthesis, characterization and antimicrobial investigations of the isomeric phthiocolates and plubaginates of tin (II) and lead (II) against some selected Gram positive, Gram negative and fungal microorganisms.

IP-30 : Synthesis, Characterization and Biological Studies on Ru(II) Ternary Complexes of Isoxazole Schiff Bases and 2,2' Bipyridyl / 1,10 Phenanthroline

Somapangu Tejaswi, Vijay Kumar Chityala and Shivaraj*

Department of Chemistry, Osmania University, Hyderabad-500007, (A.P)
E-mail: shivaraj_sunny@yahoo.co.in

Novel Ru(II) polypyridyl complexes such as $[Ru(bipy)_2(MODIIMP)]Cl_2$, $[Ru(phen)_2(MODIIMP)]Cl_2$, $[Ru(bipy)_2(MDIIMP)]Cl_2$ and $[Ru(phen)_2(MDIIMP)]Cl_2$ where MODIIMP= 2 Methoxy-6-{[(3',4' dimethyl 5'isoxazolyl)imino]methyl}phenol, MDIIMP= 4 Methyl-2-{[(3',4' dimethyl 5'isoxazolyl)imino]methyl}phenol, phen=1,10 phenanthroline and bipy=2,2' bipyridyl have been synthesized. These complexes have been characterized by Elemental analysis, IR, NMR, UV, TGA and magnetic susceptibility measurements. Based on the analytical and spectral data these complexes exhibit octahedral geometry. Antimicrobial studies of these complexes have been screened against E. coli, S. aureus, A. niger and R. oryzae.

IP-31 : Synthesis, Physico-Chemical and Antimicrobial Studies of Bidentate Oxalato Complexes of Mn(II), Fe(II) and Co(II) with Mg(II)

S. M. Vhankate[a], N. D. Dhawale[a] S. S. Pawar[a], S. A. Dhanmane[a], V. B. Tadke[a]*, G. R. Pathade[a], S. R. Sakhare[a], R. P. Pawar[b] and C. S. Patil[b]

[a]Department of Chemistry, Fergusson College, Pune
[b]Department of Chemistry, Deogiri College, Aurangabad
E-mail : vijaytadke@gmail.com

Complexes of general molecular formula $[M_1M_2(OX)_3]$ x H_2O [where M = Mn(II), Fe(II), Co(II) and M_2 = Mg(II), OX = Oxalato] have been synthesized. The synthesized metal complexes were characterized by elemental analysis, XRD, AAS, TGA as well as infrared data. Based on these characterizations, the metal complexes of the transition metal and alkaline earth suggested as polymeric. The metal complexes were formed by the coordination of two oxygen atoms of the ligand. These newly synthesized compounds have been tested for their anti-bacterial activity against *Bacillus subtilis, Staphylococcus aureus* and *Escherichia coli*. These compounds show the significant activity against these bacteria.

IP-32 : Synthesis and Characterization of Spinels Cu1-xZnx Mn1-xFexCr1-xCox O_4

S.K.Gupta[1], **K.S.Waghmode**[2] **and A.Venkatachalam**[1*]

[1]*Deptartment of Chemistry, Bhavan's College, Andheri (West), Mumbai-58*
[2]*Dept. of Chemistry, JJT University, Jhunjhunu, Rajasthan.*
**E-mail : avenkat54@yahoo.co.in*

The compounds of the system where x = 0, 0.4, 1.0 have been prepared by the co-precipitation technique using stoichiometric quantities of the respective sulphates, dissolved in minimum quantity of water and few drops of conc.H_2SO_4 to get a clear solution. They are precipitated as mixed hydroxides using 4 N NH_4OH drop by drop and the pH is raised to 9-10 for complete precipitation. The mixed hydroxides are then filtered, dried, and then incinerated at 800 °C to form mixed oxides. The mixed oxides are then pelletized by using acetone and PVA as binder. The pellets are then heated in a muffle furnace at a temperature of 800-900 ^{o}C for 40-60 hours for compound formation. The compound formation has been checked by using XRD technique. All the compositions from a single cubic spinel phase. The lattice constants have been calculated using the planes 220, 311, 22, 400, 422, 511, 440. They are further characterized by IR, magnetic hysteresis, and catalytic studies using decomposition of H_2O_2 as a simple model reaction. IR spectra for the compositions show two strong bands which are characteristic of spinels. Magnetic hysteresis studies using a field of 2000 gauss suggested a decreasing tend in the magnetization values with the substitution of Zn. Catalytic studies also suggested a decreasing trend with the substitution of Zn. Catalytic results are in accordance with the magnetization trend in the system.

IP-33 : Investigation on Oxidizing and Chlorinating Properties of Hydroxyaryltellurium Trichlorides for Oxidation of Di- and Triorganyl Phosphites

Sapana Garg, K. K. Verma, Rimpi and Sumit Kumari

Department of Chemistry, Maharshi Dayanand University Rohtak-124001
E-mail : sapanagarg1511@gmail.com

Dialkyl/diarylchlorophosphates were synthesized from di- and triorganyl phosphites using hydroxyaryltellurium trichlorides as oxidizing and chlorinating reagents in dichloromethane at room temperature under nitrogen atmosphere in good yield. The reaction probably proceeds by the attack of phosphorous centre of trivalent alkyl/aryl phosphite on the positive chlorine of $[ArTeCI_2]^{\delta+}$ $CI^{\delta-}$ which are partially ionized form of hydroxyarylltellurium(IV) trichlorides in solution. During this reaction metallic Te(0) precipitated. The authenticity of the products was established by their spectra.

IP-34 : Determination of Some Inorganic Compounds By A Newer Photochemical Method using Sodium Nitroprusside

Shailendra Singh Rathore, Ravi Sharma[1], Gayatri Prasad[2], Hardik Bakul Bhai Bhatt[3] and Ajay Sharma[4*]

P.G. Deptt. of Chemistry, Govt. College, Sirohi-307001(Raj.)
[1]Govt. College, Sheoganj, Sirohi-307027 (Raj.)
[2]Govt. College, Sirohi-307001 (Raj.)
[3]Shri N. M. Gopani polytechnic College, Ranpur, Ahmedabad
[4]P.G. Deptt. of Chemistry, Govt. College, Sirohi-307001(Raj.)
E-mail: ajneanigun@rediffmail.com, ajay395@gmail.com, gpgcsirohi@yahoo.com

A newer fast, convenient and inexpensive quantitative method for the determination of some inorganic compounds and inorganic anions using photochemical exchange reaction of sodium nitroprusside has been investigated. Sodium nitroprusside is a photolabile complex and it undergoes photchemical ligand exchange reactions rapidly. Some recent efforts have been made to utilise such reactions for the estimation of some sulphur containing anions and electron rich inorganic molecules. The progress of the reaction is observed spectrophotometrically. The effects of different parameters like pH, change of concentration of sodium nitroprusside, concentration of ligands, light intensity etc. on percentage error was investigated. The efforts were made to minimise the percentage error and some optimum conditions were obtained. Such reactions can be used for the determination of anions or inorganic molecules in the range of millimoles to micromoles, hence it is important to know whether such estimations can be done successfully and that to with the desired accuracy.

IP-35 : Complexational Behaviour of Pentaprazole Drug

Suman Malik, Bharti Jain*, Supriya Das and Jaishree More

Department of Chemistry, Sadhu Vaswani College Bairagarh, Bhopal-462030.
**Department of Chemistry, SNGGPG Autonomous College, Bhopal-462003*
E-mail : drsumanmalik@gmail.com, supriya.das.bpl@gmail.com, bhartikjain@yahoo.com

Metals have played an important role in medicine for years, ever since humans have walked the planet. Many are essential in our diet in varying quantities, although people have recently realized their significance. There are also a number of metallo-drugs and metallo-pharmaceuticals which have been utilized for the treatment of diseases and disorders or as diagnostic agents, such as gold used in anti-arthritic drug, bismuth in anti-ulcer drugs. Although a large number of therapeutic agents are known, the literature survey reveals that very little work has been done on the metal complexes of anti-ulcerative

drugs. The present work deals with the synthesis of metal complexes derived from anti-ulcerative drug. The complexes of Zn and Pd salts have been prepared. For the structure elucidation of these complexes, elemental analysis, conductivity measurements and spectral studies including IR,UV, magnetic susceptibility, ESR, TGA, XRD, SEM and mass spectral studies have been used. The stability constants of the formed complexes were as calculated by molar conductance measurement using modified Job's method. The spectroscopic results show the involvement of sulphur and azomethine nitrogen in coordination to the central metal ion and both the complexes have been proposed to be tetra-coordinated.

IP-36 : Characterization of Reaction Product of Se_4N_3Br and L-Lucine : Mass and IR Spectra

Shiv Gaurav Dixit and S. P. S. Jadon*

Department of Chemistry, S.V. College, Aligarh-202001 (UP)
E-mail : sps_ jadon@yahoo.co.in

Se_4N_3Br was heated with L - Lucine in dichloroethane for 6 h. The reaction product, formed, was separated and estimated quantitatively. On the basis of chemical data and mol.wt. 1123.6 g mol^{-1}, the Product is assigned as $(Se_4N_3)_2.[NH\text{-}CHCOOH\text{-}CH_2\text{-}CH\text{-}(CH_3)_2]_3$ which is supported by prominent mass peak at m/z 1123 observed in its Mass spectrum. The formation of the product is supported by the frequencies, found, at 940.7, 1105.6, 1400.9, 1524.6, 1703.0 and 3160.9 cm^{-1} subsequentlly for the Se –N, C- O, CH_3, C – C, COOH and C –H bands.

IP-37 : Comparative Study of Samarium(III) Chelates of 3-Nitro Lawsone and 3-Nitrolawsone Monoxime

T. S. Kadam[1], D. G. Kanase[2], P. S. Khandagale[3] and B. A. Kulkarni[4]

[1]Department of Chemistry, Fergusson College, Pune 411004
[2]MBSK, Kanya Mahavidyalaya Kedegaon, Dist-Sangli
[3]Henkel Pvt. Ltd, Jujuri, Pune
[4]Department of Chemistry, Y. M. College, Pune-38
E-mail : shivaji_takale@yahoo.co.in

Lawsone i.e. 2.hydroxy 1,4 naphthoquinone is the active constituent of *Lawsonia alba* and due to its natural occurrence it possesses biological importance. It is a powerful chelating agent which can interact with almost all metals forming a large number of metal chelates. Many of these metal lawsonates find important applications in structural, analytical and biological fields. Apart from itself, its C-3 substituted as well as oxime derivatives are equally or even more interesting and important, because the potential abilities and properties of Lawsone are enhanced in its C-3 substituted derivatives. Among these, C-3 substituted Lawsone derivatives, 3-nitro lawsone and 3-

nitrolawsone monoxime are of special interest because of the highest electro negativity of the nitro group. Therefore study of the metal chelates of 3-nitrolawsone and 3-nitro lawsone monoxime will be interesting and useful in the elucidation of the effect of C-3 substitutions on the various properties of metal lawsonates. The present communication is a part of such study in which samarium (III) chelates with 3-nitrolawsone and 3-nitrolawsone monoxime are synthesized and their comparative study has been carried out with the help of infrared and electronic spectroscopy and magnetic susceptibility measurements. The results of this study are employed to examine the effect of chelation and change of donor system on the physical, chemical and structural aspects of the parent ligand.

IP-38 : Inhibition of Copper and Tin-Lead Alloy by Macromolecules in Acidic Conditions

J. Jabali Vora[1]*, T. Rakesh Jasrai[2] and J. Jwalant Vora[3]

[1]Department of Chemistry, Hemchandracharya N. G. University, Patan-384265
[2]Shri R. K. Parikh Arts & Science College, Petlad-388450
[3]M.G. Science Institute, Ahemdabad-380009

The development of inhibitors for the corrosion of copper and tin-lead alloy in aqueous media and particularly in acid solution has been subjected of considerable interests especially from the point of view of their usefulness in industrial parts and cooking vessels. In the present study efforts have been made to study the inhibitive influence of starch in acidic conditions. The starch is considered as cheap and environmentally safe inhibitor. These carbohydrates are the organic compounds, containing heteroatom/s, used as inhibitor to reduce corrosion attack. In the present study efforts have been made to do comparison of the inhibitive influence of tapioca starch, potato starch maize starch in citric acid on the corrosion of copper and tin-lead alloy in uncoupled and coupled systems. Gravimetric method has been used to study the corrosion and inhibition by varying the concentration of inhibitor, at 35±3°C temperature.

IP-39 : Colorimetric and Fluorescent Sensing of Anions with Naphthalene based Receptor

Darshna Sharma and Suban K. Sahoo*

Department of Applied Chemistry, S.V. National Institute of Technology (SVNIT), Surat- 395007, Gujrat
E-mail : suban_sahoo@rediffmail.com; darshna_78@yahoo.in

Anions are ubiquitous and critically play major roles in many biological, medical, environmental, chemical and industrial systems. Therefore, there is a need of selective sensing methods for the detection and quantification of anions. Among the different types of chemosensors, the sensors based on colorimetric and fluorometric determination of anions have many advantages due to the simplicity and high sensitivity. In the present work, we have introduced a novel naphthalene based anion receptor (L). The binding behavior of the receptor L to various anions was investigated by UV-Vis and fluorescence analyses. In addition, IH NMR experiments were carried out to explore the nature of interaction between receptor L and acetate. Sensor L portrayed a naked-eye detectable for AcO^-, F^- and H_2PO^{4-}, where as no significant color change was observed upon addition of other anions such as Cl^-, Br^-, I^- and HSO_4^-. The processes of sensing can literally be seen through the 'naked-eye' or the sharp color changes from pale green to red. Importantly, receptor L showed selectivity for acetate anions under competitive environment. In addition, theoretical calculations using Gaussian 09W computer program have been performed to complement the experimental evidences.

IP-40 : Synthesis, Characterization and Antimicrobial Studies of Copper(II) Complexes of Biologically Active Schiff Bases

Y. Prashanthi[1,2], Vijay Kumar Chityala[1], Sathish Kumar K[1] ,
M. Ramchander[3] and Shivaraj[1*]

[1]Department of Chemistry, Osmania University, Hyderabad-500 007(A.P.)
[2]Department of Chemistry, Mahatma Gandhi University, Nalgonda-508 254 (A.P.)
[3]Department of BioChemistry, Mahatma Gandhi University, Nalgonda-508 254 (A.P.)
**E-mail : shivaraj_sunny@yahoo.co.in*

A series of metal complexes of Cu(II) have been synthesized with MIIMC, MMIIMC and CMIIMC Schiff bases derived by condensation of the 3-amino-5-methyl isoxazole with formyl chromone and substituted formyl chromones. Schiff bases and their metal complexes have been characterized by using elemental analysis, IR, UV-VIS, ^{1}H, ^{13}C, Mass spectra, magnetic susceptibility, conductance measurements and thermo gravimetric studies. Based on the data obtained, it is found that the ligands behave as neutral, bidentate coordinating through carbonyl oxygen and azomethine nitrogen and a six coordinated octahedral geometry is assigned for all the complexes. Biological studies of Schiff bases and their metal complexes have been screened against bacteria and fungi by paper disc method. The DNA binding studies of Cu(II) complexes have been investigated by UV-Vis spectroscopy. Cytotoxic activity of Schiff bases and their metal complexes investigated by MTT assay against HL60 tumor cell.

ORGANIC CHEMISTRY SECTION

Sectional President's Address

OIL-01 : Small Heterocyclic Scaffolds as Smart Antimicrobial Agents

N. C. Desai*

Dean, Faculty of Science & Head Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364 022
E-mail : dnisheeth@rediffmail.com

Combat against bacterial infections has resulted in the development of a wide variety of antibiotics. After years of misuse and overuse of antibiotics, bacteria are becoming antibiotic resistant, resulting in a potential global health crisis. Frequently, it is recommended to use new antibacterial agents with enhanced broad-spectrum potency. Therefore, recent efforts have been directed towards exploring novel antibacterial agents (Moustafa et al., 2004). Apart from this, during the past 20 years an increase of invasive fungal infections has been observed, particularly in immunosuppressed patients, which are now, cause of morbidity and mortality. However, there is still a critical need for new anti-microbial agents to treat life threatening invasive mycoses (Andriole, 1999). In order to overcome this rapid development of drug resistance, new agents should preferably consist of chemical characteristics that clearly differ from those of existing agents. In drug developing programs, an essential component of the search for new leads is the synthesis of molecules, which are novel yet resemble known biologically active molecules by virtue of the presence of critical structural features. Certain small heterocyclic molecules act as highly functionalized scaffolds and are known pharmacophores of a number of biologically active and medicinally useful molecules (Thompson and Ellman, 1996).

The increasing incidence of infection caused by the rapid development of bacterial resistance to most of the known antibiotics is a serious health problem. While many factors may be responsible for mutations in microbial genomes, it has been widely demonstrated that the incorrect use of antibiotics can greatly increase the development of resistant genotypes. As multidrug-resistant bacterial strains proliferate, the necessity for effective therapy has stimulated research into the design and synthesis of novel anti-microbial molecules. The chemistry of [1,3,5]triazine compounds has been studied.

Antibacterial and antifungal diseases are very common all over the world. Currently used antimicrobial agents are not effective due to the resistance developed by the microbes. And therefore, it is an ongoing effort to synthesize new antimicrobial agents. Over and above there is no permanent structure and activity relationship. In continuation to this, we have selected medicinally important quinazolines by modifying the third position, for the preparation of newer antimicrobial agents.

OIL-02 : In Silico Studies in Designing Organic Superbases and their Potential Applications

Bishwajit Ganguly

CSIR-Central Salt and Marine chemicals Research Institute, Bhavnagar, Gujarat

Notwithstanding, its very small in size, the proton plays a gargantuan role in chemistry and biochemistry, in particular in the proton transfer reactions. Since Alder's proton sponge was synthesized some thirty years ago and its possible application for proton transfer processes, efforts are underway to develop new ultra-strong neutral organic superbases. Designing of some novel organic super bases and their applications will be covered.

OIL-03 : Cocrystallization : A Paradigm Shift from Crystallography to Process Development Tool

Amit Trivedi

Lupin Limited, Ankleshwar
E-mail : amittrivedi@lupinpharma.com

Cocrystallization is receiving sharp interest for numerous advantages offered for the isolation and purification of complex organic molecules. It leads to diverse array of solids which have different solubility profile, crystal structures and can lead to easy purification. It offers a low –cost approach for formulating poorly water soluble molecules. When used with a study of thermodynamics and phase behavior of a system, it can expand design space for quality of efficiency by differentiating from a true polymorph and pseudopolymorphs. It can also be explored for racemic resolution.

OIl-04 : Discovery of GPCR Ligands for the Treatment of Alzheimer's and other Cognitive Disorders

Vikas Shirsath

Piramal Discovery Solutions, Shirish Research Campus, 18, PHARMEZ - Pharmaceutical Special Economic Zone (SEZ), Sarkhej Bavla Road, Matoda, Sanand, Ahmedabad, Gujarat 382213

As a part of our continuous efforts towards development of novel and selective GPCR ligands, various derivatives were envisaged. Tryptamines is one of the major chemical class of ligands identified at 5-HT$_6$ receptors and some of the known leads include, N-arylsulfonyltryptamines, e.g. MS-245 and 2-aryltryptamines, e.g. PMDT. A basic nitrogen, which could be primary binding site at the receptor aspartate residue, and two other aromatic sites which may be involved in the essential or secondary binding (staking) interactions with the receptor. In an effort to identify and map the pharmacophoric requirements for the 5-HT$_6$ receptor ligands, several diverse classes of compounds were taken up for synthesis and evaluation. Interestingly, although a lot of work has been already published on the effect of changes made in the nature of side-chain of tryptamines, the aminoalkoxy side-chains were not much studied and evaluated on the indole nucleus. Our continuing efforts towards design and discovery of selective 5-HT$_6$ antagonists have led to the identification of a new class of compounds. Unlike the compounds known so far, these aminoalkylindolyl ethers are conformationally highly flexible molecules. Our effective lead generation and optimization methods have resulted in multiple series of potent 5-HT$_6$and H$_3$receptor ligands with KI in the range of 1 - 5 nM, when tested by the *in-vitro* radioligand binding techniques. Synthesis, physico chemical properties and the *in-vitro* binding data along with the SAR has been discussed.

OIl-05 : Structure Based Drug Design

Kamala K. Vasu

B. V. Patel Pharmaceutical Education and Research Development (PERD) Centre
Sarkhej-Gandhinagar Highway, Thaltej, Ahmedabad-380 054, Gujarat

Structure-based drug design (or direct drug design) relies on knowledge of the three dimensional structure of the biological target obtained through methods such as x-ray crystallography or NMR spectroscopy. Using the structure of the biological target, candidate drugs that are predicted to bind with high affinity and selectivity to the target may be designed using interactive graphics and the intuition of a medicinal chemist.

Current methods for structure-based drug design can be divided roughly into two categories, i.e. database searching. ligand-based drug design. and receptor-based drug design. In the field of molecular modeling, docking is a method which predicts the preferred orientation of one molecule to a second when bound to each other to form a stable complex. Knowledge of the preferred orientation in turn may be used to predict the strength of association or binding affinity between two molecules using for example scoring functions. Docking is frequently used to predict the binding orientation of small molecule drug candidates to their protein targets in order to in turn predict the affinity and activity of the small molecule. Hence docking plays an important role in the rational design of drugs. Given the biological and pharmaceutical significance of molecular docking, considerable efforts have been directed towards improving the methods used to predict docking. Active site identification is the first step in this program. It analyzes the protein to find the binding pocket, derives key interaction sites within the binding pocket, and then prepares the necessary data for ligand fragment link. In present talk some case studies related to docking will be discussed in the talk.

OIL-06 : Helices and Helicates : Supramolecular Components and its Implications in Microtube Construction

P. S. Subramanian

Department of Inorganic Materials and Catalysis, Central Salt and Marine Chemicals Research Institute-CSIR, Bhavnagar- 364 002, Gujarat

Helix being bio-inspiring topology, gained significance because of its everlasting wonder in DNA, eversince Lehn coined this terminology “helicates”. Bolaamphiphile type compounds are known for their application in membrane, metal ion extraction and conducting polymers etc. The presentation covering the synthesis of series of various bolashaped diester dicarboxylic compounds, will further demonstrate various supramolecular construction components and their role in the formation of helicates and their control over the construction of “microtubular” and “bar type” materials through some simple self-assembly process.

OIL-07 : Design, Synthesis and Anti-Inflammatory Activity Study of Oxazole Coupled Iso-oxazolines and Pyrazoles

Shailesh R Shah and Sudhanva S Navathe

Department of Chemistry, Faculty of Science, The M. S. University of Baroda, Vadodara 390 002

Many of medicinal important compounds are heterocyclic compounds. Most of the drugs contain a heterocycle in their structure. Due to the presence of heteroatom, the organic compounds are able to interact with enzymes and the other biomolecules. 1,3-oxazoles are focus of research due to their biological activities and isolation of many active natural products possessing oxazole as a vital part of their structure. On the other hand, isomeric heterocycle iso-oxazole and its nitrogen variant pyrazole hold a key position among bioactive heterocycles.

We designed new iso-oxazoline and pyrazole compound in combination with 1,3-oxazole with a view to get complimentary effects on their bioactivity. In the present talk the design and synthesis of these new compounds will be presented. Out of several potential bioactivities, they were studied *in vivo* on wistar rats using carrageenin-induced paw odema standard method for their anti-inflammatory activity.

OO-CYSA-01 : Design, Synthesis and Biological Activity of Novel Vitamin E Derivatives as Potential Antitumor Agents

Naval Kapuriya,[1,2] Dasheng Wang[2] and Ching-Shih Chen[2]

[1]Shree M.& N. Virani Science College, Department of Chemistry, Saurashtra University, Rajkot-36005.
[2]The College of Pharmacy, The Ohio State University, Columbus, Ohio, USA.
E-mail : navalkapuriya@gmail.com

Despite advances in cancer treatments and therapies, cancer still remains as major public health problem in the USA as well as developing countries like India and China. Therefore, developments of novel cancer therapeutics are urgently needed to improve cancer prognosis. There is considerable interest exists in evaluating the anti-tumorigenic effects of vitamin E derivatives (α, and γ- forms of tocopherol) in light of their superior anti-inflammatory and antitumor efficacies. Recently we have also reported a series of tocopheryl succinates as potent inhibitors of cancer cell-adhesion. In the search of potent antitumor agents, we have further modified the α, and γ- forms of tocopherol scaffolds and synthesize several novel vitamin E derivatives to study their anticancer effect. It was revealed that these derivative possessed significant antitumor activity against a variety of tumor cell growths (PC-3, LNCap, MDA-MB-231). Attempts to study their molecular mechanism revealed that new tocopherol derivatives facilitate the Ser-473-specific dephosphorylation of Akt, thereby providing insights into the mode of antitumor action and a rationale for the translational development of tocopherols into novel Akt inhibitors. Detailed modification strategy, synthesis and antitumor activity of newly prepared α, and γ- forms of tocopherol will be discussed.

OO-CYSA-02 : Synthesis of Biologically Active Imidazolo and Benzimidazolo Fused Derivatives of 1,4-benzodiazepin-5-[4”-methylpiperazinyl)-carboxamide through Phenylamino Spacer

Navjeet Kaur,* Pratima Sharma, Aastha Pareek and D. Kishore

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

1,4-benzodiazepine nucleus is endowed with a wide array of biological activities ranging from the anxiety and stress related conditions to the management and control of AIDS. Due to this reason, the compounds belonging to this class are considered interesting targets for the synthesis of materials of medicinal importance. Incorporation of bioactive pharmacophores in 1,4-benzodiazepine molecular framework might allow quite interesting revelation to emerge concerning to the structural requirements for the formation of active analogues from this nucleus. Based on these observations, we have synthesized biologically active imidazolo and benzimidazolo fused derivatives of 1,4-benzodiazepin-5-[4”-methylpiperazinyl)-carboxamide through phenylamino spacer. The structures of the compounds were established on the basis of their spectral data. These final compounds have shown significant biological activity against fungus and bacteria.

OO-CYSA-03 : Synthesis, Characterization, Antimicrobial and Antioxidant Evaluation of 10*H*-Phenothiazines, their Sulfones and Ribofuranosides

Shikha Agarwal[a], Dinesh Kr. Agarwal[b], Naveen Gautam[c] and D. C. Gautam[c]

[a]Department of Chemistry, University College of Science, M. L. Sukhadia University, Udaipur (Raj.)
[b]Department of Pharmacology, Arya College of Pharmacy, Kukas, Jaipur (Raj.)
[c]Department of Chemistry, University of Rajasthan, Jaipur, (Raj.)
**E-mail : shikha_urj@yahoo.com*

10*H*-phenothiazines are synthesized via Smiles rearrangement. These prepared phenothiazines act as a base to prepare ribofuranosides by treating them with β-D-ribofuranosyl-1-acetate-2,3,5-tribenzoate. 10*H*-phenothiazines on refluxing with hydrogen peroxide in glacial acetic acid gave 10*H*-phenothiazine-5,5-dioxides. The structure of the synthesized compounds has been established by elemental analysis and elucidated using IR, UV, ^{1}H NMR, ^{13}C NMR and Mass spectra. The synthesized compounds were evaluated for their antioxidative properties through in vitro studies, and they are also screened for their antimicrobial activity. The synthesized compounds showed mixed radical scavenging activity in both DPPH and ABTS•+ assay. The antibacterial activity was performed against *Coagulase positive staphylococci* and *Coagulase negative staphylococci* and the compounds showed moderate to good activity. Regarding antifungal activity, some compounds were found moderate active against fungus *Candida albicans.*

OO-CYSA-04 : One-pot, Three Component Synthesis of Novel bis [1,2,3]triazol-2-indolinone Derivatives via Click Chemistry Approach

D. Ashok* and Srinivas G.

Department of Chemistry, Osmania University, Hyderabad-500007
E-mail : ashokdou@gmail.com

A one-pot, three component, copper-catalyzed azide-alkyne 1,3-dipolar cycloaddition (CuAAC) reaction was carried out successfully,

affording some novel bis [1,2,3]triazol-2-indolinone derivatives in excellent yields in *tert*-butanol/water. This one-pot, three component CuAAC reaction was carried out starting from an alkyl/aryl bromide, sodium azide, and terminal alkyne. All the synthesized compounds were characterized by IR, ^{1}H NMR and mass spectral analysis.

Several members of the 1,2,3-triazole family have indeed shown interesting biological properties, such as antiallergic, antibacterial and antiHIV activity. Additionally, 1,2,3-triazoles are found in herbicides, fungicides, and dyes. Click chemistry is a newer approach for the synthesis of druglike molecules that can accelerate the drug discovery process by utilizing a few practical and reliable reactions. Of the reactions comprising the click universe, the perfect example is the Huisgen 1,3-dipolar cycloaddition of alkynes to azides to form 1,4 disubstituted-1,2,3-triazoles.

OO-CYSA-05 : Constituents of *Annona Squamosa* Twigs having Major Immune Modifier to Elicit Polarized Th1 Immune Response in BALB/c Mice

Dinesh K. Yadav[a] **, Vishal Kumar Soni**[b]**, Rakesh Maurya**[c] **and Shailja Misra-Bhattacharya**[b]

[a]Department of Chemistry, University College of Science, M. L. Sukhadia University, Udaipur (Raj.)
[b]Division of Parasitology, Central Drug Research Institute, M.G. Marg, Lucknow (U.P.)
[c]Medicinal and Process Chemistry Division, Central Drug Research Institute, M.G. Marg, Lucknow (U.P.)
**E-mail : dinesh4dariyati@gmail.com*

Annona squamosa (AS) has traditionally been used as herbal medicine. Present communication deals with the phytochemical analysis and pharmacological investigation of the most active chloroform fraction that led to isolation and identification of a number of compounds whose structures were elucidated using 1D and 2D NMR spectroscopic analysis. Amongst the twelve pure compounds isolated, five compounds Lanuginosine (1), (+) -O- methylarmepavine (2), (+)-anomuricine (3), Isocorydine (4), and N-methyl-6,7-dimethoxyisoquinolone (5) were evaluated *in vivo* for their immune modifier activities in BALB/c mice after oral administration at three log doses of 0.3, 1.0 and 3.0 mg/kg for 14 consecutive days. Of these, three compounds (1, 2 and 5) showed dose dependent immune stimulating activity. However, the highest activity was noted in the compound N-methyl-6, 7-dimethoxyisoquinolone at the 3.0 mg/kg oral dose. The compound possibly acted modifying the expression of Th1- and Th2- cytokines via stimulation of pro-inflammatory Th1 cytokines IL-2 and IFN-γ. These results explore the use of the above compounds as an efficient immune-stimulant or immune-adjuvant against diseases with immune suppression.

OO-CYSA-06 : Microwave Assisted Facile and Efficient Synthesis of Some Fused Thiazoloquinazolinone Derivatives for Antimicrobial Evaluation

Manish Kumar Rawal[1] **and Pinki B. Punjabi**[2]

[1]Department of Chemistry, Vidya Bhawan Rural Institute, Udaipur-313002 (Raj.)
Microwave Chemistry Laboratory, University College of Science,
[2]M. L. Sukhadia University, Udaipur-313002 (Raj.)
E-mail : rawalmanish85@yahoo.co.in, pb_punjabi@yahoo.com

4–(4–Substituted phenyl)–2–thioxo–1,2,3,4,7,8–hexahydro-quinazolin–5(6H)–one on reaction with chloroacetic acid in the presence of fused sodium acetate afforded 5–(4–substituted phenyl)–8,9–dihydro–2H–thiazolo[2,3–b]quinazolin–3,6[5H,7H]–dione. Furthermore, its treatment with aromatic aldehydes furnished arylidene derivatives i.e. 2–(4–substituted benzylidine)–5–(4–substituted phenyl)–8, 9–dihydro–2H–thiazolo[2,3–b]quinazolin–3,6[5H,7H]–dione. Compounds on reaction with hydroxylamine, hydrazine hydrate, urea and guanidine nitrate gave its isoxazole, pyrazole, pyrimidine and amino pyrimidine derivatives under microwave irradiation. So, the present work describes the application of microwave in multi step synthesis. Structures of all the newly synthesized compounds were established on the basis of their elemental and spectral data. Synthesized compounds have been assayed for their antimicrobial activity and some of the compounds have shown significant inhibition on bacteria and fungi.

OO-CYSA-07 : Synthesis of Novel Derivative of 1, 5-Benzothiazepines from β-Diketones and their Anti-bacterial Activity

Neetu Kumari[1]**, Shilpa Jain and Y. C. Joshi**[2]

[1]Department of Chemistry, University College of Science,
M. L. Sukhadia University, Udaipur-303101 (Raj.)
[2]Department of Chemistry, University of Rajasthan, Jaipur-302004 (Raj.)
[1]E-mail : drneetuchoudhary@yahoo.com

Synthesis of six 2, 4-disubstituted-1,5-benzothiazepine have been prepared by condensation of 2-aminophenol with various 1,3-diketone in pyridine on heating mantle for about four to five hours which posses better pharmacological activity. In these compounds 1, 5-benzothiazepine ring have played significant role in medicinal chemistry. The structures of newly synthesized compounds have been elucidated by elemental analysis and spectral studies viz. IR, ^{1}H NMR and ^{13}C NMR. Newly synthesized compounds were screened for their antibacterial activity against B. subtilis, E. coli and S.typhis.

OO-CYSA-08 : Synthesis of a Novel ROMP Monomer and a Solvatochromic Betaine Dye *via* Catalytic Transfer Hydrogenation

Poorn Prakash Pande

Department of Applied Sciences, MMM Engineering College, Gorakhpur-273010 (UP)
E-mail : pppande@gmail.com

2,6-Di-*t*-butyl-phenol is a low cost commercial antioxidant. Direct nitration of this phenol fails to give the desired nitration product, however, in an improved synthesis, carrying out nitration in a two phase system, it was possible to obtain the nitro phenol “A” in 73.7% yield. In the present work catalytic transfer hydrogenation (CTH) of the nitro phenol “A” was carried out using ammonium formate as the hydrogen donor and Pd/C as the catalyst in methanol medium, under nitrogen at room temperature. Complete reduction to aminophenol “B” occurred in 10 minutes. The product, initially colourless, quickly turns to a deep red compound, even on brief exposure to air. This is expected for such hindered amino phenols, which undergo auto-oxidation to corresponding quinonimine.

We found that the aminophenol “B” can be easily converted into N-(3,5-di-*t*-butyl-4-hydroxy phenyl) maleimide “C”, through one pot synthesis, without isolating the amino-phenol. This maleimide was further converted into a novel Ring Opening Metathesis Polymerization (ROMP) monomer “D” by Diels- Alder reaction with cyclopentadiene. The aminophenol “B” was also converted into 2,4,6-triphenyl-pyridinium-3,5-di-*t*-butyl-4-phenolate “E” (a solvatochromic dye), by condensation with 2,4,6-triphenyl pyrillium hydrogen sulphate

OO-CYSA-09 : Microwave Assisted Cyclization of Acridinyl Thiourea into Dithiazolidines and their Antimicrobial Study

Pravin Kawle* and Pradip Deohate

Postgraduate Department of Chemistry, Shri Radhakisan Laxminarayan
Toshniwal College of Science, Akola-444001, Maharashtra
E-mail : pravink280685@rediffmail.com

As a part of systematic investigation of synthesis and biological activity, several [1,2,4]- dithiazolidines were synthesized by cyclization of 1-acridin-9-yl-3aryl-thiourea with N-phenyl-S-chloro-isothiocarbamoyl chloride using microwave radiation. Constitutions of synthesized compounds have been delineated on the basis of chemical transformation, elemental analysis, equivalent weight determination, IR, ^{1}H-NMR and ^{13}C-NMR spectral studies. The title compounds were screened for their antimicrobial activity against the microorganisms like *S.typhi, E. coli, B. subtilis,* and *S. aureus.*

OO-CYSA-10 : Hydroarylation of Arenes with Styrenes using Montmorillonite K-10 as an Efficient, Selective and Recyclable Catalyst

Satish R. Lanke and Bhalchandra M. Bhanage *

Department of Chemistry, Institute of Chemical Technology, N. Parekh Marg, Matunga, Mumbai, 400 019
E-mail : lanke9satish@gmail.com, bm.bhanage@gmail.com

Catalytic functionalization of arenes and heteroarenes has considerable importance in the pharmaceutical, agrochemical, fine and bulk chemical industry. Traditionally, Friedel Crafts reactions are used for such transformations. However, these methods have several limitations like the use of stoichiometric amount of Lewis acids, drastic reaction conditions, lower selectivity and large amount of salt formation. The products diarylalkanes which has great importance in various valuable biological active compounds and pharmaceutics.

Hydroarylation of styrene and its derivatives with arenes and heteroarenes was studied using Montmorillonite K-10 as an efficient, environmentally benign, economical, greener and recyclable catalyst. The reaction gives 1,1-diarylalkanes with a very excellent selectivity and excellent yields in short time with greater substrate compatibility. Solid acid Montmorillonite K-10 catalyst was thoroughly characterized with different techniques. Notable advantages offered by this metal-free reaction system are the use of Montmorillonite K-10 as a heterogeneous recyclable catalyst, simple workup procedures.

OO-CYSA-11 : Solvent Free Microwave Assisted Synthesis of 3-((*E*)-3-(2,4-dihydroxy-5-((*E*)-3-(4-oxo-4*h*-3-chromenyl)-2-propenoyl)Phenyl)-3-oxo-1-propenyl)-4*h*-4-chromenones

D. Ashok* and S. Ravi

Department of Chemistry, Osmania University, Hyderabad-500007
E-mail : ashokdou@gmail.com

The novel 3-((*E*)-3-(2,4-dihydroxy-5-((*E*)-3-(4-oxo-4*H*-3-chromenyl)-2-propenoyl) phenyl)-3-oxo-1-propenyl)-4*H*-4-chromenones have been synthesized by microwave- promoted solvent-free condensation of 1-(5-acetyl-2,4-dihydroxy phenyl)-1-ethanone and 4-oxo- 4*H*- chromene-3-carbaldehyde. The synthesized compounds have been characterized

by elemental analysis and spectral data such as IR, ^{1}H NMR and Mass.

The chromones (4*H*-1-benzopyran-4-ones) have attracted attention from the point of view of both biological activity and organic synthesis. The compounds that contain the chromone skeleton (4*H*-benzopyran-4-one) (flavones and chromones) are widely spread in nature, and they are part of the flavonoid family. These compounds have been reported to exhibit multiple biological properties, for example, anticancer, antifungal, antioxidant and anti-HIV.

OO-CYSA-12 : One Pot Synthesis of Substituted 4H-Pyrano[3,2-*c*]coumarins using Rehydrated Mg-Al Hydrotalcite in Aqueous Medium

Nanabhau B. Karanjule and Shriniwas D. Samant*

Department of Chemistry, Institute of Chemical Technology,
N. Parekh Marg, Matunga, Mumbai, 400 019
E-mail : nanakaranjule@yahoo.com, samantsd@yahoo.com

Recently multicomponent reactions (MCRs) have emerged as a highly valuable tool in modern organic synthesis and modern drug discovery. The atom economy and convergent character, the simplicity of a one pot procedure, the possible structural variations, accessible complexity of the molecules and the very large number of accessible compounds are among the desired advantages of a MCR. Pyrano[3,2-c]coumarins are of considerable interest as they possess a wide range of biological properties such as diuretic, anticoagulant, anti-cancer and anti-anaphylatic activity. Number of 2-amino 4H-pyrans are useful as photoactive materials.

The reaction of aldehydes with malononitrile/ethyl cyanoacetate and 4-hydroxycoumarin was carried out using rehydrated Mg-Al hydrotalcite (R-Mg-Al HT) (Mg/Al=2-5) in water solvent at 60^0C to obtain 4H-Pyrano[3,2-c]coumarins in good yield. Cyclic ketones, malononitrile and 4-hydroxycoumarin react under the same conditions to give spiro pyrano[3,2-c]coumarins. Aromatic ketones do not reacts under the same conditions. Knovenagel reaction, Michael reaction and hetero Thorpe-Ziegler reaction take place in a tandom manner to gave the products. Notable advantages of this process are use of heterogeneous recyclable catalyst, simple workup procedure, high selectivity, and greater substrate compatibility. With respect to aldehydes this approach is an important supplement to the existing methods.

OO-CYSA-13 : Hydrogen Bond Parameters of N-arylhydroxamic Acids

Priyanka Singh and Rama Pande*

School of Studies in Chemistry, Pt. Ravishankar Shukla University,
Raipur-492 010, Chhattisgarh
E-mail : priyankasingh0678@gmail.com

In the present investigation, the hydrogen-bond parameters of two N-arylhydroxamic acids have been measured and reported. Hydroxamic acid functional group consists of both Hydrogen-Bond Donor (HBD) and Hydrogen-Bond Acceptor (HBA) sites. The HBD and HBA strengths of these molecules ranges in between 0.6743 - 0.7014 and 2.3614 - 2.4034, respectively. Values of lipophilicity by experimentation ($\log P_{O/W}$) and calculated lipophilicity (ClogP) by Bioloom program of biobyte Co. are also reported. These data constitute the hydrophobic parameters of QSAR studies.

OO-CYSA-14 : Stereochemical Effects of the Substituents in Nucleophilic Addition of L - Cysteine on Aromatic Aldehydes

R. M. Jagtap and S. K. Pardeshi*

Department of Chemistry, University of Pune, Ganeshkhind, Pune-411007
E-mail : skpar@chem.unipune.ac.in

The natural amino acids are generous source of chiral precursors to synthesize valuable chiral organic moieties. The chirality of every natural amino acid is specific and by retaining the original chiral centre novel chiral molecules have been synthesized. In natural amino acids derived compounds (diastereomers), the chirality of newly generated chiral centre relies on parameters like; nature of the substrate, nature of the reagent, temperature, solvent used etc.

L-Cysteine is a leading amino acid with absolute configuration ‘R’. Present work reports the nucleophilic addition of L-Cysteine on alkyl, alkoxy, hydroxyl, amino, nitro and halogen substituted aromatic aldehydes to afford diasteromeric mixture of cyclic (2*R, 4R*) 2-aryl thiazolidine-4-carboxylic acids and (*2S, 4R*) 2-aryl thiazolidine-4-carboxylic acids. The diastereomeric compounds have been synthesized at room temperature in water-DMSO solvent system. Distereomeric mixtures are ascertained by using IR, H^1 NMR, C^{13} NMR spectroscopy and elemental analysis. The nucleophilic addition is studied with respect to nature and position of the substituent present in aromatic aldehydes and its influence on reactivity, time duration, NMR shifts and stereochemistry of major diastereomer product (diastereomeric excess) by LCMS analysis.

OO-CYSA-15 : Microwave Assisted Synthesis of Some Medicinally Important Heterocyclic Compounds

Urvarshi Tiwari, Sanyogita Sharma[a] and P. B. Punjabi*

Department of Chemistry, University College of Science, M. L. Sukhadia University, Udaipur (Raj.)
[a]Pacific Institute of Technology, Udaipur (Raj.)
E-mail : sanyogitasharma22@gmail.com

Now-a-days, the main focus of an organic chemist is to synthesize heterocyclic compounds exhibiting a wide spectrum of biological activities. Ethyl (1,3-benzothiazole-2-sulfanyl) acetate has been prepared by reacting mercaptobenzthiazole in ethanol with ethychloroacetate and anhydrous potassium carbonate. The compound was further subjected to reflux with hydrazine hydrate to produce 2-(1,3-benzothiazol-2-yl-sufanyl) acetohydrazide. Then cyclocondensation of substituted chalcones was furnished with it. These reactions have been carried out in the presence of glacial acetic acid. The structures of all synthesized compounds have been established by their elemental and spectral analysis.

OO-CYSA-16 : Microwave Assisted Synthesis of 10-chloro-4-methyl-8-phenyl-2*H*,8*H*-pyrano[2,3-*f*]chromen-2-ones and their Antibacterial Activity

D. Ashok* and B. Vijaya Lakshmi

Department of Chemistry, Osmania University, Hyderabad-500 007
E-mail : ashokdou@gmail.com

Synthesis of heterocyclic compounds is a powerful technique for generating new molecules useful for drug discovery. Coumarin derivatives have been reported to exhibit, antimicrobial, antioxidant, anticancer, antiviral and anti-inflammatory activities. Chromenes and fused chromenes are biologically interesting compounds with antibacterial, antifungal, antitumor, antiviral activities. It is reported in the literature that when one biodynamic heterocyclic system is fused or attached with another heterocyclic system, biological activity increases. The environmental protection has become a global concern for synthetic organic chemists. Microwave irradiation provides the environmentally benign strategies for the future sustainable growth.

Encouraged by the biological activities of coumarin and chromene we have taken up the synthesis of novel 10-chloro-4-methyl-8-phenyl-2*H*,8H-pyrano[2,3-*f*]chromen-2-ones in conventional as well as microwave irradiation methods. The structures of the compounds have been established on the basis of elemental and spectral analysis. Some of the synthesized compounds showed good antibacterial activity.

OO-CYSA-17 : Design of Topoisomerase Inhibitors as Potential Anti-cancer Agents

Ankita L. Mehta, R. S. Lokhande*, M. M. V. Ramana*[1], U. J. Joshi[2], M. K. Gadhwal[2] and Gayatri V. Gadre

School of Basic Sciences, Department of Chemistry, Jaipur National University, Jaipur.
Department of Chemistry, University of Mumbai, Vidyanagari, Santacruz (E), Mumbai-400098.
KM Kundnani College of Pharmacy 23, Jote Joy Bldg, R.S. Marg, Cuffe Parade, Mumbai-400 005.
E-mail : mmvramana@yahoo.co.in

The topoisomerase enzymes are essential for DNA metabolism, where they act to adjust the number of supercoils in DNA, a key requirement in the cellular processes of transcription and replication. Both type I and type II topoisomerases have been identified as clinically important targets for cancer chemotherapy and their inhibitors are central components in many therapeutic regimes.

In this work, we have explored the potential of computational approaches in drug discovery for designing topoisomerase inhibitors for cancer treatment. Computational drug design approach has a great potential in accelerating the drug discovery process. A structure-based virtual screening of database was performed for hit identification which can inhibit topoisomerase. The exploration of the interaction of the ligands with their binding sites in receptor is carried out for lead optimization. The prediction of ADME properties is also performed by Qikprop software.

The inhibitor identified in this study serves as a good starting point for future rational drug design of topoisomerase inhibitors. Our virtual screening approach may also be applied to discovery of new lead molecules for other drug targets.

OO-CYSA-18 : High Speed Synthesis of Isoxazoline and Study of their Antimicrobial Activity

Khushbu Yadav[1#] Abha Sharma[1] and J.N. Srivastava[2]

[1]Department of Chemistry, Agra College, Agra
[2]Department of Botany, Dayalbagh Educational Institute, Dayalbagh, Agra
E-mail : yadavkhushbu14@gmail.com

Microwave induced organic reaction enhancement (MORE) chemistry is going popularity as a non-conventional technique for rapid organic synthesis and lot of work has been reported in the direction of proving the synthetic utility of MORE chemistry in routine organic synthesis. It can be form as e-chemistry because it is easy, effective, economical and eco friendly and is believed to be a step forward green chemistry. In present study, two sets of isoxazolines were synthesized by condensation of different substituted chalcones with hydroxylamine hydrochloride in the presence of base under microwave irradiation. The purity was determined TLC and structural elucidation were carried out by spectral (IR, H-NMR, Mass spectra) studies. The antimicrobial activity of chalcones and isoxazoline was evaluated against two bacteria (E. coli and S. aureus) and three fungus (A. niger, A. fumigatus and C. albicans) by disc diffusion method. The results obtained were compared with standard antibiotics: Chloramphenicol and Ketoconazole. All derivatives exhibited better inhibiting growth of both bacteria and fungus.

OO-CYSA-19 : Synthesis and Biological Activity of Hybrid Heterocyclic Analogs Derived from Apocycin and Benzo[*b*]Furan Nucleus

Janaki P. and N. J. P. Subhashini*

Department of Chemistry, University College of Technology, Osmania University, Hyderabad, Andhra Pradesh 500 007
**E-mail : njsubhashini@yahoo.co.in*

Apocynin (4-hydroxy-3-methoxyacetophenone), a methoxycatechol first isolated from the roots of Apocynum cannabinum (Canadian hemp) in 1883, was originally used as remedies for dropsy and heart illness. Recent investigations have found that apocynin is an efficient inhibitor of NADPH oxidase. Apocynin has been investigated as a therapeutic candidate for inflammation-mediated diseases, including jaundice, asthma and cardiovascular diseases.

The benzo[*b*]furan nucleus is prevalent in a wide variety of biologically active natural and unnatural compounds. Many 2-arylbenzofuran derivatives are well known to exhibit a broad range of biological activities, including anticancer, antiproliferative, antiviral, antifungal, Immune suppressive, antiplatelet, antioxidative, insecticidal, antiinflammatory, antifeedant, and cancer preventative activity. Keeping in mind the various biological activities associated with the apocycin and benzo[*b*]furan nucleus we have synthesized a hybrid molecules consisting of benzofuran and apocynin moieties such as chalcones, Pyrazoline and Isoxazoline Derivatives. All these novel compounds were characterized by IR, ^{1}H NMR, ^{13}C NMR and MS analysis. Biological activities of these novel analogs have been screened against two Gram +ve, Gram –ve pathogens *Escheria.Coli, Pseudomonas.aeruginosa, Staphylococcus.aureus* and *Streptococus.pyogenes,* bacterial strains using ampoxycillin as standard drug.

OO-01 : A Green and Environmentally Benign Synthesis of Symmetrical N, N'-Disubstituted Thiourea Derivatives using CS_2, Amines and H_2O in Sunlight

Priyanka P. Kumavat, Asha D. Jangale, Dipak R. Patil and Dipak S. Dalal*

Department of Organic Chemistry, North Maharashtra University, Jalgaon-425 001 (M.S.)
E-mail : dsdalal2007@gmail.com

Thioureas has great importance in chemical industry due to their biological activities such as fungicide, herbicide, rhodenticide, and phenoloxidase enzymatic inhibitor as well as their metal complexes exhibit analgesic, anti-inflammatory, antimicrobial and anticancer activity. Thiourea derivatives are also useful building blocks for the synthesis of 5- and 6-membered heterocycles. They have also applications in anti-HIV, antituberculosis and antiarrythmatic.

A efficient method for the synthesis of symmetrical and unsymmetrical thiourea derivatives involves addition of CS_2 to a well stirred solution of dialkylamine in water containing NaOH at RT, stir for 1hr. To this solution add primary amine and heated at 100 ^{0}C. Also one recent method for the synthesis of thiourea derivatives was reaction of CS_2 & amines at 60 ^{0}C in water for 1-12 hrs.

We have adopted a green and operationally simple approach for the synthesis of 1,3-disubstituted thiourea derivatives using primary aromatic amines, CS_2 in water, without any catalyst and induced by free solar thermal energy. This is an environmentally benign and energy saving synthesis.

OO-02 : Synthesis and Characterization of Novel Series of Pyrazoline

H. S. Vidyshree Jois and Balakrishna Kalluraya*

**Department of Studies in Chemistry, Mangalore University,*
Mangalagangothri, Konaje- 574 199
**E-mail : bkalluraya@gmail.com*

Chalcones and their derivatives are attractive molecular scaffolds for the search of new biologically active molecules. Pyrazoline ring system has attracted significant interest in medicinal chemistry. It has been studied extensively because of their ready accessibility, diverse chemical reactivity and broad spectrum of biological activity.

A novel approach has been adopted for the synthesis of new chalcones and pyrazolines. The scheme involves the synthesis of pyrazoline from chalcone. In first step, diazotization of suitable aniline followed by coupling with heterocyclic aldehydes results in the formation of novel aldehydes. These aldehydes when treated with substituted ketone in basic medium gave chalcone in the presence of alkali, under ice bath. These chalcones were then reacted with hydrazine hydrate in glacial acetic acid medium to get the respective pyrazolines. The structures of the newly synthesized compounds were characterized by IR, ^{1}H NMR and mass spectral analysis.

OO-03 : Enhancement of Photocatalytic Activity of Some Natural Pigments Sensitized Zinc Oxide

Surbhi Benjamin, Neelam Kunwar, Rakshit Ameta and
Suresh C. Ameta*

Department of Chemistry, Pacific College of Basic & Applied Sciences,
Paher University, Debari, Udaipur - 313024 (Raj.)
E-mail : ameta_sc@yahoo.com; surbhi.singh1@yahoo.com

Photocatalytic degradation of dyes is a Green chemical and Eco-friendly method for the treatment of effluents of dyeing, textile and printing industries. An attempt has been made to study the change in photocatalytic behaviour of zinc oxide after sensitizing it with certain natural pigments like Red Sandal (*Adenanthera pavonina*) and Heena (*Lawsonia inermis*) powder. The progress of the reaction has been monitored spectrophotometrically by measuring absorbance of the reaction mixture at definite time intervals. The effect of variation of various parameters such as pH, concentration of dye, concentration of zinc oxide and light intensity on the rate of photocatalytic degradation was also observed. A tentative mechanism for the reaction has also been proposed, where hydroxyl radicals were found as active oxidizing species.

OO-04 : Design, Synthesis, Kinetics, and Antimicrobial Activity of Some Heterocyclic Hydroxamic Acids

Anita Patel[a], Surendra K. Rajput[b] and Kishor N. Bapat[c]

[a]Dept. of Chemistry, Govt. N.P.G. College of Science, Raipur, (C.G.) 492010
[b]Govt. P.G. College Bhilai-3, Durg-490021 (C.G.)
[c]Govt. N.P.G. College of Science, Raipur-492010 (C.G.)
E-mail: patelanita1988@gmail.com, skchem4450@yahoo.com
knbapat.1952@gmail.com

Heterocyclic hydoxamic acids were synthesized .The kinetics of the hydrolysis have been analysed by Bunnett, Bunnett Olsen and Cox-Yates excess acidity method . Heterocyclic hydroxamic acids and their derivatives fulfill a variety of important role in biology and medicine. The promising biology and medicine application potential of this compound prompted us to design antimicrobial activity of some heterocyclic hydroxamic acids.

OO-05 : An Ecofriendly Protocol for the Synthesis of Aliphatic Symmetrical N, N'-Disubstituted Thiourea Derivatives in Aqueous Medium

Asha D. Jangale, Priyanka P. Kumavat, Dipak R. Patil and Dipak. S. Dalal*

Dept. of Organic Chemistry, North Maharashtra University, Jalgaon-425 001 (M.S.)
E-mail : dsdalal2007@gmail.com

Thiourea derivatives are of importance in medicinal chemistry due to their biological activities such as antituberculosis, anti-HIV, analgesic, anti-inflammatory, antimicrobial, antirrythmic, fungicide, herbicides, rodenticides and as phenoxidase enzymatic inhibitors, and also used for building blocks in heterocycles. Thiourea, the sulfur analog of urea can be synthesized in a number of ways, such as from ammonium thiocynate, from primary and secondary amines with NaOH in water, mustard oils, with CS_2 at 60^0C in water for 1-12 hrs. We have attempted synthesis of 1,3-disubstituted aliphatic symmetrical thioureas using CS_2 and aliphatic amine in aqueous medium by stirring without using any catalyst. Reaction was completed within 30 minutes with excellent yields. This methodology is novel, ecofriendly and having simple workup.

OO-06 : Synthesis of Quinolines from Drug Amines by using Inorganic Composites of Transition Metals as a Catalyst

S. A. Dhanmane[a], S. M. Vhankate[a], V. B. Tadke[a], S. S. Pawar[a], P. K. Kotkar [a], T. R. Valkute[a], B. D. Vanjare[a] and R. P. Pawar[b]

[a]Department of Chemistry, Fergusson College, Pune
[b]Department of Chemistry, Deogiri College, Aurangabad-431005
E-mail : sushilkumardhanmane@yahoo.com, rppawar@yahoo.com

Quinolines were synthesized from drug amines and dimethyl formamide/$POCl_3$ using various inorganic transition metal composites as a catalyst. The yield of the quinolines obtained using this novel protocol is significantly higher than those utilizing the conventional method.

OO-07 : An α-L-rhamnosidase from *Aspergillus awamori* MTCC-2879 and its Role in Debittering of Orange Juice

Sarita Yadav and K.D.S. Yadav

Department of Chemistry, DDU Gorakhpur University, Gorakhpur-273009
E-mail : dr_saritayadav@rediffmail.com

The purpose is to purify and characterize α-L-rhamnosidase with different properties suitable for different applications. The extracellular α-L-rhamnosidase has been purified by growing a new fungal strain *Aspergillus awamori* MTCC-2879 in the liquid culture growth medium containing orange peel. The purification procedure involved ultrafiltration using PM-10 membrane and anion exchange chromatography on diethyl amino ethyl cellulose. The purified enzyme gave single protein band in SDS-PAGE analysis corresponding to molecular mass 75.0 kDa. The native PAGE analysis of the purified enzyme also gave a single protein band confirming the purity of the enzyme. The K_m and V_{max} values of the enzyme for p-nitrophenyl-α-L-rhamnopyranoside were 0.62 mM and 27.06 μmole/min/mg, respectively giving k_{cat} and k_{cat}/k_m values 39.90 s^{-1} and 54.70 $mM^{-1}s^{-1}$, respectively. The enzyme had an optimum pH of 7.0 and optimum temperature of 60° C, respectively. The purified enzyme can be used for specifically cleaving terminal α-L-rhamnose from the natural glycosides giving preparation of pharmaceutically important compounds like prunin, α-L- rhamnose. The purified enzyme can be used for the enhancement of wine aroma and debittering of orange juice.

OO-08 : The Development of Possible Substitutes to 'HAART' in Anti-HIV Chemotherapy by Incorporating the Vital Components of Etraverine on to the 2-position of Privileged Nucleus of Benzodiazepine

Aastha Pareek*, Navjit Kaur and D. Kishore

Department of Chemistry, Banasthali University, Banasthali-304022 (Raj.)
**E-mail : aastha.pareek15@gmail.com*

The advent of the 'highly active anti-retroviral therapy' (HAART) regimens comprising of three or four US-FDA approved anti-retroviral drugs in a cocktail for the treatment of AIDS has been highly encouraging as it suppressed the viral load in patients, but rapidly emerging multidrug resistant HIV-1 viral strains and severe adverse effects from long term HAART medication has necessitated this therapy to be supplanted by additional newer agents to combat this disease. Highly encouraged by the treatment option which the HAART has provided, we reasoned that an even still better treatment option could possibly emerge by joining the two or more than two enzyme inhibitors, in a single molecular framework of 1,5-benzodiazepine, by resorting to such synthetic endeavors which allowed these to unite together to become the part of the same molecule. The motivation to explore this treatment option derived its inspiration on this premise that their presence in tandem in the same molecular framework could contribute significantly to enhance the potency by providing an additive effect on the overall bio-efficacy in the resulting molecules.

OO-09 : Synthesis and Characterization of Conducting Polyanilines via Fenton and photo- Fenton Oxidation

Pinki B. Punjabi, Nirmala Kumari Jangid and
Narendra Pal Singh Chauhan[*]

Department of Chemistry, University College of Science,
M L Sukhadia University, Udaipur- 313001 (Raj.)
[*]Department of Polymer Science, University College of Science,
M. L. Sukhadia University, Udaipur- 313002 (Raj.)
E-mail : pb_punjabi@yahoo.com

Polyanilines have been prepared by catalytic oxidative polymerization of aniline in an acidic solution using H_2O_2 as an oxidant and ferrous sulphate as a catalyst in presence of light by Photo-Fenton process. The structures of polyanilines were elucidated by Ultraviolet – Visible (UV-Vis), Fourier transform Infrared (FT-IR) and Nuclear Magnetic Resonance (NMR) spectroscopy which confirmed the presence of benzenoid and quinoid rings in the polyanilines. Molecular weight and specific surface area were determined by GPC and BET analysis. The DSC results and two probe conductometry studies showed that samples had good thermal stability and electroactivity.

OO-10 : Synthesis and Characterization of Some New Pyrazolyl-thiazole Derivatives Possesing Sydnones

Balakrishna Kalluraya[*] **and Shobhitha Shetty**

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

Sydnones constitute a well-defined class of mesoionic compounds consisting of 1,2,3-oxadiazole ring system. Sydnones have been studied extensively as possible medicinal agents. It was shown that the structural features possessing partial positive charge on the heterocyclic ring and balanced by a negative charge of an exocyclic atom, they are able to interact with biomolecules such as proteins and DNA. Sydnones possessing heterocyclic moieties at the position-4 are also known for a wide range of biological properties. A number of mesoionic compounds are reported to possess activities such as anticancer, anti-infammatory, analgesic, antimicrobial etc.

Thiazole heterocyclic systems are very interesting because of their physicochemical and various pharmacological properties. Compounds incorporating the pyrazolyl structural unit are being developed in a wide variety of therapeutic areas including CNS, and metabolic diseases, also they exhibit various signiûcant biological properties.

Prompted by these reports and in continuation of our research for biologically active sydnone containing heterocycles, a substituted pyrazolyl-thiazole moiety at the 4-position of the sydnone nucleus was introduced and a series of 4-(2-{2-[(5-substituted-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene] hydrazinyl}-1,3-thiazol-4-yl)-3-aryl-sydnone were synthesized by the condensation of 4-bromoacetyl-3-arylsydnones with 2-[(3-methyl-5-substituted-1-phenyl-1*H*-pyrazol-4-yl)methylidene] hydrazinecarbothioamide.

OO-11 : Preparation and Characterization of Luminescent Eu(TTA)$_3$.Biq

Manju Bala, Rajesh Kumar, V.B.Taxak and S. P. Khatkar*

Department of Chemistry, Maharshi Dayanand University, Rohtak-124001
E-mail : s_khatkar@rediffmail.com

The complex Eu(TTA)$_3$. Biq (where TTA = 2-Thenoyl trifluoroacetone and Biq = 2,2'-Biquinoline) was synthesized and characterized by infra red spectroscopy, ^{1}H NMR spectroscopy, TGA/DTA, scanning electron microscopy, elemental analysis and energy dispersive analysis (EDS). This complex had regular shaped particles with size less than 1µm without any phase separation and on excitation at 370 nm emits bright red luminescence with main peak at 613 nm. The complex emitting red luminescence might be used to make the electroluminescent (EL) devices for display purposes.

OO-12 : Synthesis, Characterization and Molecular Docking Studies of Some New 1,3,4-Oxadiazolines Bearing 6-Methyl Pyridine Moiety

Shyma P. C.[a,b], Balakrishna Kalluraya[a,*], Peethambar S. K.[c], Sandeep Telkar[d], and Arulmoli T.[b]

[a]*Department of Studies in Chemistry, Mangalore University, Mangalagangothri, Karnataka-574 199*
[b]*SeQuent Scientific Limited, No:120 A&B, Industrial Area, Baikampady, New Mangalore, Karnataka-575 011*
[c]*Department of Bio-Chemistry, Jnanasahyadri, Kuvempu University, Shankaraghatta, Karnataka, 577 451*
[d]*Department of P.G. Studies and Research in Biotechnology and Bioinformatics, Jnanasahyadri, Kuvempu University, Shankaraghatta, Karnataka-577 451*

Two series of 3-acetyl-2-aryl-5-[3-(6-methylpyridinyl)]-2,3-dihydro-[1,3,4]-oxadiazole derivatives were synthesized from 6-methyl nicotinic acid hydrazide through multistep reactions.. Newly synthesized compounds were characterized by spectral studies. In a typical example the structure of the compound 5f was confirmed by crystallographic studies. Antimicrobial screening of the synthesized compounds were performed.. All the compounds were subjected to molecular docking studies for the inhibition of the enzyme L-glutamine: D-fructose-6-phosphate amidotransferase [GlcN-6-P] (EC 2.6.1.16). The in silico molecular docking results are matching with the in-vitro studies and they may be considered as good inhibitor of GlcN-6-P synthase.

OO-13 : Synthesis of Few Novel Chiral Pyrrole Spiro Lactam Coupled Pyridine Intermediates of API's : Impact Re-emergency and Chirality

L. N. Sharada[*], G. S. Satyanarayana Reddy, B. Sammaiah and D. Sumalatha

Department of Chemistry, Osmania University, Hyderabad-500007
E-mail : lnsharada@gmail.com

A few novel pyridine linked pyrrole spiro lactam analogues were prepared. The first key intermediate racemic 4-membered spiro lactam (8) was prepared from the precursor L-proline. The racemic spiro lactam successfully resolved via converting diasteriomer by making salt. The two separated enantiomers successfully coupled with different pyridine intermediates of API's offered few chiral spiro lactam linked pyridine analogues.

OO-14 : Greener and Facile Synthesis of S-protected Barbituric Acid Isothiocarbamides in Aqueous Medium

M. M. Sontakke[a], A. A. Jichkar[b], M. G. Dhonde[*c], C. S. Bhaskar[d] and B. N. Berad[e]

[b,*c]*Department of Chemistry, Shri Mathuradas Mohota College of Science, Nagpur-440009*
[d]*Department of Chemistry, Art's, Commerce & Science College, Koradi-441111*
[a,e]*Department of Chemistry, RTM, Nagpur University, Nagpur-440033*
E-mail : madhudash2001@yahoo.co.in, virishri@indiatimes.com, bnberad@gmail.com

A series of 1-aryl-2-(2,4,6-trioxo-1,3-diaryl(H)-hexahydropyrimidin-5-yl)-isothiocabamides(3a-l) have been synthesized by the interaction of substituted aryl/H thiocarbamides (2a-l) with monobromobarbituric acid in refluxing aqueous medium at 2.5-3 hours. The reaction is condensation reaction with elimination of hydrobromic acid. The reaction mixture was basified with aqueous ammoinium hydroxide to get free bases. The reaction was monitored by TLC and products (3a-l) were purified by column chromatography. These compounds were screened for their antibacterial and antifungal activities against different pathogens. The characterization of these newly synthesized products have been made on the basis of elemental analysis, IR, ^{1}H NMR and Mass spectral studies.

OO-15 : Stereoselective Hydroxylation of alkylbenzenes to benzylic positions

Saroj Yadav*, R. S. S. Yadav, S. Yadava and K. D. S. Yadav

Department of Chemistry, D.D.U. Gorakhpur University, Gorakhpur-273 009
**E-mail : s_saroj123@rediffmail.com*

The stereoselective hydroxylation of ethylbenzene to (R)-1-phenylethanol, 95% enantiomeric excess with 100% yield and propylbenzene to (R)-1-phenylpropanol, 80% enantiomeric excess having 100% yield of product using fungal mycelia of *Aspergillus niger* MTCC-2587. The 100% conversion yield is obtained on pH 7.0 and at room temperature. These fungal mycelia are also capable for conversion of methylbenzene to benzylalcohol and 100% product yield is obtained. Therefore, A. niger serves as a biocatalyst for stereoselective hydroxylation of alkylbenzenes to benzylic positions.

OO-16 : Synthesis and Characterization of Pyrazolo Derivatives of 2,6-dichloro-1-(N-substituted phenyl)-1,4-dihydropyridine-3,5-dicarbaldehyde

A.P. Rajput[1] and P.D.Girase[2]

[1]P.G. Research Center, Department of Chemistry, Z. B. Patil College,
Dhule-424002 (M.S.)
[2]S.V.S's Dadasaheb Rawal College, Dondaicha, Dist. Dhule (M.S.)
E-mail: aprajput@rediffmail.com, pdgirase@rediffmail.com

A number of pyrazolopyridines and its hydroderivatives exhibit a wide range of biological activities such as anxiolytic activity, dopamine D3 receptor antagonist, antiherpetic and antiallergic properties. In continuation of our interest in V-H reaction and its synthetic utility, we are reporting herein the synthesis and characterization of pyrazolo derivatives of 2,6-dichloro-1-(N-substituted phenyl)-1,4-dihydropyridine-3,5-dicarbaldehyde. The starting compounds in turn were synthesized from glutarimides using Vilsmeier-Haack reaction.

In the present work we are reporting the synthesis of dioxolane derivatives from target compounds which on condensation with hydrazine hydrate gave hydrazinodioxolane derivatives. These hydrazinodioxolane derivatives on treatment with aq. HCl at room temperature in one pot afforded pyrazolo derivatives of 2,6-dichloro-1-(N-substituted phenyl)-1,4-dihydropyridine-3,5-dicarbaldehyde. All the compounds were characterized by spectral and elemental analysis.

OO-17 : Methylation Study of Polysaccharides from the Pods of Kalanchoe Mormorate

G. C. Yadav and R. C. Verma

Department of Chemistry, Janta College, Bakewar, Etawah (U.P.)

Kalancho Mormorate Pods (Family crossulaceae) are an industrially economic plant having medicinal value. A polysaccharide has been isolated from the pods of the plant. The proposed structure was confirmed by further study. The presence of D-galactose and L-arabinose was confirmed by paper chromatography, gas liquid chromatography and quantitative study of the hydrolysate polysaccharide. The IR Spectra also confirmed the presence of D-galactose in the β-anomaric form and L-arabinose and D-galactose in α-anomeric form. Isolation and characterization of four methylated polysaccharides were identified namely, 2,4-di-O-methyl-D-galactose, 2,3,4-tri-O-methyl-D-galactose,2,3,5-Tri-O-methyl-L-arabinose and 2,3,4,6-tetra-O-methyl-D-galactose in the molar ratio 3 : 1 : 2 : 1. Thus the polysaccharide consists of main chain 1 β 6 linked β-D-glalacto pyranose unit and L-arabinofuranose units along with a D-galacto pyranose unit linked to the main chain by 1 α 3 linkages. This study showed that the polysaccharide from the Pods of Kalanchoe Mormorate may be named as arabinogalactan.

OO-18 : Green Chemical Approach to Synthesize 4-(Substituted-benzylidene-2-phenyl-1-(5-phenylthiazol-2-yl)-1H-imidazol-5(4H)-one and its Antimicrobial Studies

Dimple K. Rathor and V.K. Sharma

Microwave Chemistry Laboratory, Department of Chemistry,
M.L. Sukhadia University, Udaipur, (Raj.)
**E-mail : vkparashar53@gmail.com*

One of the key areas of Green Chemistry is the elimination of solvents in chemical processes or the replacement of hazardous solvents with environmentally benign solvents. Microwave heating has attracted the attention of investigators in that it makes it possible to shorten the length of reactions significantly, to increase their selectivity, and to increase the product yields, which is particularly important in the case of high-temperature processes that take a long time. Reactions in microwave ovens are currently in use for the synthesis of medicinally important compounds. Within the framework of 'Green Chemistry' we have now developed an environmentally benign and novel approach for the synthesis of (E)-4-(substituted benzylidene)-2-phenyl-1-(5-phenylthiazol-2-yl)-1H-imidazol-5(4H)-one.

These compounds have prepared by the reaction of 5-(pyridin-4-yl)-1,3,4-thiadiazol-2-amine with various (Z)-4-(substituted benzylidene)-2-phenyloxazol-5(4H)-one by using modified domestic microwave oven. The structure of these compounds was assigned on the basis of elemental analysis, IR, ^{1}H NMR spectral data. The compounds showed significant antibacterial and antifungal activity against *E. coli, P. aeruginosa, S. aureus , C. albicans* and *A. niger* using cup plate and agar well diffusion technique.

OO-19 : Green Synthesis and Antimicrobial Study of Some (E)-4-(4- Substituted Benzylidene-1-(Mono/ Di -Chlorophenyl)-1, 3, 4-Thiadiazol-2-Yl)-2-Phenyl-1H-Imidazol-5(4H)-One

Kalmendra Singh Sisodiya and V.K. Sharma

Department of Chemistry, Pacific University, Udaipur (Raj.)
E-mail: kalmendrasisodiya@yahoo.in

Microwave enhanced synthesis has attracted substantial attention in recent years, enabling many organic reactions to proceed much faster and with higher yields than, when conventional heating is employed. Microwave irradiation has become a powerful synthetic tool for rapid synthesis of a variety of organic compounds. Microwave assisted reactions have attracted much interest because of the simplicity in operation, milder reaction conditions, increasing reaction rates and formation of cleaner products. In view of these, it was planned to synthesize a new series of oxazolones by microwave irradiation and to evaluate the new compounds for their antimicrobial activity. The synthesis of newer class of antibacterial and antifungal agents is in need of time, especially against drug resistant bacteria and fungi which are responsible for a number of serious infections in acute and chronic care units in hospitals. In continuation to this we have undertaken green synthesis and antimicrobial study of some (E)-4-(4- substituted benzylidene-1-(mono/ di -chlorophenyl)-1, 3, 4-thiadiazol-2-yl)-2-phenyl-1H-imidazol-5(4H)-ones. These compounds were characterized by spectral techniques.

OO-20 : Charaterization and Antimicrobial Evaluation of Some Newly Synthesized Thiosemicarbazones

Sandhya Agarwal and Amit K. Agarwal

Department of Chemistry, Agra College, Agra-282002 (U.P.)
B. R. Ambedkar University, Agra (India)
E-mail : Agarwal.chem@yahoo.co.in

A large number of substituted thiosemicarbazones having 5 or 6 membered heterocyclic moieties have been reported to possess significant antimicrobial activities. Some new thiosemicarbazones viz. m-anisaldehyde thiosemi- carbazone, acetophenone thiosemicarbozone and thiophene-2-aldehyde thiosemicarbazone have been synthesized from different carbonyl compounds with thiosemicarbazide, in which primary amino group undergoes condensation with carbonyl compounds resulting the formation of respective thiosemicarbazones. All the compounds have been characterized by their repeated melting point determination, TLC, elemental analysis, IR and NMR Spectral data. They were also screened for their antimicrobial activities against two bacteria *Staphylococcus aureus* and *Escherichia coli* and two fungi *Aspergillus niger* and *Aspergillus flavus.*

OO-21 : Steroidal Glycosides and Benzoquinone Derivative from *Asparagus Curillus* (Liliaceae)

Deepak Kumar Semwal*, Ruchi Badoni Semwal and Gurjaspreet Singh

Department of Chemistry, Panjab University, Chandigarh-160014
**E-mail: dr_dks.1983@yahoo.co.in*

Phytochemical investigation of the roots of *Asparagus curillus* (Buch.-Ham.) ex Roxb. afforded a novel androstane type steroidal glycoside named 10β,13β,17α-trimethyl-17β-(21-methoxyethoxy)-androstan-2α-ol-3β-D-digitoxopyranoside; a steroidal saponin named 25*S*-5β-spirostan-3β-yl-O-[β-D-glucopyranosyl-(1→4)-β-D-glucopyranoside], and a benzoquinone derivative named 4-hydroxy-6-oxabicyclo[3.2.1]octa-1(8),4-diene-2,3-dione from the methanolic extract. The structures were elucidated by means of chemical, physical and spectral analyses including 2D NMR techniques.

OO-22 : *Berberis aristata* as an Efficient Natural Dye

Ruchi Badoni Semwal*, Deepak Kumar Semwal and Pratibha Kapoor

Department of Chemistry, Panjab University, Chandigarh-160014
**E-mail : ruchi_badoni26@yahoo.com*

The roots of *Berberis aristata* DC (Berberidaceae) were used to determine the dyeing properties with natural and synthetic mordants. The aqueous extract obtained from roots collected by sustainable manner was used for dyeing cotton. The extract of stem bark of *Myrica esculenta* (Myricaceae) was used as natural mordant whereas $SnCl_2$ and $FeCl_3$ were used as synthetic mordants. The dye solution showed remarkable increase in percentage absorption with natural mordant by 47.05% in comparison of synthetic mordants $SnCl_2$ and $FeCl_3$ by 46.02 and 36.73, respectively. This work concludes that roots extract of *B. aristata* having good dyeing properties itself and its color can be enhanced by natural mordants those are safer and eco-friendly, and can be a source of new dye stuff for textile industries.

OO-23 : Synthesis of Some New Arylidenes Derived from Phenoxazine by Microwave Technology : Novel Chemistry and Potential Applications in Pharmaceutics

S. K. Srivastava

Department of Chemistry, Synthetic Organic Chemistry Laboratory,
Dr. H. S. Gour University (A Central University) Sagar-470003 (M.P.)
E-mail : professorsks@rediffmail.com

Heterocyclic ring systems containing nitrogen and sulfur exhibit potent chemotherapeutic activites. Thiazolidinones are important synthones for various biologically active molecules. Azines and their derivatives are the important class of heterocycles because of their wide spectrum of biological activity shown by the molecules. Incorporation of 1,3-thiazolidine and 1,2,4-thiadiazole systems in phenoxazine have been considered as an important pharmacophore for introduction in the design of biologically active molecules. Hence in the present study phenoxazine containing a -NH group at position-1 was used as the target for chemical modification. Phenoxazine on treatment with bromochloropropane followed by thiosemicarbazide and H_2SO_4 and NH_3 to afford 1,2,4-thiadiazole derivatives which on reaction with various substituted aromatic aldehydes produced arylidenes. The arylidenes on further treatment with thioglycolic acid in the presence of zinc chloride afforded 1,3-thiazolideno-1,2,4-thiadiazole derivatives which on reaction with aromatic aldehydes gave various substituted aryl-4-oxo-1,3-thiazolidene-3-propyl-phenoxazine-1,2,4-thiadiazoles.The structures of the products were confirmed by spectroscopic data and chemical methods. Some of the compounds displayed antibacterial activity against E. coli and S. aureus and antifungal activity against C. albicans and A. niger.

OO-24 : A Rapid and Highly Efficient Microwave Synthesis of Some New Azetidine-2-Chloropheno-thiazines : Antimicrobial Agents

S. D. Srivastava

Department of Chemistry, Synthetic Organic Chemistry Laboratory
Dr. H. S. Gour University (A Central University) Sagar-470003 (M.P.)
E-mail : drsavitri@rediffmail.com

Heterocyclic-medicine is the boon for human beings because most of the life saving drugs are derived from heterocyclic rings and have also fewer side effects. Azetidinones are the important synthones for various biologically active molecules particularly antibiotics. A large number of antibiotics contain azetidinones moiety for examples ceftriaxone-a highly effective 3rd generation potential cephalosporin and tazobactum-a superior β-lactamase inhibitor are good in activity. According to literature a large number of antibiotics drugs contain azetidin-2-ones moiety in their structural part. 2-chlorophenothiazine have reported to have several biological activities. I have introduced azetidinoe moiety in 2-chlorophenothiazine through propane bridge with a view to obtain better drug. In this way several compounds, 4-substituted-3-chloro-2-oxo-azetidin-imino-propyl-2-chlorophenothiazines have been synthesized starting from 2-chlorophenothiazine , bromochloropropane, hydrazine hydrate, aromatic aldehydes and chloroacetyl chloride. The structures were confirmed by spectral and chemical methods. The compounds were screened for their antibacterial and antifungal activities against some selected organisms. Some of the compounds displayed pounced and acceptable biological activity.

OO-25 : Synthesis, Characterization and Antimicrobial Activity of Some 3-(2-(6-methyl-1H-benzo[*d*]imidazol-2-yl) phenyl)-2-(aryl)thiazolidin-4-ones

N. C. Desai and Atul H. Makwana*

Department of Chemistry, M K Bhavnagar University, Bhavnagar-364 002

Heterocyclic compounds have received considerable attention because of their applications in medicinal, agricultural and industrial chemistry etc. Benzimidazole and 4-thiazolidinone heterocyclic rings have proved their chemotherapeutic importance. Benzimidazole derivatives have shown pharmacological activities like antifungal, anti HIV, antihistaminic, antiulcer, antihypertensive etc. The chemistry of thiazolidinone ring system is also of considerable interest as numerous thiazolidinone derivatives have shown significant bioactivities such as anticonvulsant, antidiabetic, antihistaminic, anticancer, anti HIV etc.

Looking to the pharmacological applications of benzimodazole and 4-thiazolidinone derivatives, we have synthesized some 3-(2-(6-methyl-1H-benzo[*d*]imidazol-2-yl)phenyl)-2-(aryl)thiazolidin-4-ones. All the synthesized compounds were screened for *in vitro* antibacterial and antifungal activities on *Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Staphylococcus pyogenes, Candida albicans, Aspergillus niger* and *Aspergillus clavatus.* The structures of the compounds synthesized were elucidated by IR, ^{1}H-NMR, ^{13}C-NMR and mass spectra.

OO-26 : Design and Synthesis of Some New Modified Pyridine Substituted Coumarins and Study of their Cytotoxicity and Antimicrobial Efficiency

Rakesh R. Giri, Yogita L. Chovatiya and Dinkar I. Brahmbhatt*

Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat.
**E-mail : drdib317@gmail.com*

A new class of modified pyridine substituted coumarin derivatives has been synthesized by reacting 4-methyl-3-phenyl-6-coumarinoyl methyl pyridinium salt 1 and appropriate 2-arylidine indanones, 2-arylidine tetralones and 2-arylidene aurones respectively under Krohnke's reaction condition. All the newly synthesized compounds have been fully characterized by IR, ^{1}H NMR, APT and elemental analysis. The representative compounds have also been characterized by mass spectral analysis. All the synthesized compounds have been screened for their *in vitro* antimicrobial efficiency against a representative panel of pathogenic strains specifically *Staphylococcus aureus, Bacillus subtilis, Escherichia coli, Salmonella typhi, Candida albicans, Aspergillus niger.* Almost all the compounds showed appreciable antimicrobial activity against the tested strains. A few derivatives exhibited antimicrobial activity comparable with that of the standard drugs used for testing. The compounds have been also evaluated for their cytotoxic activity.

OO-27 : Diversity-Oriented Approach to Spiroindolines : Post-Ugi Gold-Catalyzed Diastereoselective Domino Cyclization

Sachin G. Modha[a,b], Amit Kumar[a,c], Dipak D. Vachhani[a], Jeroen Jacobs[d], Sunil K. Sharma[c], Virinder S. Parmar[c], Luc Van Meervelt[d] and Erik V. Van der Eycken[a]

[a]*Laboratory for Organic & Microwave-Assisted Chemistry (LOMAC), Department of Chemistry, KU Leuven, Celestijnenlaan 200F, Heverlee B-3001, Leuven (Belgium).*
[b] *Present address: "Mani Bhuvan", Nr. Lohana Mahajan vadi, Chhaya-360578, Porbandar*
[c]*Bioorganic Laboratory, Department of Chemistry, University of Delhi, Delhi-110 007*
[d]*Biomolecular Architecture, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, Heverlee B-3001, Leuven (Belgium).*
E-mail : sachinmodha@gmail.com

Gold-catalyzed carbocyclization and heteroannulation strategies have recently attracted much attention due to the selective and efficient activation of the C-C triple bond towards a wide range of nucleophiles. Domino approaches, involving gold-catalysis, lead to complex heterocyclic compounds under exceedingly mild reaction conditions.

Diversity-oriented approach comprising an Ugi-4CR and a diastereoselective gold(I)-catalyzed domino cyclization for the generation

of complex spiroindolines is elaborated. Mild reaction conditions were employed. Variously substituted spiroindolines were synthesized in good to excellent yields with complete diastereoselectivity.

OO-28 : Nitrogen Heterocycles as Metal Ion Sensor

Arun Kumar Padhy

National Institute of Science & Technology, Palur Hills, Berhampur-761008, Odisha
E-mail : arun_nist@hotmail.com

Application of nitrogen heterocycles now is not limited to synthetic intermediates nor in pharmaceutical industries, but they have been found in various fields such as nanoparticles, electronic devices etc. The advantage most researchers suggest is in the flexibility that the organic molecules possess in their structural entity. This paper deals with the synthesis of some imidazole derivatives and their application as metal ion sensor. Also this paper will deal with the usage of imidazole derivatives as the precursor for metal oxide nano particles. These imidazole derivatives can be prepared by reacting benzyl monoxime with aromatic aldehydes in presence of ammonium acetate and acetic acid in appreciably good yield. These imidazole derivatives are employed for the selective metal ion detection as these imidazoles bind selectively with metal ions. Some of the metals thus form complex with these synthetic imidazoles. Such metal complexes on calcinations provide the formation of metaloxide nano particles.

OO-29 : Synthetic Application of 1-Formyl-9H-β-Carboline for Generating β-Carboline Derivatives with D-Ring

Virender Singh[a], Raman Bala[b] and Sanjay Batra[C]

[a]*Department of Chemistry, Dr. B R Ambedkar National Institute of Technology, Jalandhar 144011*
[b]*Department of Environmental Science, Maharshi Dayanand University, Rohtak 124001*
[c]*Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow-226001*
E-mail : singhvirender010@gmail.com

Alkaloids comprising of β-carboline core are ubiquitously present in nature including plants, marine organisms, insects, mammalian as well as human tissues and body fluids. These alkaloids are constitutionally a large group of indole alkaloids with different scale of aromaticity. Recently an array of pharmacological applications of alkaloids belonging to β-carboline class were reviewed by Cao et al. Especially they have been demonstrated to intercalate with DNA and display activities against CNS and infectious disorders. Owing to their immense significance, synthesis of a variety of β-carboline derivatives has been a subject of intense research. Out of several subclasses of β-carboline-based alkaloids, one subclass contains additional D-ring. For example canthine, canthin-6-one, tuboflavin, maxomine, arborescidine and so on. Though there exist several elegant strategies to achieve their synthesis, we envisaged that 1-formyl-9H-β-carboline may serve as a universal precursor for obtaining β-carboline-derivatives containing D-ring.

In this context, we have engineered a novel strategy for obtaining β-carboline-1-carbaldehyde or its substituted analogs at large scale. This synthon has been demonstrated to be a useful substrate for the synthesis of highly functionalized canthi none and canthine derivatives using the Morita-Baylis-Hillman reaction. This chemistry has been extended to develop a facile synthesis of harmicine and homofascaplysin mimics and β-carboline-fused isoxazoles, isoxazoline, pyrrole and triazole derivatives. Details of these studies shall be presented and discussed.

OP-CYSA-01 : Regeneration of Carbonyl Compounds from Aldoximes and Ketoximes Over Ceric Sulphate

Sharwan K. Dewan* **and Priti Sharma**

Department of Chemistry, M. D. University, Rohtak-124001(Haryana)
E-mail : sharwankumardewan@yahoo.com

Rapid deoximation of aldoximes and ketoximes has been achieved in excellent yields in presence of Ceric Sulphate catalyst under solvent free conditions. A number of variously substituted arylaldoximes and ketoximes were reacted. The oximes of even the sterically hindered ketones such as alpha-tetralone, testosterone, androsterone underwent regeneration without any problem. Oximes obtained from a number of variously substituted (electron withdrawing and donating groups) on aldehydes and ketones, were subjected to deoximation like Benzophenone, Acetophenone, p-Bromoacetophenone, alpha-tetralone, 4-nitrobenzaldehyde, 4-bromobenzaldehyde, p-chlorobenzaldehyde , salicylaldehyde, 2,4-dichlorobenzaldehyde etc.

OP-CYSA-02 : One Pot synthesis of Nitriles from Aldehydes And Hydroxylamine Hydrochloride using Potassium Bisulphate

Sharwan K Dewan* **and Minakshi**

Department of Chemistry, M.D.University, Rohtak -124001 (Haryana)
E-mail : sharwankumardewan@yahoo.com

One pot synthesis of nitriles has been carried out from arylaldehyde and hydroxylaminehydrochloride in presence of potassium bisulphate in dry media under microwave irradiation. The nitriles were obtained in high yields. A wide variety of differently substituted, electron donating and electron withdrawing grouped arylaldehydes were attempted- p-hydroxybenzaldehyde, 2,4-dichlorobenzaldehyde, 3,4- dimethoxybenzaldehyde, 4-nitrobenzaldehyde, 3-nitrobenzaldehyde, 2-nitrobenzaldehyde, cinnamaldehyde, tolualdehyde, anisaldehyde, salicyldehyde, p-bromobenzaldehyde etc. The products were identified on the basis of their spectroscopic data.

OP-CYSA-03 : Green Synthesis of Tetraketones from Dimedone and Arylaldehydes in Aqueous Medium in Presence of Tetrabutylammoniumbromide (TBAB)

Sharwan K. Dewan* **and Anju**

Department of Chemistry, M.D.University, Rohtak-124001 (Haryana)
E-mail : sharwankumardewan@yahoo.com

The synthesis of tetraketones from dimedone and arylaldehydes has been carried out under green chemistry conditions in aqueous medium in presence of tetra butyl ammonium bromide (TBAB) at room temperature in high yields. Dimedone and arylaldehydes were taken in 2:1 ratio. The products were identified on the basis of their spectroscopic data and by comparison with authentic samples. Arylaldehydes were differently substituted - p-chlorobenzaldehyde, 2,4-dichlorobenzaldehyde, 2-nitrobenzaldehyde, 3-nitrobenzaldehyde, 4-nitrobenzaldehyde, anisaldehyde, p-tolualdehyde, 3,4-dimethoxybenzaldehyde, 2,4-dimethoxybenzaldehyde, cinnamaldehyde, Salicylaldehyde etc.

OP-CYSA-04 : Synthesis of N, N-Disubstituted Ureas from Biuret and Anilines

Sharwan K. Dewan* **and Rashmi**

Department of Chemistry, M. D. University, Rohtak-124001 (Haryana)
E-mail : sharwankumardewan@yahoo.com

Symmetrically N, N-disubstituted ureas have been synthesized from biuret and anilines. The products were obtained in good to excellent yields under solvent free conditions. The biuret and anilines were taken in 1:2 ratio. A number of anilines were reacted together to give the corresponding ureas. These included aniline, p-toulidine, anisidine, o-phenylenediamine, phenylhydrazine etc. The products were identified on the basis of their spectroscopic analysis and physical constants.

OP-CYSA-05 : Synthesis of Acylals from Arylaldehydes and Acetic Anhydride in presence of Sodium Sulphate Anhyd. Over Mont KSF

Sharwan K. Dewan* and Anil Kumar

Department of Chemistry, M. D. University, Rohtak,
Haryana and AIJAT HM College, Rohtak, Haryana-124001
E-mail : sharwankumardewan@yahoo.com

Acylals were synthesised from arylaldehydes and acetic anhydride in presence of sodium sulphate anhyd over Mont KSF under green chemistry conditions. The acylals were obtained in high yields. A number of arylaldehydes were reacted. These included aldehydes substituted with electron- withdrawing as well as electron- releasing groups. The aldehydes were taken included benzaldehyde, 3-nitrobenzaldehyde, 4-nitrobenzaldehyde, 4-chlorobenzaldehyde, 4-cyanobenzaldehyde, 3-methoxybenzaldehyde, cinnamaldehyde, furfural etc. The product were identified on the basis of spectroscopic data.

OP-CYSA-06 : Environmentally Benign Synthesis and Antimicrobial Activity of the Different Modified Sulphonamide Drug Molecules

V. R. Tembhare[a], C. S. Bhaskar[b]*, M. G. Dhonde[c] and B. N. Berad[d].

[a,b*]*Department of Chemistry, Art's, Commerce & Science College, Koradi-441111*
[c]*Department of Chemistry, Shri Mathuradas Mohota College of Science, Nagpur-440009*
[d]*Department of Chemistry, RTM, Nagpur University, Nagpur-440033*
E-mail : virishri@indiatimes.com, madhudash2001@yahoo.co.in, bnberad@gmail.com

Since sulfa drugs play an important role in a vast array of biological processes and particularly there are many advantages e.g. these are antibacterial agent. They increase activity and modify pharmacokinetic properties. They are bacteriostatic in nature and have a broad spectrum of activity. They are still an attractive group of drugs since they are very cheap. So we proposed to synthesize these molecules by involving environmentally benign method with aryl isothiocyanates.

Synthesis of different derivatives of 4-amino-*N*-[*N*-(aryl carbamothioyl)carbamimidoyl]benzene sulfonamides have been achieved with the interaction of 4-amino-N-carbamimidoyl benzenesulfonamide with different aryl isothiocyanates. These reactions were carried out in the aqueous medium for 8-10 hours. The completion of the reactions was observed with the help of TLC. The compounds were washed several times with petroleum ether (40-60). Structures of all these recently synthesized compounds have been established on the basis of certain chemical properties like elemental analysis, IR, PMR and

Mass spectral data. All synthesized compounds are tested for their antibacterial and antifungal activities.

OP-CYSA-07 : Design, Synthesis and Evaluation of Spirochromano Thiazole Derivatives as an Antibacterial Agent

Kalpesh Menpara[a] and K. D. Ladva[b]

[b]Shri M. & N. Virani Science College, Rajkot-360005, Gujarat
[a]E-mail : kalpesh.menpara@gmail.com

Synthesis of spirochromano thiazole based antibacterial agent is reported. Condensation of 2'-hydroxy-4'-methoxy acetophenone with cyclohexanone gives 7-methoxyspiro[chromene-2,1'-cyclohexan]-4(3H)-one(I). 7-methoxyspiro[chromeno[4,3-d] [1,3] thiazole-4,1'-cyclohexan]-2-amine(II) was prepared by the reaction of thiourea with(I) in the presence of iodine. The final compound (1E)-N'-(7-methoxyspiro [chromeno[4,3-d][1,3]thiazole-4,1'-cyclohexan]-2-yl)-substituted ethanimidamide(III) was synthesized by the reaction of (II) with substituted acetamide using phosphorus oxychloride and it is characterized by IR, 1H & 13C NMR, Mass & LCMS analysis and single crystal XRD.

OP-CYSA-08 : Synthesis, DNA Protection and Antimicrobial Activity of Some Novel Chloromethyl Benzimidazole Derivatives Bearing Dithiocarbamates

Priya M. Madalageri and Oblennavar Kotresh

Department of Chemistry, Karnatak Science College, Dharwad, Karnataka
E-mail : kotreshkscd@gmail.com

Organic dithiocarbamates have received much attention due to their pivotal role in agriculture and their intriguing biological activities. They have also been used as protection groups in peptide synthesis, as linkers in solid-phase organic synthesis and recently in the synthesis of ionic liquids. Furthermore, dithiocarbamates are broadly employed in medicinal chemistry and have been used in cancer treatment. Hence, a series of chloromethyl benzimidazole derivatives diverse dithiocarbamates moieties were designed and synthesized via three component reaction protocol. The synthesized dithiocarbamates were characterized by means of IR, ^{1}H NMR, mass spectral data and elemental analysis. When these were evaluated for DNA protection and anti-microbial activities some of them found to possess significant activity.

OP-CYSA-09 : Triterpenoid Saponins from Pericarp of *Sapindus mukorossi*

S. C. Sati, Maneesha D. Sati, Raman Bahuguna and Amita Sharma

Department of Chemistry, H. N. B. Garhwal University (A Central University) Srinagar, 246174, Uttarakhand
E-mail : sati_2009@rediffmail.com

A novel acetylated triterpene bisdesmoside saponin is elucidated as named Hederagenin 3-O-α-L-rhamnopyranosyl (3→1)-[2,4-O-diacetyl-α-L-arabinopyranosyl]-28-O-α-D-glucopyranosyl-(2→1) [3-O-acetyl-β-D-glucopyranosyl] ester (1)along with two known saponins hederagenin 3—O (-α-L-arabinopyranoside (1→3)- (-α-L-rhamnopyranosyl (1→2) -α-L- arabinopyranoside (2) and hederagenin-3-O-[β-D-xylopyranosyl (1→3) α-L-rhamnopyranosyl (1→2)- α-L- arabinopyranoside] (3) from the pericarp of *Sapindus mukorossi*. The structure of these compounds were characterized by means of spectral and chemical studies including advanced 2D NMR studies.

OP-CYSA-10 : Symmetry Arguments on the Properties of Molecules

M. Dhaneshwar Singh*, Ruhima Khan and Kh. Biren Singh

Department of Chemistry, Manipur University, Canchipur, Imphal-795003
E-mail : moirangthemds@yahoo.co.in

The properties of a molecule are dependent on the symmetry of the molecule. The existence or disappearance of certain physical or chemical phenomena of a system (or a molecule) can be predicted on the basis of the symmetry of the system. Certain physical and chemical properties of a molecule owe their very existence to the absence of certain symmetry operations in the molecular point group. In other words, the properties of a system vanish under some symmetry operations which are not elements of the point group. Such predictions which are based solely on the symmetry of the system are called symmetry arguments. The heart of such an argument is based on the non-equivalence brought by the absence of suitable symmetry operations. Symmetry arguments are also useful in predicting the molecular structures and the reaction mechanisms and the stereochemistry associated with certain reactions.

OP-CYSA-11 : Instrumental Approach on the Determination of Environmental Aqua Parameter of Machana River (M.P.)

M. Sallam, G. P. Sahu and S.C. Lavale*

Chemical Research Laboratory, J. H. Govt. P. G. College, Betul 460001 (M.P.)

The authors have used various instrumental technique/ probe viz.

pH-metry, conductometry, colourimetry, spectrophotometry, voltammetry well striping technique for the detection and determination of various component present in the water samples, Specially of organic type of the various tube-wells of distinct spots of Betul belt, the spot wise water quality parameters have been computed in the tabular form DO, BOD, COD, Total hardness have also been reporting WQI (Water Quality Index) and almost organic was calculated using weight arithmetic index method. It is observed that metallic concentration have been obtained <2 mg level in the industrial area. The bacteria, Coliform, E. coli, and other organic componenets dissolved have been analysed using polarographic estimation. Special empasis given to the organic polarographic method for the estimation at low level organic dissolved.

OP-CYSA-12 : Facile Synthesis of Some New Dihydropyrazole Derivative from 3-(substituted)-N-phenyl-2-enamides Under the Frame Work of Green Chemistry

Arpit Kumar Pathak, Urvashi Tiwari and Pinki B. Punjabi

Microwave Chemistry Laboratory, Department of Chemistry,
University College of Science M.L. Sukhadia University Udaipur, 313001 (Raj.)
E-mail : arpitpathak2009@gmail.com

The pyrozole nucleus has been proven to be fertile source of medicinal agent such as antibacterial, antifungal, antiamoebic, anesthetic etc. In the present work MW assisted synthesis of dihydropyrazoles by cyclocondensation of 3-(substituted)-N-phenyl-2-enamide with the hydrazide derivatives of benzotriazole in presence of glacial acetic acid (GAA) has been reported. The synthesized compounds have been characterized by their infra red, proton nuclear magnetic resonance and mass spectral studies. The synthesis of these compounds has also been carried out under conventional conditions. The yield of the products by microwave irradiation was significantly higher as compared to conventional condition.

OP-CYSA-13 : Evaluation of Antimicrobial Activities of Polar and Non Polar Flavanoids from Leaves of Ocimum tenuiflorum

P. S. Pande

Department of Chemistry, Shankarlal Khandelwal Arts,
Science and Commerce College, Akola (M.S.)

Polar flavanoids and non polar flavanoids have been isolated from the leaves of Ocimum tenuiflorum by chemical method. The isolated extract was screened for antimicrobial activities against

Proteus vulgaris, Staphylococcus aureus, Escherichia coli and Salmonella typhi. The extracts showed good to moderate activity against the pathogens.

OP-CYSA-14 : Phytochemistry and Antifungal Activity of Various Extracts of the Plant *Cassia fistula*

V. D. Mane[1], P.R. Rajput[2] and M.O. Malpani[3]

[1,3]Post graduate Department of Chemistry, S. K. College, Akola
[2]Post graduate Department of Chemistry, V.B.M.V. Amaravati
E-mail : vivekvdm@rediffmail.com

The present work is for evaluation of antifungal response of various extract of *cassia fistula* leaves and pod on pathogenic fungas. The litature survey revels that the water extract and organic solvent extract of the leaves and pod of the plant Cassia fistula is act as a antifungal agent against the pathogenic fugi. In this experiment we extract the leaves and pod in water and ethanol chloroform and we examine the antifungal activity of these extract by using the cup plat method. The result of our experiment found that there is good to moderate inhibition zone on the plat hence we can predict that the various extract of Cassia fistula plant have antifungal activity.

OP-CYSA-15 : Synthesis, Characterization and X-ray Crystallographic Studies of 2,4-dimethyl Benzopyrylium Salts

Pratik Ambasana, Manisha Parmar and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : pratikambasana@gmail.com, parmar_manisha01@yahoo.com, anamik_shah@hotmail.com

The development of the chemistry of pyrilium salts observed in recent years is associated not only with the great theoretical interest in the reaction of carboxoniumcation but also with the possibility of using such salts for the synthesis of diversified compounds, which sometimes cannot be obtained by other processes.

A relatively simple and efficient method has been adopted for the synthesis of benzopyrilium salts, with application of perchloric acid and sulfuric acid. The crystallographic study of the compounds 2,4,7-trimethylchromenylium perchlorate, 2,4,7,8-tetramethyl chromenylium perchlorate and 7,8-dihydroxy2,4-dimethyl chromenylium perchlorate has been confirmed the structure of the compounds which are of biological interest.

OP-CYSA-16 : Selective Oxidation Cyclohexane Over Mn(Salen) Intercalated Alpha-zirconium Phosphate Using Thbp as an Oxidant

Savita Khare, Rajendra Chokhare and Priti Shrivastava

School of Chemical Sciences, Takshashila Campus, Khandwa Road
Devi Ahilya University, Indore-452017 (M. P.)
E-mail : kharesavita@rediffmail.com

A heterogeneous catalyst, Mn(Salen) intercalated α-zirconium phosphate, abbreviated as {α-ZrP.Mn(Salen)} was synthesized in situ by the flexible ligand method. The resulting compound was characterized by BET surface area, X-ray diffraction, energy dispersive X-ray analysis, Fourier transform infrared, electron paramagnetic resonance and atomic absorption spectroscopy. The catalytic activity of α-ZrP.Mn(Salen) was tested for the oxidation of cyclohexane using dry *tert*-butylhydroperoxide as an oxidant under solvent free condition. In the oxidation reaction, cyclohexane was oxidized to cyclohexanol and cyclohexanone. Influence of various reaction parameters viz. reaction temperature, catalyst and oxidant concentration was studied. Under the optimized conditions, oxidation of cyclohexane gave a maximum 8.00% conversion. The major product followed the order of selectivity: cyclohexanol > cyclohexanone. The catalyst was reused for two cycles. The hot filtration experiments proved that the catalyst was heterogeneous.

OP-CYSA-17 : Stereoselective Synthesis of Novel Spiropyrrolidine Library through 1,3-dipolar Cycloaddition Reactions

Balakrishna Kalluraya[*] and Sahana Mallya

Department of Studies in Chemistry, Mangalore University, Mangalagangothri-574 199
[*]E-mail : bkalluraya@gmail.com

The chemistry of azomethine ylides have been investigated intensively in recent years as it serves as an significant route for the construction of nitrogen containing five-membered heterocycles. The 1,3-dipolar cycloaddition of azomethine ylides with olefinic and acetylenic dipolarophiles offers an excellent route for the construction of pyrrolidines and pyrrolizidines. The spiropyrrolidine and pyrrolizidine ring systems form the core structure of many pharmacological agents and alkaloids. Because of their remarkable biological activities of spiropyrrolidines and pyrrolizidines ring systems, significant efforts have been devoted to their synthesis.

Here in a series of novel spiropyrolidines have been synthesized through 1,3-dipolar cycloaddition reaction of azomethine ylide with

1,3-disubstituted propenones as dipolarophiles. The structure of the new synthesized cycloadducts were established upon their elemental analysis, IR, ^1H NMR and ^{13}C NMR. Study of anti-oxidant property of newly synthesized compounds is on progress.

OP-CYSA-18 : A Facile Synthesis, Characterization and Study of Biological Activity of Some Novel Series of 3-substitued-4-(4/5-subtituted-3-indolylidene) Amino-5-mercapto-1,2,4-triazoles and their Mannich Bases

R. Gururaja*, Suresh Marakala[1], Aravinda Kumar Madugula[1] and Srinivasa Rao Pedada[1]

**Department of Chemistry, Sarada Vilas College, University of Mysore, Mysore-04, Karnataka*
E-mail : dr.gururaja@gmail.com

In recent years, a large number of indole derivatives have been shown to possess an array of biological properties like anticonvulsant, anti-depressant, antihistamine, antidiabetic, etc 1,2,4-Triazoles are well known compounds and are found to possess varied pharamacological activities. The analgesic, diuretic, antiviral antibacterial, and antifungal properties exhibited by various 3-substituted-5-mercapto-1,2,4-triazoles. Further indole associated with active heterocycles like imidazole, thiazole, oxazole etc. at 3-position has reported promising potent biological activity.

Keeping in view of above, it was thought fit to synthesize Indole derivatives containing 1,2,4, triazole at 3-position. Condensation of 3-substituted-4-amino-5-mercapto-1,2,4-triazole and 5/6-subtituted-Indole-3-carbaldehyde in ethanol and catalytic amount of conc. HCl, yield Schiff bases. Interaction of the resultant schiff's bases with suitable active primary/secondary amine in ethanol and formaldehyde gave title compounds. The newly synthesized compounds were characterized by spectral data.

OP-CYSA-19 : A Rapid and Facile Synthesis of some 3,5-Dicyano-1,4-dihydropyridines and their Novel Mannich Bases

Sabera Bijani, Vaibhav Ramani and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : saberabijani@gmail.com, anamik_shah@hotmail.com

Recent studies have revealed that 1,4-dihydropyridines exhibits several medicinal applications which include neuroprotectant and platelet anti-aggregratory activity, in addition to acting as a cerebral antiischemic agent in the treatment of Alzheimer's disease. These examples clearly demonstrate the remarkable potential of novel DHP derivatives as a source of valuable drug candidate.

Present work covers the synthesis of Mannich reaction of 1,4-dihydropyridines containing hydroxyl group on phenyl ring. The Mannich bases of 3,5-dicyano-4-(substituted phenyl)-2,6-dimethyl-1,4-dihydropyridines are novel which are potent to have significant biological activity. All the newly synthesized compounds have been well characterized by IR, Mass,^{1}H NMR and ^{13}C NMR and Elemental Analysis.

OP-CYSA-20 : A Rapid Microwave Assisted Synthesis of Novel 1,4-dihydropyridines Derivatives Under Aqueous Medium

Vicky Jain, Shailesh Thakarar and Anamik Shah

Department of Chemistry, Saurashtra University, Rajkot-360005.
E-mail : vickydjain@yahoo.com, anamik_shah@hotmail.com

An environment friendly synthesis of 1,4-dihydropyridine derivatives was developed by one pot multi component reaction of pyrazole aldehyde, EAA/MAA, 3-amino crotononitrile and Fe^{+3} montmorillonite clay K-10/ HY-zeolite under microwave irradiation in aqueous medium. The structures of all synthesized compounds were well characterized by Mass, FT-IR, ^{1}H NMR and elemental analysis.

The aim of current work is to prepare dihydropyridine which have a hybrid moiety where at C3 position possess a cyano group while at C5 position various esteric groups are present. This will ultimately give structural and molecular diversity of unsymmetric nature. We have exhibit green protocol for the synthesis and cyclization reaction of pyrazole aldehydes, EAA/MAA, 3-amino crotononitrile in water. This method is rapid, high yielding, environment friendly and water is easily available green solvent.

OP-CYSA-21 : Synthesis and Characterization of Some Cyanopyridine Derivatives Comprised with Furan Nucleus

Prachi Trivedi*, Radhika Vasani and Ranjan Khunt

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : drrckhunt12@yahoo.com

A series of cyanopyridine derivative have been synthesized via different reaction series. The 5(4-fluorophenyl) furfural was reacted with different aromatic ketones in presences of basic catalyst such as sodium hydroxide, pipiridine, etc. to furnish α, β-unsaturated ketocompounds, which on cyclization with malononitrile to furnish respective cyanopyridine derivatives. All the synthesised products have been confirmed by spectral analysis such as 1HNMR, IR and Mass spectrometry. Further it is confirmed by elemental analysis. All the synthesized compounds evaluated for their antimicrobial screening against *Gram- +ve* and *Gram-ve* bacterial strains.

OP-CYSA-22 : Synthesis and Molecular Docking Studies of Benzimidazole Incorporated Chalcone Derivatives

J. J. Vora[1] and L.S. Bhutadiya[2]

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

A series of chalcone derivatives *(5a-j)* were achieved upon reaction of newly synthesized ketone *(4)* with various aromatic aldeydes in alcohol. Ketone *(4)* was synthesized by reaction of p-amino acetophenone *(1)* and 2-mercapto-5-methoxy benzimidazole *(3)* with chloroacetyl chloride. All the synthesized compounds have been characterized by spectral analyses like IR, ^{1}H NMR and Mass and also screened for their microbial activities against selected organisms. The synthesized compounds were studied for molecular docking studies for antitubercular activity using GOLD 3.1 program.

OP-CYSA-23 : Synthesis and Anti-HIV Activity of Some New Fused Heterocyclic Compounds

Denish C. Karia*[1] and Anamik Shah[2]

[1]Department of Chemistry, Patel JDKD Science College, Borsad, Gujarat
[2]Department of Chemistry, Saurashtra University Rajkot, Gujarat
**E-mail : denishkaria@yahoo.com*

Number of 4-hydroxy -2H, 5H pyrano (3,2-C) chromene – 2,5 – dione are active as a potential photo reagents and also known for their pronounced anticoagulant properties. But recently, 3-acetoacetyl coumarins/pyranobenzopyrans have been explored for the inhibitory activity against HIV-1 and HIV-2 type of viruses.

In the present work, 4-hydroxy coumarinis treated with phosphorus oxychloride and zinc chloride to give 4-hydroxy -2H,5H pyrano (3,2-C) chromene – 2,5 - dione which was converted to 3- acetyl 4-hydroxy -2H,5H pyrano (3,2-C) chromene – 2,5 – dione when treated with acetic acid and phosphorous oxy chloride on heating with ethyl acetate and pulverized sodium metal for several hours afforded 4-hydroxy-3-(3-oxobutanoyl)2H,5H pyrano(3,2-c)chromene-2,5-dione which when treated with 3,4-diaminobenzophenone/o-phenylene diamine and glacial acetic acid to give 3-(7-benzoyl-3H-benzo[b][1,4]diazepin-2-yl)-4-hydroxypyrano [3,2-c]chromene-2,5-dione and 3-(4,7-dimethyl-3H-benzo[b][1,4]diazepin-2-yl)-4-hydroxypyrano[3,2-c]chromene-2,5-dione.

Several of similar derivatives were also synthesized. The structures of the synthesized compounds have been assigned on the basis of elemental analyses, IR, NMR and mass spectral studies.

OP-CYSA-24 : Synthesis and Biological Evaluation of Novel N-benzylidene-5,6-dimethoxy-8H-indeno[1,2-d]thiazol-2-amine Derivatives

Vimal Patel[a], Pralav Bhatt[b*] and Hasmukh Joshi[a]

[a]Department of Chemistry, Saurashtra University, Rajkot 360 005, Gujarat
[b]School of Chemistry, University of KwaZulu-Natal, Durban 4000, South Africa
E-mail : drvimalpatel@rediffmail.com

Thirteen N-benzylidene-5,6-dimethoxy-8H-indeno[1,2-d]thiazol-2-amines 3 were synthesized. 5,6-dimethoxy-8H-indeno[1,2-d]thiazol-2-amine 2 prepared from reaction of 1 with iodine and thiourea, reacted with aromatic aldehydes in presence of catalytic amount of p-toluenesulfonic acid to provide the title compounds in 59–85% isolated yields. The structures of compounds 3 were confirmed by ^{1}HMR, ^{13}CMR, MS and elemental analysis. All compounds have been evaluated for their *in vitro* antibacterial activity and compared with standard drugs.

OP-CYSA-25 : Synthesis of Bisazo Reactive Dyes Based on 4,4'-Bis o-Toludine and Their Application on Various Fibres

Rajesh B. Patel[a] and Keshav Patel

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395001
B.P. Baria Science Institute, Sayaji Road, Near fuwara, Navsari, Gujarat

Some bisazo reactive dyes have been synthesized by coupling diazotized 4,4'-methylele bis o-toluidine with various o-toluidino cyanurated coupling components. Their dyeing performance as reactive dyes has been assessed on silk, wool and cotton fibres. The purity was checked by thin layer chromatography. The IR spectra showed all characteristics bands and representative PMR spectra showed all the expected signals. The dyeing performance of all these dyes on silk, wool and cotton gave fair to good light fastness.

OP-CYSA-26 : Synthesis of Arylene Azo p-hydroxy Benzoic-formaldehyde Oligomeric Dyes and Their Application on Various Fibres

Paresh S. Patel[a] and Keshav Patel

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395001
Narmada College of Science and Commerce, Zadeshwar, Bharuch-392011

A series of oligomeric azo dyes has been synthesized by coupling various aromatic diazonium salts to p-hydroxy benzoic acid-formaldehyde (p-HBAF) oligomer. They were evaluated in terms of their softening point, yields, UV-visible spectra, IR spectra and PMR spectra. Dyeing on polyester and nylon resulted in yellow to red shades having moderate to good fastness to light and good to very good fastness to washing.

OP-CYSA-27 : Antioxidant Activty of Synthesized Ascorbyl Ester

Priyanka Vyas and Jaiswar Gautam

Department Of Chemistry, IBS, Khandari Agra
E-mail : vyaspriyanka640@gmail.com

In the present study the use of antioxidant of L- ascorbyl ester were demonstrated. This class of antioxidant find wide extensive use in the fields of food preservation, and in various diseases which associated with the generation of the free radicals. The L-ascorbyl ester were synthesised by chemical method in which L-ascorbic acid treated with different fatty acid such as valeric acid, myristic acid, stearic acid and sulphur containing like thiomalic acid in 98% concentrate H_2SO_4 acid. The products obtained were characterized by U.V. and I.R. The antioxidant activities was screened by FRAP Method (Ferric reducing antioxidant procedure).The anti-microbial studies were carried out to evaluate the minimum Inhibitory concentration(MIC).

OP-01 : Facile Synthesis, Characterisation and Biological Activities of Novel 2,4-Disubstituted-[1,3]-Thiazoles

Sumangala V[a,b], Boja Poojary[a,*], Chidananda N[a], Arulmoli T[b] and Shalini Shenoy[c]

[a]Department of Studies in Chemistry, Mangalore University, Mangalagangothri, Karnataka, 574 199
[b]Sequent Scientific Limited, No: 120 A&B, Industrial Area, Baikampady, New Mangalore, Karnataka-575 011
[c]Department of Microbiology, KMC Mangalore-575001, Karnataka
[*]E-mail: bojapoojary@gmail.com

Thiazole is an important scaffold in heterocyclic chemistry and

[1,3]-thiazole ring is present in many pharmacological active substances. Thiazole derivatives have attracted a great deal of interest owing to their antibaterial, antifungal, anti-inflammatory, CNS depresent, antitumor and anthelmintic activities. Encouraged by the above reports, it was planned to synthesize new [1,3]-thiazole derivatives, with the hope that the resulting molecules would exhibit promising biological properties. The present study describes the synthesis of 2,4-disubstituted-[1,3]-thiazoles (3a-l) and evaluated their cytotoxicity and antimicrobial activity against pathogenic strains.

The novel 2,4-disubstituted-[1,3]-thiazoles (3a-l) were synthesized by the reaction of 2-chloro-6-fluoro-/2-fluoro-benzaldehyde thiosemicarbazone (2a,b) with phenacyl bromides. 2-Chloro-6-fluoro-/ 2-fluoro-benzaldehyde thiosemicarbazone was obtained by treating aldehydes (1a,b) with thiosemicarbazide in the presence acetic acid. All structures of the newly synthesized compounds were characterized by spectral studies and were evaluated for their cytoxicity and antimicrobial activity. Some of the compounds exhibited promising activity.

OP-02 : Preparation and Characterization of Luminescent Sm(TTA)$_3$.bipy

Satish Kumar, V. B. Taxak, Rajesh Kumar, Manju Bala and S. P. Khatkar*

Department of Chemistry, Maharshi Dayanand University, Rohtak-124001
E-mail : s_khatkar@rediffmail.com

The complex Sm(TTA)$_3$.diph (where TTA = 2-Thenoyl trifluoroacetone and bipy = 2,2'- Bipyridyl) was synthesized and characterized by infra red spectroscopy, ^{1}H NMR spectroscopy, TGA/ DTA and scanning electron microscopy. This complex had regular shaped particles with size less than 1μm without any phase separation and on excitation at 390 nm emits orange red luminescence with main peak at 604 nm. The complex emitting orange red luminescence might be used to make the electroluminescent (EL) devices for display purposes.

OP-03 : Synthesis of Nanoparticles (Nanosorbents) and Applications in Defluoridation of Drinking Water

Kalpana Gupta

R. R. Govt. College, Alwar
E-mail : 27guptakalpna@gmail.com

Fluoride contamination in drinking water due to natural and anthropogenic activities has been recognized as one of the major problems worldwide imposing a serious threat to human health. There are many methods have been developed for removal of fluoride and other contaminants from water were adsorption, ion exchange, electrodialysis and precipitation and membrane process. However, many of these methods cannot be applied in developing countries and low-income areas, because of their high cost and complexity.

Among several treatment technologies applied for fluoride removal, adsorption process has been explored widely and offers satisfactory results especially with mineral-based and/or surface modified adsorbents. Therefore objective is to develop new nanoadsorbent find their adsorption capacities under various conditions available in the literature. It is evident from the literature survey that various adsorbents have shown good potential for the removal of fluoride. However, still there is a need to find out the practical utility of such developed adsorbents on a commercial scale, leading to the improvement of pollution control. Therefore we are looking for new and effective adsorbents Nanoparticles have much larger surface area than bulk particles and less expensive method for fluoride method.

OP-04 : Synthesis of Biologically Potent Pyrazole and Isoxazole Incorporated Derivatives of 1,5-benzodiazepine

Pratima Sharma, Navjeet Kaur, Rachna Mishra and Dharma Kishore

Department of Chemistry, Banasthali University, Banasthali-304022 (Raj.)
E-mail : misspratima29@gmail.com

Benzodiazepine and their derivatives demonstrated as potent anti-cancer, anti-HIV agent, and anti-convulsant. This has stimulated us further interest in pyrazole, isoxazole , thiadiazole pyrazole derivatives etc. which have the proven record of biological potential when incorporated on pharmaceutically active molecules tend to exert a profound influence on the bioefficacy of the molecule. The conceived synthetic plan for the preparation of these materials proceeded through the acceptable protocol which emerged from the face ‘c’ cyclohexano substituted 1,5 benzodiazepine bearing the thiomethylether function on its 2-position that in turn resulted from the reaction of o-aminothiophenol with 2-oxoketenedithioacetal derivative of cyclohexanone . Its treatment with p-hydroxyacetophenone afforded the corresponding p-acetyl substituted derivatives. Its treatment with benzaldehyde afforded the corresponding chalcone, which further react with hydroxyl amine hydrochloride and hydrazine hydrate formed p-formyl and p-acetyl substituted derivatives. The p-formyl and p-acetyl derivatives on its reaction with IBA (iodoxybenzoic acid) formed the thiadiazole derivative isoxazole incorporated analogues in good yield. The impact of this substitution on the biological activity of the molecule are under study. The structure of the compounds has been established on the basis of IR, ^{1}H NMR, and Mass spectral data.

OP-05 : Nanocomposites : Future High-rated Materials

Arvind Dixit*[1], Anuradha Tewari[1], Vishal Verma[2], K. N. Pandey[2]
[1]Department of Chemistry, V.S.S.D. College, Kanpur-208002
[2]Central Institute of Plastics Engineering & Technology, Lucknow
**E-mail : dixit_arvind2@yahoo.co.in*

The term nanocomposite represents a new exciting field in materials science and technology. The nanocomposites have actually been used for centuries by the nature. It is only recently that characterization and control of structures as the nanoscale have been studied, investigated and exploited by research scholars and scientist. Consequently the nanocomposite technology has emerged as an efficient powerful strategy/tool to upgrade the structural and functional properties of natural and synthetic polymers. Polymer nanocomposites have attracted great attention worldwide due to the exhibition of superior properties such as strength, decreased thermal expansion coefficient, decreased gas permeability, enhanced ionic conductivity, decreased flammability, toughness and various properties far from those of conventional micro composites and comparable with those of metals. Polymer Nanocomposite, overall improved properties result from nanoscale dispersion within the polymer matrix which leads to the tremendous interfacial contents between the polymer and inorganic filler leading to the superior properties than those of bulk polymer phase. The present paper reviews the preparation methodology of various types of nanocomposites and their characterization by several advance analytical techniques such as TEM, SEM, AFM, TGA, DMA, FTIR etc.

OP-06 : Synthesis, Characterization and Antimicrobial Studies of Uranium and Cerium Complexes with Lorazepam

Praveen Kumar Verma[1], K. Chaturvedi[2] and R. Chaturvedi[3]
[1]Department of Chemistry, Sainath Group of Education, Agra.
[2]Department of Chemistry, Agra College, Agra.
[3]Forensic Science Laboratories, Agra

Lorazepam [LZM] and other 1, 4 benzodiazepine drugs are the Schiff bases tend to react with the metals to form the complexes. Present paper revels that ligand LZM reacts with uranium and cerium metals to form the drug-metal derivatives. Synthesized complexes were characterized by elemental analysis, potentiometric and spectroscopic methods. The general formula of the synthesized complexes have been given by $[L_1M(NO_3)_4]$ and the geometry of the complexes were found to be octahedral. Where L_1= lorazepam, and M = uranium or cerium metal. Antimicrobial study shows that all the synthesized complexes are bioactive. Biological studies have been carried out on some selected bacteria *(E. coli, S. aureus, S. typhi)* and fungi *(A. niger, A. flavous, P. triticena)* at different concentrations.

OP-07 : Preparation and Characterization of Luminescent $Eu(TTA)_3$.diph

Rajesh Kumar, V.B.Taxak, J. K. Makrandi and S. P. Khatkar*

Department of Chemistry UIET, Maharshi Dayanand University, Rohtak-124001
E-mail : s_khatkar@rediffmail.com

The complex $Eu(TTA)_3$.diph (where TTA = 2-Thenoyl trifluoroacetone and diph = 5,6-Dimethyl-1,10-phenanthroline) was synthesized and characterized by infra red spectroscopy, ^{1}H NMR spectroscopy, TGA/DTA, scanning electron microscopy, elemental analysis and energy dispersive analysis (EDS). This complex had regular shaped particles with size less than 1µm without any phase separation and on excitation at 370 nm emits bright red luminescence with main peak at 612 nm. The complex emitting red luminescence might be used to make the electroluminescent (EL) devices for display purposes.

OP-08 : Synthesis, Characterization and Antimicrobial Evaluation of Some Novel Alkyl Derivatives of 2-(1H-azol-1-yl)-N-(substituted phenyl) Acetamides

Ambarsing P. Rajput*[a] and Rambhau P. Gore[b]

[a]*Department of Chemistry P.G. Research Centre, Z. B. Patil College, Dhule, 424002 (M.S.)*
[b]*School of Chemical Technology, North Maharashtra University, Jalgaon, 425001 (M.S.)*
E-mail : aprajput@rediffmail.com, gorerp@gmail.com

The N-alkylation of some secondary amides, 2-(1H-azol-1-yl)-N-(substituted phenyl) acetamides, was carried out under different conditions basic, microwave and Mannich reactions. Some studies on N-alkylation of amides have shown the complex nature of N-alkylation reaction, majority of methods are having limitations such as harsh reaction condition, functional group tolerance, low yield and less selectivity, along with N-alkylation facilitates O-alkylation, C-alkylation and C, N-dialkylation due to ambident properties of amide anions.

Relatively few reports are on studies of anions in which there is competition between C and heteroatom usually O, N, S have been reported.

Considering all the possibilities of N-alkylation we tried alkylation in some azole amides 2-(1H-azol-1-yl)-N-(substituted phenyl) acetamides. The synthesis strategy is proved simple in ambident nature substrate and selectively yields tertiary amides in moderate yields. The biological activity data showed that the secondary amides are more active than the tertiary one.

OP-09 : Metal Triflate : A Simple and Efficient Catalyst for the Synthesis of Quinoxalines

L. N. Sharada*, D. Sumalatha, B. Sammaiah and G. S. S. N. Reddy

Department of Chemistry, Osmania University, Hyderabad-500007
E-mail : lnsharada@gmail.com

Quinoxalines are a versatile class of nitrogen containing heterocyclic compounds and they constitute useful intermediates in organic synthesis and medicinal chemistry. Quinoxaline derivatives possess a broad spectrum of biological activities including anti-bacterial, anti-viral, anti-inflammatory, anti-cancer, and kinase inhibitors. In addition, quinoxaline derivatives have been evaluated as anthelmintic agents, semiconductors, dyes and biocides. Therefore, a variety of synthetic strategies have been developed for the preparation of substituted quinoxalines. Conventionally, quinoxalines synthesis can be achieved by the reaction of *ortho*-pheny lenediamine with two-carbon synthones such as α-dicarbonyls, α-halogeno carbonyls, α-hydroxycarbonyls, α-azocarbonyls, epoxides, and α, β-dihalides. Among the reported procedures, the most common method is the condensation of an aryl-1, 2-diamine with 1, 2-diketone compounds in refluxing ethanol or acetic acid or using different catalysts and reaction conditions.

The development of simple, convenient environmentally benign and improved method for the synthesis of quinoxalines derivatives would certainly be useful in generating combinatorial libraries for drug discovery. As part of our research program, we have developed a simple and efficient methodology for the synthesis of Quinoxalines using Phenacyl bromide and *ortho*-phenylene diamine in presence of a mild Lewis acid metal triflate as a catalyst.

OP-10 : Application of Organobismuth (III) Compounds Synthesized via Diazotization Route in N-arylation of Amines Under Copper Catalysis

Balaso D. Jadhav and Satish K. Pardeshi*

Department of Chemistry, University of Pune, Ganeshkhind, Pune-411007
E-mail : skpar@chem.unipune.ac.in

The synthesis of diazonium salts of different aromatic amines is done by diazotization reaction at 0-5°C and they are trapped as a ion pair by using acidic solution of trivalent bismuth salt. The ion pair complexes are well characterised by FT-IR spectroscopic technique and melting point measurement. These complexes were decomposed to stabilized R_2BiCl or $RBiCl_2$ type intermediates by metalic copper/ zinc powder as a reducing agents. Solvents like ethanol, dimethyl sulphoxide in combination with sodium iodide are used to get mono or dichlorobismuthine. In order to get the maximum conversion of the aryl diazonium salts to corresponding organobismuthines, hydrazine hydrate reduction was employed. Reaction condition was optimised in Dimethyl sulphoxide to avoid the hydrogenation of aryl radical formed during reaction in comparision to hydrogen donar solvent like ethanol. The organobismuth compounds are isolated and well characterized by FT-IR, ^{1}HNMR and ^{13}CNMR spectroscopic techniques.The synthesized organobismuthines are used in N-arylation of amines under neutral conditions catalysed by copper powder at room temperature. This method gives high yields of corresponding N-aryl amines which finds applications in the pharamaceutical industry.

OP-11 : Self Compacting Concrete : Concrete of the Future

Anuradha Varshney and Nalini Jain

Department of Chemistry, Dayanand Girl's PG College, Kanpur
E-mail : anurmc@gmail.com

Self Compacting concrete is the greatest advancement and most revolutionary development in concrete technology over last 30 years. Self compacting concrete is the concrete which flows under its own weight without any segregation and maintaining its homogeneity through all shapes and obstructions, without any need of vibrations. Self compacting Concrete requires low yield stress and high resistance to segregation (high viscosity). Addition of water decreases the yield stress but lowers the viscosity. Superplasticizers also lowers the yield stress, but slightly. Viscosity of the mix can be improved by taking a proper mix design. Addition of viscosity modifier, when added, increases yield stress of the paste. An attempt has been made to use modern superplaticizers (based on carbolxylic ethers) which promotes good workability due to electrostatic repulsion in combination with steric hindrance. Increased quantity of polymer admixture and use of flyash gives Self Compacting Concrete with higher slump. Various testing methods used are : Slump flow Test, L Box Test and Fill box Test.

OP-12 : Cost Effective Hardener for Epoxy Resin Based on Fatty Acid

Firdous Habib and Madhu Bajpai

Department of Oil & Paint Technology, Harcourt Butler Technological Institute (HBTI) Nawabganj, Kanpur 208002
**E-mail : firdaus24@gmail.com*

At present epoxy resins are extensively used in technical applications such as coatings, composites and as structural adhesives. There is a lot of scope and need for improving the properties of epoxy resins to be used in advanced applications. For example, epoxy resin with superior thermal stability is needed for using as molding compounds and encapsulation materials in advanced electronic components. Generally, modifying epoxy resin with polyamides or imido compounds provides a convenient approach of enhancing the thermal stability of epoxy resins. Therefore, epoxy resins were cured with reactive polyimides polyamic acid and imidomodified curing agents to introduce imide structure into epoxy resin. The present project deals with synthesis and characterization of dimer fatty acid base hardener known as for two component epoxy resin. Since dimmer fatty acid is a natural produce and eco friendly product and available abundantly, along with environment friendly it is also a cost effective. Such hardener can be synthesized by Primary amines for example Diethylene triamine (DETA) and Triethylentetramine (TETA). Polyamide resin is produced by the reaction of dimer fatty acid and amine has excellent resistance towards good solvent, acid, water both distilled and saline and alkali.

OP-13 : Design of New Leads Against Ubiquitin Like Enzyme RV1 : A Novel Drug target of Cancer

Ramatenki Vishwanath, U. S. H Raghavendra Prasad,
Sarita Rajender P., Ramakrishna Dumpati and Uma Vuruputuri*

Department of Chemistry, Nizam College, Osmania University, Basheerbagh, Hyderabad - 500001
E-mail : vuma1957@gmail.com; vuma@osmania.ac.in

Cancer prevention is a global precedence, but history indicates that the journey towards achieving the goal is complicated. Ubiquitin dependent proteolysis by the 26s proteasome plays a crucial role in cell cycle progression as well as in tumorigenesis. In this pathway

RV1 binds with ubiquitin ligase (E3) and transfers ubiquitin to the specific substrate protein. However, it is predicted to be a potential contributive factor for ubiquitin conjugation enzyme to control tumorigenesis.

In the present study the enzyme RV1, is targeted for designing a new lead compound against cancer. The enzyme RV1 3D model was generated by comparative modeling techniques using Modeller 9v7. The generated 3D-structure of the RV1 was validated and active site was identified using software tools and literature. The active site was considered for structure based virtual screening of small molecules using an in-house library. Insilico screening of the molecules against RV1 was carried out using virtual screening work flow of Schrödinger suite. The new leads are identified as potent RV1 antagonist for cancer therapy.

OP-14 : Novel Application of Dimethylamino-methylene Ketone Intermediate in the Synthesis of Pyrimidino Substituted Derivative of 1,4-Benzodiazepin-5-carboxamide linked at its 2-Position Through a Oxyphenyl Spacer

Navjeet Kaur, Pratima Sharma, Aastha Pareek and D. Kishore

Department of Chemistry, Banasthali University, Banasthali-304022 (Raj.)
[*]E-mail : nvjithaans@gmail.com

A survey of literature on the synthesis of this material revealed that the reaction of methanolic solution of hexamine on N-chloroacetylisatin provided an every convenient synthetic entry to this nucleus. Under these conditions, the lactam function of N-chloroacetylisatin undergoes a facile cleavage of the ring to give the ring opened product whose concurrent cyclocondensations leads to ring enlargement to form the seven membered ring of the 1,4-benzodiazepine nucleus with a carbomethoxy substituent at the 5-position in 3. The reaction of the carbomethoxy function of 3 with N-methylpiperazine produced the corresponding C_5-carboxamido derivative. This on treatment with $POCl_3$ + dimethylaniline formed the corresponding 2-chloro derivative whose subsequent reaction with p-hydroxyacetophenone afforded its incorporation on 2-position of 1,4-benzodiazepine nucleus to give. 6 reacted smoothly with commercial dimethylformamide dimethylacetal to yield the corresponding dimethylaminomethylene ketone derivative. The intermediate 7 underwent a facile cyclocondensation reaction with urea and thiourea to generate the desired pyrimidine derivatives 8 and 9 respectively in good yield. The structure of the compounds had been established on the basis of IR, ^{1}H NMR, ^{13}C NMR and MS spectral data. The exploration of the biological properties of derivatives are in progress.

OP-15 : Preparation, Charaterization and Ion-Exchange Properties of 2-Hydroxyacetophenone-Melamine- Formaldehyde Terpolymer Resin

W. B. Gurnule[a*] and R. H. Gupta[b]

[a]*Department of Chemistry, Kamla Nehru College, Sakkardara,*
Nagpur 440010, Maharashtra
[b]*Department of Chemistry, Laxminarayan Institute of Technology,*
Rastrasant Tukdoji Maharaj Nagpur University, Nagpur 440010, Maharashtra

The terpolymer resin 2-HAMF has been synthesized by the condensation of 2-hydroxyacetophenon and melamine with formaldehyde in 2:1:4 molar ratio in presence of 2M hydrochloric acid as catalyst. The newly synthesized copolymer resin has been characterized by UV-visible, IR and proton NMR spectral studies. The copolymer 2-HAMF proved to be a selective chelating ion exchange polymer for certain metals. Chelating ion-exchange properties of this polymer were studied for Fe^{3+}, Cu^{2+}, Ni^{2+}, Co^{2+}, Zn^{2+}, Cd^{2+} and Pb^{2+} ions. A batch equilibrium method has been employed in the study of the selectivity of metal-ion uptake involving the measurements of the distribution of a given metal ion between the copolymer sample and a solution containing the metal ion. The study was carried out over a wide pH range and in media of various ionic strengths. The polymer showed higher selectivity for Fe^{3+}, Cu^{2+}, Ni^{2+} than for Co^{2+}, Zn^{2+}, Cd^{2+} and Pb^{+2} ions. Study of distribution ratio as a function of pH indicates that the amount of metal ion taken by resin increases with the increasing pH of the medium. The quantitative separation of metal ions from binary Cd(II) - Pb(II) and ternary Zn(II)-Cu(II)- Ni(II) synthetic mixture were done by batch equilibrium method. The constitute of brass were also analyzed by selective sorption on column at optimized distribution coefficient values.

OP-16 : Partial Acid Hydrolysis Technique used for the Identification of Oligosaccharide from *Peltophorum ferrugineum* Benth. Seeds Polysaccharide

R. B. Singh

Department of Zoology, School of Life Sciences, Dr. B. R. Ambedkar University,
Khandari Campus, Agra-282002 (U.P.)
E-mail : rbsinghugc@gmail.com

Polysaccharide was extracted from *Peltophorum ferrugineum* Benth seeds (Caesalpiniaceae) as D-galactose and D-mannose in the molar

ratio 2:5. Plant is known as *Gulmohar ke Yellow Flower.* Present study mainly deals with the isolation and structure elucidation of oligosaccharide by partial acid hydrolysis of seeds polysaccharide with sulphuric acid and identified by paper chromatographic analysis which afforded 3-di-and 2-trisaccharides. Each oligosaccharide was characterized by their optical rotation, derivative (disaccharide), degree of polymerisation and periodate oxidation studies. Oligosaccharides were identified as: (I) 4-O-β-D-mannopyranosyl-(1→4)-O-β-D-mannopyranose, (II) 6-O-α-D-galactopyranosyl-(1→6)-O-α-D-mannopyranose, (III) 4-O-β-D-galactopyranosyl-(1→4)-O-β-D-mannopyranose, (IV) O-α-D-galactopyranosyl-(1→6)-O-α-D-mannopyranosyl-(1→4)-O-β-D-mannopyranose and (V) O-β-D-mannopyranosyl-(1→4)-O-β-D-mannopyranosyl-(1→4)-O-β-D-mannopyranose. Oligosaccharides I, III & V clearly indicates that the main polymer chain of polysaccharide is composed of D-galactose and D-mannose with (1→4)-β-type linkages. Oligosaccharide II & IV shows that the branches of main chain consists of single unit of non-reducing D-galactopyranose which are glycosidically linked to D-mannopyranose unit of main chain through (1→6)-α-type linkages. Oligosaccharide II supports the fact that branches of main chain consist of D-mannopyranose unit linked together with (1→6)-α-type and (1→4)-β-type glycosidic linkages. The earlier proposed seeds polysaccharide structure obtained after methylation and periodate oxidation studies from *Peltophorum ferrugineum* Benth. seeds polysaccharide has been fully confirmed by the above finding oligosaccharide results.

OP-17 : Regioselective, Photochemical Chlorination of Aromatic Compounds using *N*-Chlorosuccinimide

Prakash K. Chhattise

Department of Chemistry, H. V. Desai College, Pune-411 002
E-mail : pk3600se@gmail.com

A regioselective nuclear chlorination of aromatic compounds has been investigated using *N*-Chlorosuccinimide (NCS) as a chlorinating agent under UV irradiation (Philips HPL-N (250 W, λ_{max} = 200–600 nm) to afford the corresponding chlorinated compounds. The reaction proceeds at ambient temperature (30 ± 2 °C) in acetonitrile without any catalyst. It represents a simple and efficient method for chlorination of a wide range of mono- and di-substituted aromatic substrates under mild reaction conditions. In most of the reactions, regioselectively mono chlorinated products are obtained in good to high yields. The conversion and selectivity for mono chlorination depends upon the nature of the substituent on the aromatic ring. Optimization of the reaction conditions for photochemical chlorination of phenol with N-chlorosuccinimide is investigated as a model transformation. A simple methodology leads to regioselective nuclear chlorination with selectivity of about 78% for para chlorophenol.

OP-18 : Synthesis and Biological Evalution of Some Novel Aceto Nitrile and Acetamide Derivatives

Jayesh V. Padaliya*

Department of Chemistry, H & HB Kotak Institute of Science,
Dr. Yagnik Road, Rajkot-360 005 (Gujarat)
E-mail : jayeshpatel123@yahoo.com

Literature survey reveals that aceto nitrile are endowed with a wide range of biological activities like hypnotic antiinflammatory, antifungal, antitubercular, analgesic properties. Looking to the significant properties of aceto nitrile it was contemplated to synthesis aceto nitrile bearing therapeatically active PAS nucleus in search of more potent agents having better potency. Acetamide derivatives are well known pharmacological agents having antibacterial, antifungal, anthelminitic, analgesic, antipyretic properties. These observation gave us impetus to synthesise few novel acetamide derivatives bearing pharmalogically active thiosemicarbazide nucleus. 2-Ethoxy-4-acetamido benzoyl hydrazine was prepared by condensation of 2-ethoxy-4-acetamido methyl benzoate & hydrazine hydride. ∝–($2^{|}$ –ethoxy-$4^{|}$ – acetamido benzoyl hydrazino) – aryl aceto nitrile was further synthesised by condensation of $2^{|}$-ethoxy-4-acetamido benzoyl hydrazine with aromatic aldehyde in presence of pottasium cyanide and acetic acid at 0°C. when N-aryl chloro acetamide reacts whith $2^{|}$ –methoxy phenyl thiosemicarbazide in presence of potasium carbonate gives 3-(2 –methoxy phenyl thiosemi Carbazide) – N – aryl acetamide. The constitution of all these derivatives has been supported by elemental analysis, IR and PMR spectra. These compounds were screenes for their antimicrobial activity and most of the compounds displayed significant activity. The anticancer activity of some selected compount are tested by (SPECHEM, the Czech, Republic) for biological screening.

OP-19 : Synthesis and Characterization of N-substituted Pyrazoline Derivatives Bearing Hydroxyl Coumarine Nucleolus

Jayant Rathod[a], Bhavna Lavadia and Anamik Shah*

Department of Chemistry, Saurashtra University Rajkot
**E-mail : anamik_shah@hotmail.com, [a]jayant_rathod@ymail.com*

N-Substituted pyrazoline core structure possesses the interesting biological activities, including analgesic, antimicrobial, antiviral, anti-inflammatory and antitumor. More over coumarine derivatives found very good pharmacological activity in the field of medicinal chemistry. So it have stimulated considerable work in recent years advantage to synthetic utility of the various derivatives and large class of naturally occurring and synthetic biologically active phenolic compounds made up of benzo-2-pyrane nucleus. The above facts lead us to synthesize some pyrazole derivatives comprised with coumarine nucleolus. Series of N-substituted pyrazoline derivatives bearing coumarine moiety were prepared by using the Pechmann synthesis method followed by the esterification and reaction with hydrazine furnished hydrazide derivatives of coumarine 4-acetic acid which on cyclisation with various 1,3 diketone derivatives. All the synthesized compounds have been confirmed by spectroscopic methods such as ^{1}HNMR, IR and Mass spectrometry. Further it is confirmed by elemental analysis.

OP-20 : Synthesis, Characterization and Thermal Behavior of 4-Oxo-Thiazolidine Compounds

Dinesh R. Godhani*[1], Anand A. Jogel[1] and Anil M. Sanghani[2]

[1]Department of Chemistry, (DST-FIST sponsored Department), Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar- 364022, Gujarat

[2]Chemistry Department, Sir P. P. Institute of Science, Bhavnagar-364002, Gujarat

A series of compounds of 4-oxo-thiazolidine derivatives was synthesized by condensation reaction. These synthesized compounds have been characterized by various spectral techniques such as FT-IR, ^{1}H-NMR, ^{13}C-NMR and mass spectroscopy. The thermal stabilities of these compounds were investigated by simultaneous TGA-DSC methods. The decomposition steps and thermal behaviour of five compounds were investigated. The kinetic parameters such as order of reaction (η), energy of activation (E_a), pre-exponential factor (A), entropy of activation ($\Delta S^{\#}$), enthalpy of activation ($\Delta H^{\#}$) and free energy of activation ($\Delta G^{\#}$) were calculated using Freeman-Carroll method. The one step degradation for each compound and its correlation with thermal behaviour was also elucidated.

OP-21 : Antimicrobial Assay of Aerial Parts of *Cassia* Species

Jignasu P. Mehta*, Pravin H. Parmar, Sohil H. Vadia and Kahan I. Pandya

Analytical Chemistry Division, Department of Chemistry, (DST-FIST-sponsored Department) Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar 364002

This study was designed to evaluate the antimicrobial assay of the extracts from the aerial parts two plants of *Cassia* species *viz.*

Cassia siamea (Lam.) and *Cassia javanica* (Linn.). Total eight solvents were used to extract various secondary metabolites from aerial parts of *C siamea*, and *C javanica*. Antibacterial assay of eight extracts was done against bacteria *Staphylococcus aureus*, *Streptococcus pyogenes*, *Escherichia coli* and *Pseudomonas aeruginosa*. The results were compared against standard antibiotics. Antifungal assay of eight extracts was done against fungi strains *Candida albicans, Aspergillus niger* and *Aspergillus clavatus* and results were compared against standard antifungal agents. The overall results provided evidence that the leaf extract of *C. siamea* in acetone might be a potential source of new antimicrobial drug against gram positive and gram negative bacteria studied in present work. It is concluded from the results that phytochemicals are responsible for such inhibition of multi resistance microorganisms and four major families of phytochemicals were identified by GC-EI-MS method.

OP-22 : Chemistry of Novel Spiro Oxazolo-thiadiazoles Derivatives – Synthesis, Characterization and Biological Evaluation

Vijay Dabholkar* and Abhishek Karekar

Organic Research Laboratory, Department of Chemistry, K.C. College,
Dinshaw Waccha Road, Churchgate, Mumbai-400 020
E-mail : orlkcc@rediffmail.com

1, 3, 4-Thiadiazoles have wide applications in many fields. The earliest uses were in the pharmaceutical area as an antibacterial with known sulphonamides drugs. Some of the later uses are as antitumor and anti-inflammatory agents, pesticides, dyes, lubricants and analytical reagents. 1,3,4-thiadiazole and its derivatives possess wide range of therapeutic activities like anticonvulsant, herbicidal, pesticidal, amoebicidal, CNS depressant, antibacterial , antiviral. A mixture of Hippuric Acid and substituted aromatic aldehyde were refluxed in presence of acetic anhydride and sodium acetate to yield 4-substitutedbenzylidene-2-phenyloxazol-5-one, which further, on treatment with thiocarbohydrazide, in presence of catalytic amount of conc. sulphuric acid , to form thiocarbohydrazine derivative , which further allowed to reacted with acetic anhydride and sodium acetate, to obtained target molecule. Representative samples were screened for their anti-microbial activity against gram-negative bacteria, *E coli* and *Paeruginosa* and gram-positive bacteria, *S. aureus*, and *C. diphtheriae* using disc diffusion method.

OP-23 : Traditional use and *in-vivo* anti Inflammatory Activities of *Cassia* Species

**Jignasu P. Mehta[1*], Pravin H. Parmar[1], Sohil H. Vadia[1],
Mahendra K. Patel[2] and Chandrabhanu B. Tripathi[2]**

[1]Analytical Chemistry Division, Department of Chemistry, (DST-FIST sponsored Department) Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
[2]Department of Pharmacology, Government Medical College, Bhavnagar-364001

Cassia species are native to Southeast Asia and sub-Saharan Africa and are commonly used as food and also for a broad variety of medicinal applications. *Cassia* species are widely used in India, but there are few reports in the literature of studies on its chemical compositions and biological properties. In this study the antioxidant and anti-inflammatory activities of two plants of *Cassia* species namely *Cassia siamea* (Lam.) and *Cassia javanica* (Linn.) were evaluated and the total phenolic compounds and flavonoid contents were also determined.

The antioxidant activity of the extracts was measured using scavenging of 2, 2'-Diphenyl-1-picrylhydrazyl hydrate (DPPH), bleaching of β-carotene and % inhibition of H_2O_2. The anti-inflammatory activity was evaluated using carrageenan induced paw edema method on *Wistar* albino rats.

The etahnolic extracts of aerial parts of *C. siamea* and *C. javanica* were evaluated for *in-vivo* anti-inflammatory activity against animal model of female *Wistar* albino rats. Ethanol extracts showed significant and dose-dependent anti-inflammatory effects. The contents of flavonoids and total phenolic compounds could be correlated with the antioxidant and anti-inflammatory activities observed for *C. siamea* and *C. javanica*. Our findings suggest that aerial parts of *C. siamea* and *C. javanica* contain potential antioxidant and anti-inflammatory compounds, which could be tested as drug candidates against oxidative and inflammation-related pathological processes in medicinal chemistry studies.

OP-24 : Synthesis and Biological Studies of Oxadiazolo-thiadiazines

Vijay Dabholkar[*] and Prem Naik

Organic Research Laboratory, Department of Chemistry, K.C. College,
Dinshaw Waccha Road, Churchgate, Mumbai-400 020
E-mail : orlkcc@rediffmail.com

In recent years, interest in 1,3,4-thiadiazines has increased in connection with a high biological activity such as antimicrobial, ant irradiation and ant parasitic. In addition, 1,3,4-oxadiazole is a versatile lead molecule for designing potent bioactive agents. This interesting group of compounds possesses diverse biological activity such as antimicrobial, anti-inflammatory, antitubercular, anticonvulsant, anticancer, anti-HIV, hypoglycemic and genotoxic activities. A mixture of substituted triazoles and substituted aromatic aldehyde were refluxed in presence of alcoholic KOH to yield 4- substituted banzylideneamino-5-substituted-4H-1,2,4-triazole-3-thiol, which further, on treated with ethyl chloro acetate in presence of catalytic amount of K_2CO_3 undergoes a cyclization reaction to form tthyl 6,7-dihydro-6-substitutedbanzylidene-3-substituted-5H-[1,2,4] triazolo[3,4-b][1,3,4]thiadiazine-7-carboxylate. Furthermore undergoes a nucleophilic addition reaction with hydrazine hydrate in presence of ethanol to yield 6,7-dihydro-6-substitutedbanzylidene-3-substituted-5H-[1,2,4]triazolo[3,4-b][1,3,4]thiadiazine-7-carbohydrazid which on further treatment with carbon disulfide yielded 5-(6,7-dihydro-6-substitutedbanzylidene-3-substituted-5H-[1,2,4]Triazolo[3,4-b][1,3,4]thiadiazine-7yl)-1,3,4-oxadiazole-2-thiol. The structures of the products were confirmed by IR, ^1H, ^{13}C NMR and elemental analysis. Representative compounds were screened for their antimicrobial activity.

OP-25 : Synthesis and Microbial Evaluation of Novel Tetrazolo-triazole Derivatives

Vijay Dabholkar* **and Navnath Shinde**

Organic Research Laboratory, Department of Chemistry, K.C. College,
Dinshaw Waccha Road, Churchgate, Mumbai-400 020
E-mail : orlkcc@rediffmail.com

Azides are considered to be very important compounds due to both their industrial as well as biological applications. They have been used in rubber vulcanization, polymer cross linking, dyes, tire cord adhesives, foaming of plastics, pharmaceuticals, pesticides and herbicides. Many azide compounds show mutagenic activities. They have also been used as fungicides, herbicides, light stabilizers, fluorescent whiteners, optical brightening agents, and corrosion retardants. 5-(4'-bromomethyl-1, 1'-biphenyl-2-yl) -1H-tetrazole was converted into its azide derivative using sodium azide, which on further treatment with malonitrile, diethyl malonate, ethyl acetoacetate and isopropyl acetoacetate to yielded the respective tetrazole-triazole derivatives. The structures of the synthesized compounds were confirmed by physico-chemical test and spectral techniques, representative samples were screened for their antimicrobial activity against gram positive and gram negative bacteria.

OP-26 : Synthesis and Studies of Some Bio-active Thieno[2,3-*d*]pyrimidine Derivatives

Himanshu D. Patel[1], Keshav C. Patel[2]* and Paresh S. Patel[3]

[1]Department of Chemistry, Silvassa Institute of Higher Learning,
DNHUSS, Silvassa - 396 235 (D&NH)
[2]Department of Chemistry, Veer Narmad South Gujarat University,
Surat - 395 007(Gujarat)
[3]Department of Chemistry, Narmada College of Science and Commerce,
Zadeshwar, Bharuch - 392011(Gujarat)
E-mail : himanshu4p_2765@yahoo.com

Several thieno[2,3-*d*]pyrimidine derivatives were synthesized from 2-aminothiophene-3-carboxylic acid esters analogs. The formed compounds have been evaluated by physical methods (melting point and elemental analyses) and upon spectral data (IR and NMR). All newly synthesized compounds have been tested for their antibacterial activity against gram (+)ve and gram (-)ve bacteria and also on different strains of fungi.

OP-27 : Synthesis, Characterization and Antimicrobial Activity of Some New Benzimidazole Containing Sydnone Derivatives

Vikunjana K. Akbari[a], Himanshu D. Patel[b], Shreyas A. Patel[a] and Keshav C. Patel[*]

*[*a]Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007, Gujarat*
[b]Department of Chemistry, Silvassa Institute of Higher Learning, Dnhuss, Silvassa.

A series of sydnone derivatives, namely 3-(4-chlorophenyl)-4-{2-(substitutedphenyl)-1*H*-benzo[d]imidazol-1-ylsulfonyl}sydnones 9(a-j) were synthesized starting from 4-chloroaniline 1. The characterization of the newly synthesized compounds was established by IR, ^{1}H NMR, ^{13}C NMR and Elemental analysis. All the compounds were screened *in vitro* for their antimicrobial activity against several microbes.

OP-28 : Mass Spectrometric Identification of Supramolecular Assemblies

Naisargee Parikh and Asit K. Chakraborti

National Institute of Pharmaceutical Education and Research (NIPER),
S.A.S. Nagar, Punjab - 160062
E-mail : naisasargiparikh@yahoo.co.in

Understanding the reaction mechanisms is a very tactful task for organic chemists as it offers us insights into how molecules (substrates, substrate-catalyst, substrate-solvent) react, enable us to manipulate the course of known reactions, aid us in predicting the course of known reactions using new substrates, and help us to develop new reactions and reagents. In order to underline the reaction mechanisms, identification of reactive intermediates and its characterization by various analytical techniques has become essential to validate the proposed mechanism. Among various analytical techniques, mass spectrometry (MS) is gaining priority as an analytical tool to analytical/organic/pharmaceutical chemists and biologists due to its appealing features like ability to identify short lived non covalent species or ion, ease of sample preparation, operational simplicity and ease of spectral interpretation. Mass spectrometric technique holds the place at the crucial stage of analysis such as structural confirmation, purity determination, and conversion. Often interpretation/prediction of the desired product depends upon the understanding of the reaction mechanism. The MS techniques particularly ESIMS is a solution provider towards this end through 'ion fishing' of charged species as reactive intermediates. However, revealing reaction pathways that proceed through noncovalent short lived species remains the challenging task and MALDI and ESI MS techniques are being increasingly used for the purpose that adds a new dimension to analytical techniques. This presentation will summarise about a special application of ESI-MS to 'fish' the noncovalent complextion directly from solution phase to gas phase that gives insight into the reaction mechanism and proves it on the basis of trapped reactive intermediate.

OP-29 : Synthesis and Characterization of Some New Pyrazole Containing 4-oxothiazolidine Derivatives Endowed with Broad Spectrum Antimicrobial Potency

G. M. Kotadiya, V. V. Joshi and N. C. Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@rediffmail.com

The emergence of microbial strains resistant to the present antibiotics highlights the need for search of new antimicrobials. In continuation to this, the present paper deals with the synthesis and antimicrobial activity of a novel series of 2-(5-(3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl)-3-(aryl)-4,5-dihydro-1H-pyrazol-1-yl)thiazol-4(5H)-ones. The structures of these compounds were characterized by IR, ^{1}H-NMR, ^{13}C-NMR and mass spectra. All bio-active molecules were tested for their *in vitro* antimicrobial activity by serial broth dilution method. Compounds were screened for *in vitro* antibacterial activity against the representative panel of Gram-positive (*Staphylococcus aureus*, *Streptococcus pyogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria. All newly synthesized compounds were also tested for their inhibitory action against three strains of fungi (*Candida albicans*, *Aspergillus niger*, *Aspergillus clavatus*) and have exhibited moderate to excellent growth inhibition of bacteria and fungi. On basis of statistical analysis, it was observed that these compounds showed significant co-relation.

OP-30 : Efficient Synthesis of Thiazolidin-4-one, Quinoline and Barbitone Hybrids as New Scaffold with Antimicrobial Interest

H. M. Satodiya and N. C. Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

In the present investigation, it was of interest to synthesized some new derivatives containing 1-(2-(5-((2-chloroquinolin-3-yl)methylene)-2-(2-hydroxyphenylimino)-4-oxothiazolidin-3-yl)-2-oxoethyl)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione moiety incorporated with different biologicaly active heterocycles such as thiazolidin-4-one, barbitone and 2-chloroquinoline-3-carbaldehyde derivatives. The structures of synthesized compounds were elucidated by IR, ^{1}H NMR, ^{13}C NMR, and mass spectral data. The newly synthesized final compounds were evaluated for their *in-vitro* antibacterial and antifungal activities. Preliminary results indicated that most of the compounds demonstrated moderate to good antimicrobial activity, comparable to standard drugs. Structure–activity relationship studies revealed that the nature of the substituent at the 6th and 8th positions of the quinoline nucleus had a significant impact on the *in-vitro* antimicrobial activity of this class of potent antimicrobial agents.

OP-31 : Synthesis of Promising Antimicrobial Agents: A New Class of n-(5-phenyl-1, 3, 4-thiadiazol-2-yl) Carboxamide Derivatives

Ramesh Senta, Mitesh Pandya and N C Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

Some new substituted N-(5-Phenyl-1, 3, 4-thiadiazol-2-yl) carboxamide derivatives have been synthesized and evaluated for their in vitro antimicrobial and antifungal activities on *Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Staphylococcus pyogenes, Candida albicans, Aspergillus niger*, and *Aspergillus clavatus*. Some of the molecules have exhibited significantly potent inhibition on several strains of microbes. The structures of the compounds were elucidated by IR, NMR, and Mass spectra.

OP-32 : A New Synthetic Approach and *In Vitro* Antimicrobial Evaluation of Imidazoline Incorporated Thiazolidine Motifs

Hasit V. Vaghani, Vivek V. Joshi and N. C. Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

The emergence of microbial strains resistant to the present antibiotics highlights the need for search of new antimicrobial. In continuation to this, the present paper deals with the synthesis and antimicrobial activity of a novel series of 2-[1,2-diaza-3-(4-{4-[(aryl)methylene]-2-(4-nitrophenyl)-5-oxo(2-imidazolinyl)}phenyl)but-2-enylidene]-1,3-thiazolidin-4-ones. The structures of these compounds were characterized by spectral (IR, ^{1}H-NMR, ^{13}C-NMR, mass spectra) analysis. All bio-active molecules were tested for their *in vitro* antimicrobial activity by bioassay namely serial broth dilution. Compounds were screened for *in vitro* antibacterial activity against the representative panel of Gram-positive (*Staphylococcus aureus*, *Streptococcus pyogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria. All newly synthesized compounds were also tested for their inhibitory action against three strains of fungi (*Candida albicans*, *Aspergillus niger*, *Aspergillus clavatus*) and have exhibited moderate to excellent growth inhibition of bacteria and fungi. On basis of statistical analysis, it was observed that these compounds showed significant co-relation.

OP-33 : Synthesis and Characterization of Some 2-thioxothiazolidine, Quinoline Derivatives as Potential Antimicrobial Agents

Malay Bhatt, Niraj Shihory and N. C. Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

Several new substituted {4-[1-aza-2-(aryl)vinyl]-3-phenyl-2-thioxo(1,3-thiazolin-5-yl)}-*N*-[1-aza-2-(2-chloro-8-methyl(3-quinolyl))vinyl]carboxamides derivatives have been synthesized and evaluated for their in vitro antimicrobial and antifungal activities on Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, Staphylococcus pyogenes, Candida albicans, Aspergillus niger, and Aspergillus clavatus. Some of the molecules have exhibited significantly potent inhibition on several strains of microbes. The structures of the compounds were elucidated by IR, ^{1}H NMR, ^{13}C NMR, and Mass spectra.

OP-34 : Synthesis, Characterization and Antimicrobial Evaluation of Some Benzimidazolyl Pyridine Carbonitriles Incorporated Thiazolidinone Derivatives

Kandarp Bhatt, Darshan Pandya and N C Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

A series of 6-benzimidazol-2-yl-4-(aryl)-2-[2-(3-nitrophenyl)-4-oxo-(1,3-thiozolidin-3-yl)]pyridine-3-carbonitrile derivatives were synthesized in good yields by a multi-step synthetic procedure.. All the synthesized compounds were screened for in vitro antibacterial and antifungal activities on against *Escherichia coli* (MTCC-442), *Pseudomonas aeruginosa* (MTCC-441), *Staphylococcus aureus* (MTCC-96), *Streptococcus pyogenes* (MTCC-443), *Candida albicans* (MTCC-227), *Aspergillus niger* (MTCC-282) and *Aspergillus clavatus* (MTCC-1323) by serial broth dilution. The structures of the compounds were elucidated by IR, ^{1}H-NMR, ^{13}C-NMR, and Mass spectra. On basis of statistical analysis, it was observed that these compounds showed significant co-relation.

OP-35 : Synthesis and Antimicrobial Activity of Clubbed 1, 3-benzoxazine and 2-oxopyridine (2-pyridone) Derivatives

Hardik Somani, Nayan Bhatt and N. C. Desai*

Division of Medicinal Chemistry, Department of Chemistry, Mahatma Gandhi Campus, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar-364002
E-mail : dnisheeth@gmail.com

The emergence of microbial strains resistant to the present antibiotics highlights the need for search of new antimicrobial. In continuation to this, the present paper deals with the synthesis and antimicrobial and antifungal activity of a novel series of 1-[2-(4-(2*h*,4*h*-benzo[*e*]1,3-oxazin-3-yl)phenyl)- 1-azaprop-1-enyl]-2-[1-aza-2-arylvinyl]-6-oxo-4-phenylhydropyridine-3,5-dicarbonitriles. The structures of these compounds were characterized by spectral (IR, ^{1}H-NMR, ^{13}C-NMR, mass spectra) analysis. All bio-active molecules were tested for their *in vitro* antimicrobial activity by bioassay namely serial broth dilution. Compounds were screened for *in vitro* antibacterial activity against the representative panel of Gram-positive (*Staphylococcus aureus*, *Streptococcus pyogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa*) bacteria. All newly synthesized compounds were also tested for their inhibitory action against three strains of fungi (*Candida albicans*, *Aspergillus niger*, *Aspergillus clavatus*) and have exhibited moderate to excellent growth inhibition of bacteria and fungi. On basis of statistical analysis, it was observed that these compounds showed significant co-relation.

OP-36 : Green Nanotechnology : Towards Synthesis of Pharmaceutically and Biologically Pertinent Moieties

A. Dandia*, **S Bhaskaran, S. L. Gupta and V. Parewa**

Centre of Advanced Studies, Department of Chemistry, University of Rajasthan, Jaipur-302004
E-mail : dranshudandia@yahoo.co.in

In view of ever increasing demand for novel medicinally active compounds, the most important goal for chemists is to ensure that the next generation of synthetic protocols for drugs and fine chemical synthesis is more sustainable and greener than the current generation. Thus, we modified the laborious process of lead discovery by accumulating Green methodologies and nanotechnology in combination with aqueous media which disguised as the natures reaction enforcers for synthesis “in water” and “on water”. This resulted in synthesis of a wide variety of novel spiro heterocycles and biologically important scaffolds via facile tandom reactions using non-conventional energy sources, e.g., ultrasound and infrared radiation, which dramatically reduced chemical waste and reaction times along with increased selectivity of the process. Furthermore, the procedure is found to be capable of generating multiple bonds in single step with simultaneous generation of spiro and chiral center in single reaction which enhances the biocidal profile or may create new medicinal properties.

PHARMACEUTICAL CHEMISTRY SECTION

Sectional President's Address

PCIL-01 : Pharmacological Importance of Quinolone Analogous : Their Synthesis and Antimicrobial Activities

Navin B. Patel

Department of Chemistry, Veer Narmad South Gujarat University,
Surat-395 007, Gujarat
E-mail: drnavin@satyam.net.in

Fluoroquinolones are broad spectrum antimicrobial agents. They are DNA gyrase, topoisomerase IV inhibitors, which cause an interruption in DNA supercoiling. Long DNA can not longer remain in the cell without supercoiling, results in bacterial death. Study of structural activity relationships provided scope to perform structural variation at C-3, C-6, C-7 positions of 4-quinolones as amides of fluoroquinolones and pyridoquinolones. New synthetic route was developed for fluoroquinolone their analogous especially on C-3 position have been carried out and also synthesized pyridoquinolones.

The structural activity relationship performed after the study of antimicrobial activity against Gram positive, Gram negative and fungal microbes for library of 4-quinolones and pyridoquinolones.

PCIL-02 : Generic Pharmaceuticals – Facts, Hurdles and Advantages

R.R. Soni

Adventus Laboratories India Private Limited, 495/7, GIDC, Makarpura,
VADODRA. 390010
E-mail : rohitsoni@adventus.co.in

Generic Pharmaceuticals are identical or within the acceptable bioequivalence range to the branded pharmaceuticals with respect to Pharmacokinetic and Pharmacodynamic properties. The key note in lecture describes the advantages, disadvantages and hurdles of Generic drugs for approval of generic drug.

PCIL-03 : Perspectives and Challenges in Drug Stability : Bringing Chemists and Pharmaceutical Scientists Together

Sharwan K Dewan

Department of Chemistry, M.D University, Rohtak, Haryana-124001
E-mail : sharwankumardewan@yahoo.com

The Stability of the drug products is directly related to well-being of patients. Problems associated with drug stability can have serious clinical consequences. The inconvenience, discomfort and expenses associated with the use of subpotent drugs or those with a range of potencies are unacceptable. The drug products can undergo degradation. Drug Products safety, efficacy and quality are of utmost importance. Drugs are susceptible to many types of degradation-Physical, Biological including Microbiological etc. Many drugs undergo chemical degradation when formulated in either liquid or solid dosage forms leading to a reduction in their potency. That is why there are strict drug stability regulations. Naturally, a question arises about enhancing the stability of drug products. Evidently, that can be best done by preventing decomposition of the products which can be achieved only when we know the mechanism of their degradation. The idea behind this lecture is to inspire chemists to work in collaboration with pharmaceutical scientists for the well-being of patients-human and vet.

PCIL-04 : Iodine Deficiency Disorder : Diagnosis and Therapy

N. S. Rajurkar

Department of Chemistry and Department of Environmental Science
University of Pune, Pune 411 007
E-mail : rajurkar@unipune.ac.in

Iodine is an essential trace element and is of much interest in nutritional research. It is essential for the production of the hormones in the thyroid gland. However, deficiency or excess of iodine can cause disorders, commonly known as iodine deficiency disorders. The safe and adequate intake of iodine is in the range of 50-200 $\mu g.d^{-1.}$ Iodine deficiency disorders can cause a spectrum of disorders like mental retardation and stunted growth in children, hair loss and other effects in adults. In a recent survey it has been reported that, in India, out of 324 districts surveyed, 264 have been found to be endemic for iodine deficiency disorders (IDD). There are several cases of goiter reported in Maharastra. Children and pregnant women are found to be more susceptible to IDD. The talk will cover different methods used for the diagnosis of the IDD, the emphasis will be given on radioimmuno assay technique. Treatment measures for treating the iodine deficiencies will also be discussed.

PCIL-05 : Studies on Chemotherapeutically Potential Heterocyclic Class of Privileged Scaffolds and their Combinations, Prediction of their Bioactivity, Biological Evaluation and their Structure Activity Relationships : Syntheses of Some Alkoxy Derivatized Novel Combinations

G. L. Talesara

Department of Chemistry, M L Sukhadia University, Udaipur (Raj.) 313001
E-mail : glntalesara@yahoo.com

Current interest of medicinal scientist is focused on design and synthesis of new drugs with improved pharmacokinetic properties. Heterocycles have been recognized as privileged structure and emerged guiding principal for modern drugs discovery. Intense global efforts have been under way to develop biologically active material from various heterocycles. Heterocyclic chemistry has increased great prominence over the years in the field of research. The presence of one or more hetero atoms within the carbocyclic analogues are accountable for better biological activities in the heterocycles. It has been apprised that more than 60-65% of all published research paper and reviews of chemical studies deal in one or another way with heterocyclic systems. Heterocyclic chemistry persist an interesting psychology as it is a vast and expanding area of chemistry due to multiple applications of their compounds in pharmacy, medicine, agriculture and other fields. Their study is of great interest both from the theoretical as well as practical standpoint. It may fairly be said that heterocyclic chemistry although cover one third of all organic chemistry, has started to receive as much attention as it merits.

About half of the ten million or so compounds recorded in the chemical abstracts are heterocyclic. Working on oxygen substituted hydroxylamine derivatives a number of medicinally important molecules have been synthesized by our research group and tested for various biological activities *viz* antimalarial, antibacterial, antifungal, anticancer, antiviral, anti-inflammatory, antitubercular *etc.* Histological and cytotoxic effects of synthesized compounds have also been investigated.

Few series of N-ethoxyphthalimido 3-(4-substitutedphenyl)-6,6-diphenyl-3,3a-dihydro-2H-imidazo[2,1-b]pyrazolo[3,4-d][1,3]thiazol-7(6H)-one, 4-(4-substituted phenyl)-2-(N-ethoxyphthalimidoamino)-7,7-diphenylimidazo[20,10:2,3][1,3]thiazolo[4, 5-d]pyrimidin-8(7H)-one,3-{[7-

(2,4-dichlorophenyl)-5-(4-methoxyphenyl)]pyrido[2,3-d]pyrimidin-4-yl}-2-substituted -imidazolidin-4-one ,8-[(1*N*-ethoxyphthalimido-2-oxo-1,2-dihydro-3*H*-indol-3-ylidene)amino]-3,6-bis(substitutedphenyl)-1,3,3*a*,9*a*-tetrahydro-isoxazolo[3',4':4,5][1,3] thiazolo[3,2-*a*]pyridine-5,7-dicarbonitrile , *N*-(5,7-dicyano-3,6-bis(substitutedphenyl)-2*N*-ethoxyphthalimido-2*H*,6*H*-pyrazolo[3',4':4,5][1,3]thiazolo[3,2-*a*]pyridine-8-yl) benzamides and many other have been synthesized in our research programme & tested for their biological activity. Activities of these compounds have been estimated/predicted/computed using various software techniques including PASS and assayed/evaluated/screened activities have been compared with above and a correlation have been established in order to achieve structure activity relationship, in the field of drug design.

PCIL-06 : Recent Advances in Pharmaceutical Sciences-Green Chemistry

K. R. Desai

Department of Chemistry, Ukatarsadia University, Bardoli, Surat,
E-mail : k_r_desai@rediffmail.com

We have to adapt and respond to new challenges more rapidly than ever before. Delay is no longer an option. We are learning that we need to innovate solutions and systems that are both locally appropriate and globally relevant.

Discovery of a new drug is a time consuming and very expensive business. Only one out of 5000 compounds may have a chance to be placed on the shelf of a chemist. It has been estimated that it takes 8-10 years of sustained efforts of chemists, pharmacologists and physicians to bring a new product in to the market as a drug. Despite the high cost, efforts are being continuously made to develop new drugs as the annual global sale of drugs crosses US $ 500 billion.

We live in times of major change. We are constantly learning more and at the same time becoming aware of how much we do not know about our global system.

The demands for green and sustainable synthetic methods in the fields of pharmaceutical industries, healthcare and fine chemicals combined with the pressure to produce these substances expeditiously and in an environmentally benign fashion, pose significant challenges to the synthetic chemical community. Green chemistry protects the environment, not by cleaning it up but by inventing new chemistry and new chemical processes that do not pollute. This objective can be achieved through the development using green chemistry techniques like Microwave heating, supercritical carbon dioxide as an important commercial, industrial green solvent, Ionic liquid, Sono chemistry, aqueous hydrogen peroxide for clean oxidation, super critical water oxidation, Biocatalyst in chemical synthesis, Biofuel, Hydrogen fuel etc.

PCIL-07 : Docking, Synthesis, Antioxidant and Anticancer Studies of Cyclic Heptapeptide *Wainunuamide* and Its Analogues Using Solution Phase Technique

M. Himaja

Pharmaceutical Chemistry Division, School of Advanced Sciences, VIT University, Vellore-632014.
E-mail : dr_himaja@yahoo.com

Wainunuamide was isolated by Marcel et al. in 2005 from the Western Pacific marine sponge *Fijian* species. It is a cyclic heptapeptide: cyclo-[L-phenylalanyl-prolyl-histidyl-prolyl-prolyl-glycyl-leucine]. The isolated *Wainunuamide* exhibited strong *in vitro* cytotoxicity against A2780 ovarian tumour and K562 leukaemia cancer cell line.

Wainunuamide and its analogues were designed by Schrodinger drug design software. Following analogues were designed by incorporating D-proline, thiazole and oxazole moieties in the ring:

- Cyclo-[D-prolyl-L-phenylalanyl-prolyl-histidyl-prolyl-prolyl-glycyl-leucine]
- Cyclo-[thiazolyl-L-phenylalanyl-prolyl-histidyl-prolyl-prolyl-glycyl-leucine]
- Cyclo-[oxazol-L-phenylalanyl-prolyl-histidyl-prolyl-prolyl-glycyl-leucine]

The designed cyclic peptide and its analogues were docked with target protein for cancer (1h2K) to predict the anticancer activity of the synthesized compounds. The results of the docking studies clearly confirm that the designed cyclic peptides are active against the cervical cancer cell lines. Based on the docking score, the designed cyclic peptides were synthesized by solution phase peptide technique using EDC/TEA in chloroform. The synthesized compounds were evaluated for antioxidant activity by DPPH method and were screened for their anticancer activities against HeLa cancer cell lines. All the synthesized compounds showed potent anticancer activity against HeLa cancer cell lines.

PCIL-08 : Pharmacologically Active Agents from Plants : Global Resurrection Opens New Opportunities

D. N. Singh

K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Faizabad-224001
E-mail : dnsinghsaket@ yahoo.com

India's traditional system of medicine, primarily based on Aurveda has been exploited by companies in the west by filling patents. It was estimated that a majority of the patents granted by the US PTO and EPO on medicinal plants were plants of Indian origin and till now, India has lost over 1500 patents of medicinal plants to the west.

Pharmacologically active agents, ephedrine isolated from Chinese system of traditional medicine from *Ephedra sinica* is currently used as a decongestant and for the treatment of bronchial asthma and artemisinin isolated form *Artemisia annua* is found to be effective for the treatment of drug resistant malaria and it is first effective antimalarial drug which was discovered after chloroquin in 1940s. It has recently been found that plant products are effective in cancerprevention and major breakthrough in cancer chemotherapy was the introduction of taxol and camptothecin isolated from the bark of *Taxus brevifolia,* and *Champtotheca acuminate* respectively. Pharmacologically active compounds isolated from plants which are currently in the market for clinical use and the some active constituents isolated in our laboratory will be discussed in details.

PCIL-09 : Green Synthesis of Bis Heterocycles as Potential Pharmaceutical Agents

D. Ashok

Department of Chemistry, Osmania University, Hyderabad-500 007
E-mail : ashokdou@gmail.com

The environmental protection has become a global concern and the chemists are searching the ways of developing and applying more efficiently and environmentally benign strategies for future sustainable growth. One of the thrust areas for achieving this target is use of green chemistry. It is essentially a way of thinking rather than a new branch of chemistry. Green chemistry presents new opportunities to create better materials and products. Applications of green chemistry in the environmental protection have created conditions to improve environment and control pollution, which will breakthrough progress into environmental science. It involves pulling together tools, techniques and technologies that can help chemists in research, development and production to develop more eco-friendly and efficient products and processes, which may also have significant financial benefits. Green chemistry also aims to reduce hazards and the risk to people as well as to the environment. This involves concepts such as inherently safe design of reactions and substitution of hazardous chemicals or those that pose a high risk. In practice, green chemistry embraces concepts such as atom efficiency - designing processes to maximize the amount of raw material that is converted into the product, energy conservation - designing more energy efficient processes, waste minimization - recognizing that the best form of waste disposal is not to create waste in the first place, substitution - using safer, more environmentally benign raw materials and solvents or solvent free processes. Chemists can use their knowledge of green chemistry and its benefits to justify research into 'cleaner and greener' processes. In recent years green chemistry techniques such as Microwave Assisted Organic Synthesis (MAOS), Ultrasound Assisted Organic Synthesis (UAOS), Ring Closing Metathesis (RCM), Aqueous Phase Organic Synthesis (APOS), Solvent Free Organic Synthesis (SFOS), and Enzyme Catalyzed Organic Synthesis (ECOS) attracted the attention of chemists. The salient features of these methodologies are enhanced reaction rate, easy workup, high yields, operational simplicity, greater selectivity and experimental ease of manipulation, low cost and economy. Organic chemistry is the heart of our society as it provides a multitude of consumer goods without which modern life would not have been possible. Organic compounds display a wide variety of pharmacological properties, many of which can be exploited for medicinal purposes and are also essential for the human well-being. Therefore methods for the synthesis of such systems are of significant interest. In view of these advantages of the above environmental benign approaches and as a part of our ongoing research programme towards the green chemistry techniques; the concept of Green chemistry has been adapted for the rapid and efficient synthesis of some novel organic compounds of pharmacological interest.

PCO-CYSA-01 : Phytochemical Scanning and Antioxidant Activity of Different Extracts of *Anthocephelus cadamba*

Ajay Gupta and Jaiswar Gautam

Department of Chemistry, Institute of Basic Science, Dr. B. R. Ambedkar University, Agra
E-mail : ajaygt18@gmail.com

Anthocephalus cadamba is an ethnomedicinally suggested medicinal plants which is used in the treatments of diseases like, fever, anaemia, leprosy, blood & skin diseases and for improvement of semen quality.

The main characteristic of an antioxidant is its ability to trap free radicals. Highly reactive free radicals and oxygen species are present in biological systems from a wide variety of sources. These free radicals may oxidize nucleic acids, proteins, lipids or DNA and can initiate degenerative disease. Antioxidant compounds like phenolic acids, polyphenols and flavonoids scavenge free radicals such as peroxide, hydroperoxide or lipid peroxyl and thus inhibit the oxidative mechanisms that lead to degenerative diseases. The present study is carried out to analyze the chemical composition of the aqueous, methanolic, acetonic, and n-hexane extracts of flowers and leaves of *anthocephalus cadamba* by GC-MS technique. The standard methods are used for preliminary phytochemical screening of these different extracts and the antioxidant activity of these different extracts are also be determined by different methods such as DPPH radical scavenging assay etc. The obtained result shows that many of these extract possess antioxidant activity.

PCO-CYSA-02 : Synthesis and Characterization of Iron Bhasma

N. S. Rajurkar*[1], Vivek Rathod[1] and Shailesh Kantak[2]

[1]Department of Chemistry, University of Pune, Pune 411007
[2]Prayag Hospital, Deccan Gymkhana, Pune - 411004
E-mail : rajurkar@unipune.ac.in

Medicinal preparation called "*Bhasma*" is unique to the Ayurvedic and Siddha system of medicine. These are made from a variety of base materials. In this paper Louha bhasma was prepared as per ayurvedic methods viz "*Shodhan*" and "*bhasmikarana*". The process of Shodhan was done by heating iron sheets till red hot and dipping it in different media i.e. tila taila, takra, gomutra, kanji, kulatha kwatha. In the process of Bhasmikarana, the purified Iron was repeatedly calcined at 700°C in different media. The characterization of the bhasma is done by using various techniques like FTIR, AAS, and XRD. The iron content of Final product was found to be 48.42%.

PCO-CYSA-03 : Synthesis, Interaction with DNA, Cytotoxicity, Cell Cycle Arrest and Apoptotic Inducing Properties of Ru(II) Molecular "Light Switch" Complexes

C. Shobha Devi, Yata Praveen Kumar, N. Deepika and S. Satyanarayana

Department of Chemistry, Osmania University, Hyderabad
E-mail : ssnsirasani@gmail.com

In an endeavor towards development of metal based anticancer drugs, we present here the design, synthesis and characterization of a ruthenium(II) functionalized phenanthroline complexes with extended π-conjugation. These complexes have been shown to act as promising DNA (calf thymus) intercalators and DNA light switches, as evidenced by UV visible, luminescence titrations, steady-state emission quenching by $[Fe(CN)_6]^{4-}$, DNA competitive binding with ethidium bromide, salt dependent studies and viscosity measurements.

All three Ru(II) complexes $[Ru(Hdpa)_2PPIP]^{2+}$ (**1**), $[Ru(Hdpa)_2PIP]^{2+}$ (**2**), $[Ru(Hdpa)_24HEPIP]^{2+}$ (**3**) where (PPIP=2-(4'-phenoxy-phenyl) imidazo[4,5-][1,10]phenanthroline), (PIP = 2-phenyl-1H-imidazo [4, 5-f][1,10](phenanathroline), (4HEPIP = 2-(4-hydroxy, 3-ethoxy-phenyl)-1H-imidazo[4, 5-f][1, 10](phenanathroline) and Hdpa(2,2'-bipyridylamine), Further, all three complexes synthesized were screened for their antimicrobial activity.Cell viability experiments indicated that the Ru(II) complexes showed significant dose dependent cytotoxicity to A549 (Human alveolar adenocarcinoma cell line), Du145 (Human Prostate cancer cell lines), HeLa (Human cervical cancer cell line) and MCF-7 (Human breast adenocarcinoma cell line). The cytotoxicity of all three complexes was evaluated by the MTT method. Ru(II) complex **1** exhibited promising growth inhibitory effects and showed slightly higher cytotoxicity than cisplatin on HeLa cells. The apoptosis and cell cycle arrest were also investigated. The complexes were docked into DNA-base-pairs using the docking program.

PCO-CYSA-04 : Electroanalytical Studies and Spectroscopic Investigations on the Interaction of An Anti-fungal Drug, Methylparaben with Bovine Serum Albumin

Keerti M. Naik and Sharanappa T. Nandibewoor*

**P. G. Department of studies in chemistry, Karnatak University, Dharwad 580003*
E-mail : stnandibewoor@yahoo.com, keertiraman@gmail.com

The electroanlytical determination of an antifungal drug, methylparaben at gold electrode has been studied by different voltammetric techniques. The oxidation of methylparaben shows an irreversible and exhibits a diffusion controlled process in phosphate buffer of pH 7.4, a physiological pH. The effect of scan rate, pH, different electrolytes, etc on electrochemical behaviour of methylparaben was investigated. A square wave voltammetry (SWV) method with reasonable accuracy and precision was developed for the assay of methylparaben in the concentration range of 0.04 to 1.0 mM with a limit of detection was 1.7 µM. The developed method was successfully applied to the determination of methylparaben in pharmaceutical products and urine as real samples. Spectroscopic techniques viz., UV–vis absorption, IR and fluorescence were employed to the interaction between methylparaben and bovine serum albumin (BSA). The binding constant and binding sites were calculated. Based on the spectroscopic results, the quenching mechanism was dynamic. The distance between methylparaben and BSA according to the Foster energy transfer and the thermodynamic parameters according to the Van't Hoff equation were calculated. The proposed study finds its applications in quality control laboratories and pharmacokinetics and may serve as a reference for the interaction of methylparaben with BSA in the natural environment of living cells.

PCO-CYSA-05 : Synthesis and *in-vitro* Anticancer Activities of 3, 4-dihydropyrimidin-2-(1*H*)–ones

D. D. Kumbhar[a], B. Y. Waghamare[a], B.A. Chopade[b], S. K. Pardeshi[a]*

[a]Department of Chemistry, University of Pune, Ganeshkhind, Pune-411007
[b]Institute of Bioinformatics and Biotechnology, University of Pune, Ganeshkhind, Pune-411007
E-mail : skpar@chem.unipune.ac.in

3, 4-Dihydropyrimidin-2-(1*H*)-ones of different groups have been prepared from a three-component one-pot condensation reaction by modified procedure of Biginelli reaction. All the fourteen synthesized 3, 4-dihydropyrimidin-2-(1*H*)-ones were characterized by different spectroscopic techniques, and subjected for their *in-vitro* anticancer activity against human epithelial cervical cancer (HeLa) cell line using Mitomycin C as standard. The title compounds were tested at the concentration of 10-100 µg. Compounds exhibited activity ranging from weak to moderate and, from moderate to high in terms of percentage cytotoxicity. Among them, compounds 5 and 6 exhibited significant anticancer activity.

PCO-CYSA-06 : Synthesis, Characterization and Biological Study of Some New Pyrimidine Derivatives from 2-Amino Benzimidazole

Shah Nirav M. and H. S. Joshi

Department of Chemistry, Saurashtra University, Rajkot-360 005
E-mail : drhsjoshi49@yahoo.com

Among the various biological active fused heterocyclic systems, the most important are those containing nitrogen ring system. A large number of heterocycles derived from chalcones and reported as active biological entities. Pyrimidine derivatives have attracted much attention as important structural motifs in medicinal chemistry owing to their significant therapeutics and biological activities. 2-Amino benzimidazole bearing NH-C-NH type component, which is used for the synthesis of pyrimidine. So, from the above facts it is worthwhile to synthesize some good potential pyrimidine compounds bearing 2-amino benzimidazole as core part.

In our present study, we have synthesized different chalcones using furfural with various substituted acetophenones. The synthesized chalcones were refluxed with 2-Amino benzimidazole, using catalytic amount of piperidine in ethanol solvent, to obtained new pyrimidine derivatives. All synthesized compounds were characterized by IR, ^{1}H NMR and Mass spectroscopy. As pyrimidine derivatives showing various types of biological activities, we have evaluate all synthesized compounds for their antimicrobial activity against gram positive and gram negative bacteria which showed moderate to good activity.

PCO-CYSA-07 : Antifungal Activity of *Amaranthus Spinosus* against Dermatophytes

Sharma K. K., Kotoky J.*

Division of Life Sciences, Institute of Advanced Study in Science and Technology, Guwahati-35, Assam
E-mail : jkotoky@gmail.com

The antimycotic effect of chloroform, methanol and water extracts from leaves and roots of *Amaranthus spinosus* Linn. (Amaranthaceae) was examined against some human pathogenic fungi, commonly involves in superficial diseases of the skin. The antifungal assay was performed by agar cup diffusion and broth macro-dilution techniques, used to determine the inhibition zones and minimum inhibitory concentrations respectively. The extracts from the roots showed slightly higher antifungal activity than the extracts from the leaves of the plant. The methanol extract of the roots exhibited strong activity against the tested fungi with inhibitions zones 33-21 mm at the maximum tested concentrations. MICs ranged between 2.5-10 mg/ml and above for the different extracts. The results showed that the plant has good inhibitory activity against the tested organisms and provides preliminary scientific validation for the traditional use of this plant against skin diseases.

PCO-CYSA-08 : CoRILISA : A Novel 3D-QSAR Formalism for Investigating the Drug-receptor Interactions

Vijay M. Khedkar* and Evans C. Coutinho

Computer-Aided Molecular Design Laboratory, Department of Pharmaceutical Chemistry, Bombay College of Pharmacy, Kalina, Santacruz (E), Mumbai
E-mail : vijaycpn@gmail.com

Molecular similarity has been extensively used in drug design, in the selection of analogs for chemicals, in the estimation of molecular properties, in the rational selection of candidates from large databases and in some QSAR approaches. Based on the similarity principle, a novel 3D-QSAR technique termed CoRILISA (derived from CoRIA and LISA) has been developed. It is an extension to our recently developed technique-LISA in a receptor-based setting finding its roots in another *in house* technique- CoRIA. The formalism is based on the calculation and comparison of similarity between the molecules (in terms of a local similarity index, LSI) at each and every residue in the receptor active pocket. The local similarity indices, calculated on the basis of Petke's formula, at all the residues surrounding the molecules are then used as descriptors in formulating the QSAR and the models are derived with genetic algorithm incorporated partial least square analysis (G/PLS) statistics. The major highlight of the method are: (a) adaptation of the QSAR formalism in a receptor setting to answer both the type (qualitative) and the extent (quantitative) of ligand–receptor binding; (b) global molecular similarity is broken into local similarity at each residue surrounding the molecules and is used as a QSAR descriptor giving an account of the complete thermodynamics of the ligand–receptor binding. The methodology was developed using the complexes of HIV-1 protease with its inhibitors as a test bed and was further validated using two additional datasets- Glycogen phosphorylase *b* (GP *b*) and Cyclin dependent kinase 2 (CDK 2) inhibitors. The QSAR models derived using G/PLS statistics are found to be comparable to the ones obtained by Comparative Residue Interaction Analysis (CoRIA), Comparative molecular field analysis (CoMFA) and Comparative molecular similarity indices analysis (CoMSIA) techniques. The primary objective is to extract not only from the reference molecule but also from the remaining ones in the series, the crucial features which contribute positively to the biological activity and to utilize them to design novel compounds and/or optimize existing leads. The CoRILISA models permit an understanding of the binding mechanisms of ligand with the enzyme and allow fine-tuning of the molecules at the local level to improve their activity. The generality of the method and the transferability of the protocol with essentially no changes to any other protein-ligand system are emphasized.

PCO-CYSA-09 : Synthesis and Pharmacological Evaluation of Newer 1,2,4-triazoles Clubbed Benzimidazoles

N.B. Patel* and Imran H.Khan

Department of Chemistry,Veer Narmad South Gujarat University, Surat (Gujarat)
E-mail : imu4u_786@yahoo.com, drnavin@satyam.net.in

The triazole analogues were obtained via. multistep synthesis sequence in beginning with tetra and pentafluoro ethyl benzoate **2** which on treatment with hydrazine hydrate yields hydrazide compound 3. Intermolecular cyclisation of 3 with various acids 4a-g in presence of phosphorous oxy chloride affords 2-(penta / tetra fluorophenyl)-5-substituted heterocycles-1,3,4-oxadiazole 5a-g and 6a-g. Condensation of 5a-g and 6a-g with 2-hydrazino benzimidazole 7 results in 3*N*-[3-(penta / tetra fluorophenyl)-5-substituted heterocycles-4*H*-1,2,4-triazol-4-yl]-1*H*-benzimidazol-2-amine 8a-g and 9a-g analogs. All the compounds have been characterized by elemental analysis, IR, ^{1}H NMR, ^{13}C NMR and mass spectral data. The compounds are evaluated for antimicrobial and antitubercular activity.

PCO-01 : Synthesis, Antimicrobial Activity, in vitro Antitubercular Evaluation and QSAR Study of Substituted Pyrimidine Derivatives Bearing the Quinoline Nucleus

Ranjan Khunt[1*]

Chemical Research Laboratory, Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : drrckhunt12@gmail.com

A new series of substituted pyrimidine derivatives bearing quinoline nucleus have been synthesized by cyclo-condensation reaction of chalcone with urea or thiourea. All the synthesized compounds were subjected to *in vitro* screening against two Gram positive bacteria (*Bacillus subtilis, Bacillus coccus*), two Gram negative bacteria (*Escherichia coli, P. Vulgaris*), fungi (*A. niger*) and antitubercular evaluation against *Mycobacterium tuberculosis H37Rv.* Reviewing the data, the compounds were found to show 25 to 95% inhibition against *Mycobacterium tuberculosis H37Rv* at *6.25* µg/ml concentration. Recursive partitioning analysis was carried out to develop a classification model for identifying structural characteristics of the molecules responsible for different affinity profiles. The decision tree derived from the classification model provided meaningful insight into structure-activity relationship in the dataset which will guide the design of improved inhibitors.

PCO-02 : Synthesis and Biological Evaluation of Imidazole Derivatives Bearing Quinoline Nucleus

Devandra Kaneria[1*] **and Ranjan Khunt**[2]

M & N Virani Science College, Rajkot
Chemistry Department, Saurashtra University, Rajkot-5
E-mail : devendrakaneriya@gmail.com

From the last decade interest has been create on fine membered heterocycles containing “N” atom due to their vast range of biological diversity. From the survey realize that immediate process antitubercular, antibacterial and anti-inflamer activity. Over above quinoline has prominent structure in the field of medicines & natural chemistry due to their pharmacological importance.

Above observation create a interest to couple imidazole with quinoline giving which may possess potent activity. To approach this goal we have synthesise series of imidazole compound bearing quinoline nucleus via series of reaction. All the synthesized product have been confirmed by spectral technique & further supported by elemental analysis.

All the synthesized compounds evaluated for their biological activity towards different strains of Gram +ve & Gram –ve bacterial & fungi also.

PCO-03 : In vitro Bioaccessibility of Minor Elements from Some Indian Medicinal Plants

N. S. Rajurkar*[1] and S.M.Hande[2]

[1]Department of Chemistry, University of Pune, Pune-411007
[2]Department of Chemistry, Haribhai.V. Desai College, Pune-411002
E-mail : rajurkar@unipune.ac.in

The present work deals with the studies on bioaccessibility of the trace elements from some Indian medicinal plants *viz. Ocimum tenuiflorum, Aegle marmelos, Casearia esculenta, Phyllanthes emblica and Eugenia jambolana* using in vitro digestion model. For this purpose initially total elemental content was determined using ICP-AES technique. Bioaccessibility of elements was then determined by in vitro gastric and gastro-intestinal digestion. Our results indicated significant changes of mineral bioaccessibility among the samples. As expected, it is observed that bioavailability during gastrointestinal digestions were higher than gastric digestion indicating higher absorption of minerals in gastro-intestinal tract at neutral pH. The total concentration of the elements was found to vary in the order Fe > Mn >Zn >Cu. Iron was found to show highest bioaccessibility.

PCO-04 : Synthesis, Characterization, Antimicrobial Studies of Certain Piperazine Containing s-Triazine Derived Compounds

K. N. Sarmah* and Talha V. Patel

Department of Chemistry, Shree Jayendrapuri Arts & Science College,
Bharuch, Gujarat. 392001.
E-mail : talha.patel9@gmail.com

Some new substituted 1,3,5-triazine with Chloro benzhydryl piperazine and substituted urea/thiourea were synthesized and evaluated for their *in vitro* antimicrobial activity against Gram positive and Gram negative strains using a microdilution procedure. Synthesized compounds 2a to 2k prove to be effective with MIC (µg/ml), among them 2b, 2d, 2g showed good activity against a panel of microorganisms. The newly synthesized compounds were characterized using IR, ^{1}H-NMR.

PCO-05 : Estimation of Selegiline Hydrochloride in Bulk and Tablets by UV Spectrophotometric Method

A. Narayana[a], C. Narasimha Rao[b], P. Venkateswarlu[b] and K. Siva Kumar[a*]

[a]*Department of Chemistry, S. V. Arts U.G and P.G College (TTD'S), Tirupati-517502, A.P.*
[b]*Department of Chemistry, S.V. University, Tirupati-517502, A.P.*
E-mail : sivakumark78@gmail.com

A simple, accurate, reproducible and cost effective Spectrophotometric method has been developed for the estimation of Selegiline Hydrochloride in bulk form and tablets. The drug was highly soluble in water, so it was selected as a solvent for estimation of Selegiline in bulk and formulations. For UV spectrophotometric method, maximum absorption was found to be at λ_{max} 205 nm.

The percentage recovery of Selegiline Hydrochloride ranged from 98.83 ± 0.08% in tablets. The developed method was validated as per ICH guidelines with respect specificity, precision, linearity and accuracy (recovery). The analysis data has been subjected to statistical analysis and the results of this study are validated. Beers law was obeyed in the concentration range of 1 to 10 µg/ml having linear equation of $Y= 0.0407x+0.0034$ with correlation coefficient of 0.9999.

PCO-06 : In vitro Studies of Chalcone Containing Pyrazolyl Quinazolin-4(3H)ones as Potential Antimicrobial Agent

N.B. Patel* and G.G. Barat[1]

**Department of Chemistry, Veer Narmad South Gujarat University, Surat-395007*
[1]*Department of Chemistry, Art's, Science and Commerce College, Pilvai(N.G.)-382850*
E-mail : drnavin@satyam.net.in; gamanbarat@gmail.com

A new series of 2-[2-(2,6-dichloro phenyl)amino]phenyl methyl-3-[(1-phenyl-5-substituted phenyl)-5-hydro-1*H*-pyrazol-3-yl-amino]-6,8-dibromoquinazolin-4(3*H*)-ones C1-13 have been synthesized by the reaction of 2-[2-(2,6-dichloro phenyl)amino]phenyl methyl-3-substituted phenyl chromen amido-6,8-dibromoquinazolin-4(3H)-ones with phenyl hydrazine in the presence of glacial acetic acid. The chalcone B1-13 have been synthesized by the condensation of 2-[2-(2,6-dichloro phenyl)amino]phenyl methyl-3-acetamido-6,8-dibromoquinazolin-4(3*H*)-one A with different substituted aromatic aldehyde. The structures of newly synthesized compounds have been confirmed on the basis of their elemental analysis and spectral data IR, ^{1}H NMR, ^{13}C NMR. All the compounds have been screened for antibacterial and antifungal activity.

PCO-07 : Use of Different Brands of Black Tea Extracts as Antioxidants : A Comparative Study

Dipti Soni, Abhilasha Tripathi, Rakshit Ameta and Suresh C. Ameta*

Department of Chemistry, Pacific College of Basic & Applied Sciences,
PAHER University, Udaipur (Raj.)
E-mail : soni_mbm@rediffmail.com

Black tea extracts show antioxidant properties. As we know that the extracts contain Epicatechin (EC), Epigallotechin (EGc), Epicatechin Gallate (ECg) and Epigallocatechin Gallate (EGCg). Dye-Sensitized photooxidation of thiourea by singlet oxygen has been carried out in presence of tea extracts of various brands. The effect of different concentrations of solution of tea extracts (prepared in ethanol and acetone) was observed based on the yield of sulphur. It was observed that in all the brands, as the concentration of tea extracts was increased, the yield of sulphur was found to decrease. On the basis of observations, it was concluded that as the concentration of tea extracts was increased, the effectiveness of tea extracts also increases.

PCO-08 : Some Thermodynamic Studies on Nicotinamide – Khellin Drug System

Himanshu Shekhar[1] and Vishnu Kant[2]

Department of Chemistry, V. K. S. University, Ara-802301
E-mail : hshe2503@rediffmail.com[1], imvishnukant@gmail.com[2]

Nicotinamide (NA), isolated from *Mallotus Faponicus* leaves and Khellin (KH), extracted from fruits of *Khella* were used as different pharmacological actions. Nicotinamide and Khellin, very small biomolecules are reported as emerging and challenging biomolecules of 21st century as different kind of therapeutic action with their marvelous activities against *Pellegra, M. tuberculosis, HIV infection, angina, vitiligo, psoriasis, renal colic, diuretic, kidney stone, coronary and bronchial asthma* etc. Nicotinamide adenine dinucleotide (NAD) and nicotinamide adenine dinucleotide phosphate (NADP) function as coenzymes in a wide verity of enzymatic oxidation-reduction reactions essential for tissue respiration, lipid metabolism and glycogenolysis. In the present communication active pharmaceutical ingredient Khellin (KH) with pharmaceutical excipient Nicotinamide (NA) has been undertaken as solid dispersed binary products. These products have been prepared through melting/fusion method. The solid-liquid equilibrium data of NA-KH system infers the formation of an eutectic (E) at 0.135 mole fraction of KH and melting temperature 120.6°C. The composition and temperature of non eutectic alloys A1-A8 have also been discussed. . The activity co-efficient model based on enthalpy of fusion is employed to calculate the excess partial and integral thermodynamic functions such as g^E, h^E and s^E. The positive value of excess Gibbs free energy predicts the stronger molecular interaction between the like molecules as compared to unlike molecules. The spontaneity of mixing of eutectic and non eutectic alloys was discussed by the partial and integral mixing quantities G^M, H^M. and S^M. The positive value of integral Gibbs free energy of mixing suggests the mixing is not spontaneous for all alloys. The critical radius r* is found in *nm* scale which may be very surprising for the drug world. The binary interface structure of alloys has been discussed in the light of Jackson model of interface structure. The surface roughness, $\alpha > 2$ predicts the faceted growth leads in all the alloys and parent components of the system.

PCO-09 : Angiogenesis : Targeting Signaling Pathways for the Identification of New Leads of Cancer

Navaneetha Nambigari, Rajender Vadija Bhargavi Kondagari and Uma Vuruputuri*

Department of Chemistry, Nizam College, Osmania University, Basheerbagh Hyderabad – 500 001. Andhra Pradesh
E-mail : vuma@osmania.ac.in, vuma1957@gmail.com

Despite continued interest of scientific community around the world in cancer research, the mortality rate remains high and cancer remains leading cause of death [1]. Tumor growth is highly dependent on the supply of oxygen, nutrients and host-derived regulators [2]. Angiogenesis is a multi-step process governed by Oncogenes that are over expressed and have been attractive targets for therapy. Pro - angiogenic factors like Angiopoietins, FGFs have been shown to be involved in various stages of angiogenesis. The emerging fields of systems biology provide methods for conceptualizing and analyzing the entire circuitry of cancer, and thus facilitate identification of specific pathways of oncogene addiction [3, 4]. The present study treats pro – angiogenic factors as novel targets for designingantagonists for specific growth factors.

Computational techniques are applied to the pro - angiogenic factors like Ang - 1 and KGF -7 proteins for identification of novel leads against cancer. The3D structural evaluation, identification of the active site and virtual screening studies were carried out using standard insilico procedures [5,6]. A case study of identification of leads for inhibition of angiogenesis against the novel targets will be discussed.

Treatment regimens that combine molecular targeted agents with other anticancer agents could provide an optimal strategy for treating and preventing cancer. The drug designing strategies having distinctive target cells and mechanisms of action, lead to an increased therapeutic efficacy with minimal toxicity.

PCO-10 : Screening of Potential Therapeutic Leads as Anatogonists for Anti-Apoptotic Protein CIAPIN1

Ramasree Dulapalli and Uma Vuruputuri*

Department of Chemistry, Nizam College, Osmania University, Basheerbagh, Hyderabad – 500 001. Andhra Pradesh
E-mail : vuma1957@gmail.com; vuma@osmania.ac.in

Cytokines regulate positively or negatively the growth, differentiation and survival of cells. Cytokines induce phosphorylation and activate cell surface kinases like tyrosine kinases. Activated tyrosine kinases transmit mitogenic and antiapoptotic signals through simultaneous activation of downstream signalling molecules including Ras/MAPK, PI3K/Akt, signal transducers and activators of transcription resulting in cancer. Cytokine-Induced Apoptosis Inhibitor 1 (CIAPIN1) is an antiapoptotic protein that mediates RAS signalling pathway[1]. The anti-apoptotic activity of CIAPIN1induces cell cycle G1/S arrest and promotes cell proliferation leading cancer. The expression of CIAPIN1 protein in cancer is responsible for drug resistance against cancer therapy. The protein CIAPIN1 is important therapeutic target for cancer[2].

In the present study comparative modeling method was used to generate the 3D structure of the CIAPIN1protein. The generated 3D structure of the protein was energy minimized, validated and active site identified[3]. Structure based virtual screening of in-house database of molecules was carried out for the protein CIAPIN1.The novel lead molecules identified were structurally optimized by docking studies and predicted ADME properties. The molecules identified are novel chemical entities that can act as potential cancer therapeutics by antagonising the activity of CIAPIN1.

PCO-11 : Synthesis, Characterization and Antimicrobial Activity of N-Substituted Tetrahydroisoquinolines via a Pictet-Spengler Approach

Arun L. Patel

Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390 002
E-mail : arunpatel_5376@yahoo.co.in

The chemistry of tetrahydroisoquinoline(THQ) alkaloids has attracted significant interest over the last few decades due to their potent biological activities. A wide range of N- substituted 1,2,3,4 - THQs has been found to be a useful starting material for the synthesis of a variety of medicinally useful compounds. The natural alkaloids are generally optically active compounds possessing antihypertensive, hemostatic, smooth or skeletal muscle relaxant, antispasmodic, antitussive, antimalarial, narcotic, analgesic or antipyretic activities. Papaverine is also a naturally occurring benzylisoquinoline alkaloid isolated from opium. Few N-acyl derivatives of papaverine and related compounds show variety of activities against AIDS, glucoma and fungal infections.

In quest for biologically more potent compounds we have synthesized few N-substituted THQ derivatives. Present work is reporting a four step synthesis that gives N-substituted THQ derivatives. Further, a new bis-isoquinoline derivative, namely, 1,2,3,4-tetrahydro-1-(4-(1,2,3,4-tetrahydro-6,7-dimethoxyisoquinolin-1-yl)phenyl)-6,7-dimethoxyisoquinoline is also synthesized. The synthesized compounds were characterized by IR, NMR (^{1}H and ^{13}C), Mass spectral data. All the compounds were screened for their antimicrobial activities.

PCO-12 : Selective Removal of Silver Impurity from Oxaliplatin by Sorption on Functionalized Polymer

Pradipta Kumar*, Khursheed B. Ansari and Vilas G. Gaikar

**Department of Chemical Engineering, Institute of Chemical Technology (ICT), Nathalal Parikh Marg, Matunga, Mumbai-19.*
E-mail : kumarpradipt@gmail.com

Oxaliplatin was first reported by Kidani et al., is an alkylating agent frequently used against metastatic colon and rectal cancer. A general method for preparation is described in U. S. pat-No-4,169,846. Oxaliplatin prepared this way is, however, accompanied with silver ion as one of the impurities. The US and EP Pharmacopeia demands, the silver content in the drug should be less than 5 ppm. It becomes, therefore, imperative that the silver content is reduced to the minimum acceptable level as it creates intense adverse effects in the therapeutic uses of oxaliplatin. Conventionally, NaI/KI are used for the removal of Ag^+ but these salts also react parallel with the intermediate product producing *cis*-mono-iodo and *cis*-di-iodo Pt(II) complexes as additional impurities and thus effectively reducing the yield of the desired product to 52%. Thus a need exists to remove Ag^+ in a more effective way without generation of side products with improved yield. Herein we report, synthesis of thiourea grafted-polystyrene resin for selective removal of Ag^+ to produce 92.8 % Oxaliplatin with a desired impurity profile for silver. The process eliminated the formation of impurities because of exceptionally high value of separation-factor ($\lambda_{Ag/Pt}$=1155) of the resin with maximum sorption capacity (Q_{max}=101.58 mg/g).

PCO-13 : Synthesis, Characterization and Anti Inflammatory Activity of Silver Nanoparticles of Diclofenac Sodium

Bhavna A. Shah[a*], Pravin S. Patil[a] and Hirva A. Shah[b]

[a]Department of Chemistry, Veer Narmad South Gujarat University,*
Udhana Magdalla road, Surat, 395007, Gujarat
[b]S K Patel College of Pharmaceutical Education and Research, Ganpat University, Kherva, Mehsana, 384012, Gujarat
E-mail : bhavna606@gmail.com

Silver nanoparticles of diclofenac sodium were prepared in alkaline medium. UV-Vis spectrophotometric, transmission electron microscopy (TEM) and viscometric techniques were used for characterization of diclofenac sodium based silver nanoparticles (SN-DS). Silver from silver nitrate solution was reduced by diclofenac sodium in alkaline condition. TEM results show spherical nature with highly dispersed aggregates of silver nanoparticle in aqueous solution. The silver nanoparticles of diclofenac sodium exhibited excellent anti inflammatory activity against acute and chronic paw models edema in mice when compare to standard diclofenac sodium.

PCO-14 : Synthesis, Solution Behaviour and Gene Transfer Activities of Novel Dimeric Surfactants Possessing Biocompatible Spacers

Kushan P. Parikh and Sanjeev Kumar*

Department of Chemistry, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390 002
E-mail : drksanjeev@gmail.com

The novel dimeric surfactants (16-s-16, s = CH_2-COO-$(CH_2)_2$-COO-CH_2 and CH_2-CONH-$(CH_2)_2$-CONH-CH_2) were synthesized (dimeric I and II, respectively). The chemical structures (Scheme) of the synthesized compounds were confirmed by FT-IR, ^{1}H NMR, ESI mass and element analysis. Micellization behavior of dimeric surfactants with various novel spacers has been studied by conductance and steady state fluorescence quenching (*SSFQ*) measurements and compared with conventional cetyl trimethyl ammonium bromide (CTAB). Critical micelle concentration (cmc) values were found nearly same for a few surfactants by both the techniques. Conductance measurements are used exclusively to obtain cmc and degree of dissociation (á) at various temperatures (278.15 to 338.15 K) while *SSFQ* measurements were used to get aggregation number (N_{agg}). A decrease in cmc and N_{agg} values and an increase in α were observed for dimeric surfactants when compared with CTAB. These surfactants were used as gene delivery agents. Dimeric surfactants induced better transfection activity than their monomeric counterpart (CTAB). This may be due to the presence of biocompatible spacer groups present in dimeric surfactants. Work is currently underway in our laboratory to assess gene trasfection potential in such type of material.

PCP-CYSA-01 : Synthesis, Characterization and *in vitro* DNA Binding Studies of Organotin(IV) Schiff base Complexes Derived from 3–formylchromone and Ethanolamine : Antibacterial Studies

Imtiyaz Yousuf, Rahman Alizadeh and Farukh Arjmand*

Department of Chemistry, Aligarh Muslim University, Aligarh–202002
E-mail : farukh_arjmand@yahoo.co.in

The chemistry of organotin compounds is gaining paramount attention on account of their interesting structural features. There is, however, promising and recent success in using different organotin(IV) derivatives, which have shown acceptable in vivo cytotoxicity and antiproliferative activity as new chemotherapy agents. In this work, we describe here the synthesis and characterization of new organotin(IV) Schiff base complexes 1–3 derived from the condensation reaction of 3–formylchromone with ethanolamine. These complexes were characterized thoroughly by various spectroscopic methods (IR, NMR, ESI–MS), elemental analysis and molar conductance values. The *in vitro* DNA binding properties of complexes 1–3 have been investigated by electronic absorption spectra, fluorescence spectroscopy and viscosity measurements suggesting that all the complexes have the ability of binding to CT DNA through electrostatic mode of interaction. The intrinsic binding constant, K_b values suggested that complex **3** binds to CT DNA most efficiently as compared to 1 and 2.

PCP-CYSA-02 : Rapid Synthesis and Biological activity of 1-alkyl -4,6-dimethylpyrimidine-2-ones

Deepika

College of Pharmacy, Pt. B.D. Sharma University of Health Sciences, Rohtak-124001
E-mail : kumari.deepika967@gmail.com

The title compounds were synthesized from monosubstituted ureas and acetylacetone, a β-diketone. The ureas included N-methyl urea, N-ethyl urea, N-propyl urea, N-isopropyl urea, N-isobutyl urea, N-allyl urea etc. The condensations were carried out both in the presence as well as in the absence of the catalyst. The products were obtained in excellent yields. The characterization of the products was done on the basis of their spectroscopic data. The antimicrobial activity of the products was assayed by agar well diffusion method as recommended by CLSI. The four representative were namely *S. aureus* ATCC 25923, *E. coli* ATCC 25922, *P. aeruginosa* ATCC 90028 bacterial strains. The method developed is very convenient, practical, clean and environmentally friendly as no solvents are used and the work-ups of the reactions are also very simple. Some of the new synthesized compounds have shown moderate antimicrobial activity to gram positive bacteria.

PCP-CYSA-03 : Thermal, Conducting Behavior and Antimicrobial Properties of Emeraldine Base (EB) Form of Polyaniline (PANI)

Nirmala Kumari Jangid and Narendra Pal Singh Chauhan

Department of Chemistry, University College of Science, M. L. Sukhadia University, Udaipur (Raj.)-313001
E-mail : nirmalajangid.111@gmail.com,

Emeraldine base (EB) form of polyaniline (PANI) powder is prepared by chemical oxidative polymerization using different acidic media (HCl or CF_3COOH) at different temperature. These polyanilines are soluble in DMSO (dimethyl sulfoxide), DMF (dimethyl formamide). The softening temperature of different EB range from 87.8 – 116.4°C, which is believed to be an indication of cross – linking. The chemical structure, thermal characterization and conducting behavior are studied by FTIR spectroscopy, differential scanning calorimeter (DSC) and two – probe conductivity method. Conductivity of emeraldine base of PANI is around $(0.8 - 1.5) \times 10^{-6}$ S/Cm. Wide – angle XRD technique indicates that PANI – EB base is amorphous in nature. Antibacterial and antifungal studies of synthesized polyanilines have also been carried out.

PCP-CYSA-04 : Synthesis and Anti Tubercular Activity of Isoxazole Derivatives Bearing Pyrazole Nucleus

Khushal M. Kapadiya*, Parth A. Manvar* and Ranjan C. Khunt

Department of Chemistry, Saurashtra University, Rajkot
E-mail : drrckhunt12@yahoo.com

The compounds bearing isoxazole nucleus have been of great interest to synthetic and medicinal chemists for a long time due to their different biological activities like antiviral, antitumor, anticancer, and antiinflammtory. Moreover pyrazole have been also found to possess wide range of biological activities such as anticonvulsant, insecticidal, analgesic and antifungal. Our approach towards the synthesis of isoxazole derivatives is to show the biological importance at products bearing pyrazole nucleus.

The present study deals with anti tubercular activity of some Isoxazole derivatives bearing pyrazole nucleus. Preparation of isoxazole by condensation of chalcone with hydroxylamine hydrochloride in presence of sodium acetate.

All the synthesized compounds have been confirmed by spectroscopic techniques such as PMR, CMR and IR; further supported by mass spectra and elemental analysis. The entire synthesized compounds have been also evaluated for anti bacterial and anti fungal activity.

PCP-CYSA-05 : Synthesis of 3-(substituted phenyl)-4,5-dihydro-5-(1H-imidazole-4-yl)pyrazol-1-yl)(pyridine-4-yl)methanones

N. M. Panchani and H. S. Joshi*

Chemical Research Laboratory, Department of Chemistry,
Saurashtra University, Rajkot- 360 005
E-mail : drhsjoshi49@gmail.com

Several 1-(substituted phenyl)-3-(1*H*-imidazol-4-yl)prop-2-en-1-one derivatives (chalcones) were synthesized by the reaction between 1*H*-imidazole-4-carbaldehyde and different substituted acetophenone using PEG-400 as an alternative reaction solvent. This product was treated with isonicotinohydrazide to get 3-(substituted phenyl)-4,5-dihydro -5-(1*H*-imidazole-4-yl)pyrazol-1-yl)(pyridine-4-yl)methanone. The constitution of all the synthesized compounds have been characterized by Elemental analyzer, FT-IR, ^{1}H NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds has been checked by thin layer chromatography.

PCP-CYSA-06 : Studies and Biological Evaluation of Some New Salicylic Acid-1,3,4-oxadiazole Derivatives

Vaishali M. Goswami and H. S. Joshi

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : drhsjoshi49@gmail.com

The wide occurrence of the heterocycles in natural products has made them important synthetic targets. 1,3,4-Oxadizole moiety was selected for the synthesis because of its diverse biological activities. In the present work some newer salicylic acid 1,3,4-oxadiazole derivatives were synthesized by conventional method. The five-membered ring was synthesized by the condensation reaction of substituted salicylic acid with catalytic amount of conc.H_2SO_4 and ethanol. The obtained ester (2) was refluxed with hydrazine hydrate in ethanol to get hydrazides (3). The hydrazides (3) on cyclo-condensation reaction with different aromatic acids using phosphorous oxytrichloride ($POCl_3$) lead to the cyclized formation of some new salicylic acid-1,3,4-oxadiazole derivatives. All the compounds were purified by column chromatography. The structures of compounds were characterized by spectroscopic studies and elemental analysis. After structural elucidation, all the synthesized compounds were evaluated for their antimicrobial activity against gram positive and gram negative bacteria.

PCP-CYSA-07 : Synthesis of Some Aminopyrimidines Derivative Bearing Pyrazole Nucleus and Their Microbial Evaluation

Rupali Mehta*, Kishor M. Kavadia* and Ranjan C. Khunt

Department of Chemistry, Saurashtra University, Rajkot-360005
E-mail : drrckhunt12@yahoo.com

Recent studies showed that aminopyrimidines derivatives with lipophilic groups have significant anti-tubercular activity. These compounds are widely used as anticonvulsant, antianxiety, analgesic, sedative, anti-depressive, hypnotic agents and anti-inflammatory agents. In the last decade, the area of biological interest of aminopyrimidines has been extended to several diseases such as cancer, viral infection and cardiovascular disorders. The above importance of pyrimidine leads us to synthesise aminopyrimidines derivative comprised with pyrazole nucleus. The present paper deals with the synthesis of aminopyrimidines derived from chalcones and their evaluation for antimicrobial, antitubercular and antifungal activity. The chalcones have been prepared by the condensation of different aromatic ketone with pyrazole aldehyde which on cyclisation with aminoguanidine to furnished aminopyrimidines derivatives.

All the synthesised products have been confirmed by spectroscopic method such as 1HNMR, IR and Mass spectrometry. It is further supported by elemental analysis. The synthesised products have been evaluated for antimicrobial as well as antifungal activity.

PCP-CYSA-08 : Phytochemical and Biological Studies of *n*-Hexane Extract of Leaves of *Corchorus fascicularis* Lam

A. P. Rajput[*] and T. A. Rajput[†]

[*]P. G. Research Centre, Department of Chemistry, Z. B. Patil College,
Dhule 424002 (M.S.)
†Department of Chemistry, R. C. Patel A.C.S. College, Shirpur Dist. Dhule
425405 (M.S.)
E-mail : aprajput@rediffmail.com, tejenrajput@gmail.com

The present study aim was to identify and characterize the active principles from the leaves of *C. fascicularis* Lam. For isolation of compounds, the dried leaves powder of *C. fascicularis* Lam was subjected to cold maceration using *n*-Hexane as solvent. The Two compounds HEC-1, HEC-2 were isolated and purified from chloroform. Mass spectrum of HEC-1 and HEC-2 showed a parent molecular ion peak at m/z 456 which corresponds to molecular formula $C_{30}H_{48}O_3$. The compounds were characterized by using physical, chemical and molecular spectroscopic analytical methods which concluded the isolation of two isomeric phytoconstituents Oleanolic acid (HEC-1) and Ursolic acid (HEC-2).

Minimum Inhibitory Concentration (MIC), Minimum Bactericidal Concentration (MBC) and Minimum Fungicidal Concentration of values of HEC-1 and HEC-2 were determined. The results of each isolated compounds for MIC, MBC and MFC values were potent against *Escherichia coli, Staphylococcus aureus, Bacillus subtilis, Pseudommonas aeruginosa, Candida albicans, Aspergillus niger* tested bacterial and fungal strains.

PCP-CYSA-09 : Synthesis and Biological Evaluation of 2-(5-(4-(substituted) phenyl)-1,3,4-oxadiazol-2-yl)pyrazine

Jalpa R. Pandya and H. S. Joshi*

Chemical Research Laboratory, Department of Chemistry, Saurashtra University,
Rajkot- 360 005
E-mail : drhsjoshi49@gmail.com

Pyrazine nucleus possesses remarkable pharmaceutical importance and biological activities. Pyrazine play an important role as intermediates for pharmaceuticals, agricultural and chemical species. Extensive literature survey revealed very few published data on pyrazine derivatives as potential anti-inflammatory agents. This observation prompted us to synthesize this nucleus so as to enhance the overall activities at resulting moieties can be evaluated. It was consider of interest to design and synthesize some pyrazine2-carboxylic acid derivatives.

The importance of this study is to prepare various pyrazine2-carboxylic derivatives by introducing the pyrazine core into several molecules to explore the possibilities of some altered biological activities. Series of 2-(5-(4-(substituted) phenyl)-1,3,4-oxadiazol-2-yl)pyrazine 6(a-j) were synthesized in satisfactory yield. The constitution of all the synthesized compounds have been characterized by Elemental analyzer, FT-IR, ^{1}H NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds has been checked by thin layer chromatography.

PCP-CYSA-10 : Synthesis of new 1,3-thiazolidine-2,4-dione Derivatives Incorporated with 4-(6-Methylbenzo [d] thiazol-2-yl) Benzenamine as Antimicrobial, Antitubercular and Anti-HIV-1 Agents

Navin B. Patel[a]*, Faiyazalam M. Shaikh[a] and Nilesh B. Chauhan[b]

[a]*Organic Research Laboratory, Department of Chemistry, Veer Narmad South Gujarat University, Udhana-Magdalla Road, Surat-395 007, Gujarat*
[a, b] *J. P. Arts and Science College, Bharuch*
E-mail : faiyaz_online007@yahoo.co.in, drnavin@satyam.net.in

A new series of (E)-*N*-(4-(6-methylbenzo[d]thiazol-2-yl)phenyl)-2-(5-substituted benzylidene-2,4-dioxothiazolidin-3-yl)acetamides have been synthesized. These compounds are prepared by molecular hybridization of two different biologically active moieties benzothiazole and thiazolidinedione. The structures of the newly synthesized compounds were established on the basis of spectral data (IR, ^{1}H and ^{13}C NMR) and elemental analyses. All the synthesized compounds were screened for a variety of biological activities like *in vitro* antibacterial, antifungal, antitubercular and anti-HIV-1 activity.

PCP-CYSA-11 : Effect of Gamma Irradiation on the Natural Antioxidants in *Malaxis acuminata*

Nilima S. Rajurkar* and Kunda N. Gaikwad

Department of Chemistry, University of Pune, Pune 411007
E-mail : rajurkar@unipune.ac.in

Malaxis acuminata is used in the treatment of rheumatism, seminal

weakness, insect bites and burning sensation. In present investigations, the effect of gamma radiation on natural antioxidants of *Malaxis acuminata* (Family: Orchidaceae) was studied. For this purpose, sample was extracted in different solvents and irradiated in Co-60 irradiator (Gamma chamber-900) to 0, 1, 3 and 5 kGy at ambient temperature. Antioxidant activity was investigated by DPPH scavenging activity assay, ABTS scavenging activity assay and total phenolics. The results demonstrate that irradiation of extracts leads to the formation of MRPs which further help to increase antioxidant activity. ABTS scavenging activity and DPPH scavenging activity in ethanol extract was found to increase by 6.9 % and 2.55 % respectively after irradiation. Hence gamma irradiation could be an efficient method to increase antioxidant activity.

PCP-CYSA-12 : New 2-Benzylsulfanyl-nicotinic Acid based 1,3,4-thiadiazoles Bearing Different Heterocycles : Synthesis and their Biological Evaluation

Navin B. Patel* and Amit C. Purohit

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007
E-mail : drnavin@satyam.net.in

A novel series of 2-benzylsulfanyl-nicotinic acid based thiadiazoles namely 5-(2-benzylsulfanyl-pyridin-3-yl)- 2-(substituted)-sulfanyl-1,3,4-thiadiazoles 5a-j has been synthesized from the key intermediate 5-(2-Benzylsulfanyl-pyridin-3-yl)-[1,3,4]thiadiazol-2-ylamine 4. Nucleophilic substitution reactions with different electrophiles (E+), such as haloacetate and haloalkyl groups, which show different biological properties, were performed to get target compounds. These newly synthesized compounds were characterized by NMR, mass spectral, IR spectral study, C, H, N analyses and were evaluated for their antimicrobial and antimycobacterial activity. Some of them showed significant activity. The other compounds exhibited moderate activity when compared to standard substances.

PCP-CYSA-13 : Green Synthesis and Pharmacological Properties of 4-(Substituted benzylidene)-2-phenyl-1-(5-(pyridin-4-yl)-1, 3, 4-thiadiazol-2-yl)-1H-imidazol-5(4H)-one

Kalmendra Singh Sisodiya and V. K. Sharma

Department of Chemistry, Pacific University Udaipur (Rajasthan).
E-mail : kalmendrasisodiya@yahoo.in

Microwave-induced organic reaction enhancement (MORE) has

gained popularity as a non-conventional technique for rapid organic synthesis in the last few years. Reactions in domestic microwave ovens are currently in use for the synthesis of medicinally important compounds. Within the framework of 'Green Chemistry' we have now developed an environmentally benign and novel approach for the synthesis of (E)-4-(substituted benzylidene)-2-phenyl-1-(5-(pyridin-4-yl) 1, 3, 4-thiadiazol-2-yl)-1H-imidazol-5(4H)-one. The title compounds were prepared by the reaction of 5-(pyridin-4-yl)-1, 3,4-thiadiazol-2-amine with various (Z)-4-(substituted benzylidene)-2-phenyloxazol-5(4H)-one by using modified domestic microwave oven. The structure of these compounds was assigned on the basis of elemental analysis, IR, ^{1}H NMR spectral data. The compounds showed significant antibacterial activity against *B. subtilis* , *S. aureus* (gram-positive) and *E. coli* (gram-negative) bacteria and antifungal activity against *C. albicans* and *A. niger* fungi.

PCP-01 : Synthesis and Biological Evaluation of Coumarin Based Chalcones and their Analogues

Divyesh K. Patel[a] **and Navin B. Patel**[b]

[a]*Applied Chemistry Department, S. V. National Institute of Technology, Surat-395007, Gujarat*
[b]*Department of Chemistry, V. N. South Gujarat University, Surat-395007*
E-mail : dkpatel11984@gmail.com

A novel series of coumarin based chalcone analogues have been synthesized from the intermediate 4-(4-acetyl-phenylamino)-chromen-2-one. Cyclization reaction of chalcones with hydroxyl amine hydrochloride and thiourea gives the corresponding isoxazoles and pyrimidinthiones analogues. The newly synthesized compounds were evaluated for their antimycobacterial activity and antimicrobial activity against eight bacteria (S. *aureus*, *B. cereus*, *E. coli*, *P. aeruginosa*, *K. pneumoniae*, *S. typhi*, *P. vulgaris and S. flexneri*) and four fungi (*A. niger*, *C. albicans*, *A. fumigatus* and *A. clavatus*).

PCP-02 : Synthesis, Antioxidant and Anticancer Activity of Some Novel 1,3,4-Oxadiazoles

A.M.A. Khader* and Precilla Pathrao

**Department of Studies in Chemistry, Mangalore University,*
Mangalagangothri-574 199, Karnataka
E-mail : amakhader@yahoo.com

A series of S-alkylated 1,3,4-oxadiazoles were synthesized by reacting 5-[(naphthalen-1/2-yloxy)methyl]-1,3,4-oxadiazole-2-thiols with appropriate alkylating agents in the presence of triethylamine. The newly synthesized compounds were initially evaluated for antioxidant property using DPPH radical scavenging assay. Few of them exhibited good radical scavenging capacity with concentration of 100µg/mL in comparison with the standard ascorbic acid. Our aim was to systematically analyse their bio activities with an emphasis on their anti cancer effects. The anticancer activities of the newly synthesized compounds were evaluated against HepG2 cell line. 5 compounds showing promising activity against HepG2 cell line were further evaluated for their cytotoxicity against MCF-7 (human breast cancer cell line) and V79 (Chinese hamster lung fibroblast V79 cells). Compound 1-({5-[(naphthalen-1-yloxy)methyl]-1,3,4-oxadiazol-2-yl}sulfanyl)propan-2-one was found to have lowest IC_{50} value about 195.3µg/ml in human breast cancer cell line and was found to be safe upto 200 µg/ml tested concentrations in normal cell line.

PCP-03 : Efficient Catalyst and Organic Solvent Free Multi-component Protocol for Synthesis of (Z)-5-[(arylamino)methylide]-2-thioxodihydropyrimidine-4,6-(1*H*,5*H*)-dione Derivatives in Water and their Biological Evaluation

Bhaveshkumar D. Dhorajiya* and Bharatkumar Z. Dholakiya

Department of Applied Chemistry, S.V. National Institute of Technology,
Ichchhanath, Surat-395007, Gujarat
E-mail : bhavesh.orgchem@gmail.com

A novel multicomponent, eco-friendly protocol for Synthesis (Z)-5-[(arylamino)methylide]-2-thioxodihydropyrimidine- 4,6-(1*H*,5*H*)-dione derivatives in water has been developed. In this protocol appropriate amines reacts with formic acid to afford formamides and in situ these formamide derivatives reacts with active methylene group of α,β-unsaturated thiobarbituric acid under catalyst free condition in aqueous medium. Water plays an excellent role for catalyst as well as solvent for both formylation and Knoevenagel condensation reactions. The structures were elucidated by FT-IR, ^1H NMR, ^{13}C NMR, UV–Spectra, Mass and Elemental analysis. The newly synthesized compounds were evaluated for their antimycobacterial activity and antimicrobial activity.

PCP-04 : Design of Novel Lead Molecules for Cardiomyopathy - A Computational Study

Raghavendra Prasad, S. H. Uppala, Vishwanath Ramatenki,
Ramasree Dulapalli and Uma Vuruputuri*

Department of Chemistry, Nizam College, Osmania University, Basheerbagh,
Hyderabad-500001, Andhra Pradesh
E-mail : vuma@osmania.ac.in; vuma1957@gmail.com

Cardiomyopathy is a prominent disorder observed in cardiovascular diseases.USH-2 has a major role in muscle fibers contractions which is dependent on the variable expression of sarcomeric proteins and calcium ions signaling.USH-2 is a key regulatorsarcomeric protein involved in initiation of muscle contraction in skeletal and cardiac muscles of *Homo sapiens* and all vertebrates. In the present study the USH-2 is treated as novel target to design antagonists for cardiomyopathic therapy.

The protein USH-2 is subjected to 3D structural evaluation using comparative modelling techniques and is validated. The active site is identified by using the Schrodinger module SITE MAP. The protein is further considered for Virtual Screening studies using various databases of molecules using Standard Protocol.Novel ligands that are antagonistic toUSH-2 activity are identified, which are of potential therapeutic value for cardiomyopathy.

PCP-05 : Synthesis and Biological Evolution of Amino Based Tetrazole Compounds

M. H. Malani and B. Z. Dholakiya*

Department of Applied Chemistry, S.V. National Institute of Technology,
Ichhanath, Surat-395007, Gujarat
E-mail : maheshmalani.svnit@gmail.com

Tetrazole based cyano-biphenyl like motif used as a non peptide angiotensin II receptor antagonist used in the regulation of hypertension, heart strokes, diabetic, neuropathy and congestive heart diseases. We synthesize various amino based tetrazole like moieties. Synthesized compounds were characterized by spectral techniques. Compounds were tested in vitro anticonvalsant activity on Gaba T- Receptor Antagonist. Two compounds showed very excellent activity comparable with slandered drugs.

PCP-06 : Isolation and Chemical Characterization of Biosalts of Medicinal Plant Origin

Sujata Kale[1], Sonali Dhamal[2], Vividha Dhapte[3], V. V. Dhapte[2], B. A. Kulkarni[2] and S. S. Kadam[3]

[1]Abasaheb Garware College of Arts, Science and Commerce, Pune 04
[2]Department of Chemistry, Yashwantrao Mohite College Pune 38.
[3]Bharati Vidyapeeth University, Poona College of Pharmacy Pune 38.
E-mail : shivaji_takale@yahoo.co.in

Biosalts are the inorganic products isolated from the burnt ashes of medicinal plants. Due to their biological origin, they possess certain medicinal properties which are not shown by the equivalent synthetic salts. In ayurvedic system of medicine, these biosalts are recognized by a different name and they are called as *ayurvedic kshars*. The medicinal importance of these *kshars* was identified and well

established in ayurvedic system of medicine since antiquity and their origin goes back to the time of Charak and Sushrut.

Although several attractive medicinal applications are ascribed to these ayurvedic *kshars* or biosalts and *kshar* therapy was claimed to be superior to surgical treatments in some critical conditions, it is rarely used at present. This is because (a) only expert ayurvedic physicians can make use of *kshar* therapy and the number of such authorities is negligibly small (b) lack of advance research to reinvestigate the science of these *kshars* or biosalts from the modern scientific approach. Therefore, we have selected this challenging field for advance research to explore the chemistry, medicinal utility and isolation techniques from pharmaceutical and biomedicinal point of view.

This communication is a part of above refered project in which three medicinal plants, *Punica grantum, Erum indicum* and *Citruleus cololynthis* are selected whose biosalts / *kshars* were isolated and characterized using modern analytical techniques.

PCP-07 : Transformation of Macroscopic Iron State into Nanometric Bhasma State through Ayurvedic Process of *Bhasmikarana*

R. W. Jawale[1], Rupali Lad[2], Shivaji Takale[3], M. P. Wadekar[4], Sonali Dhamal[1] and Vineeta Bendale[4]

[1]College of Engineering, Bharati Vidyapeeth University, Katraj Pune 43.
[2]B. J. S. College of Arts, Science and Commerce, Pune.
[3]Bharati Vidyapeeth, Technical Campus, College of Engineering, Lavale, Dist-Mulshi, Pune-412 115
[4]Ayurved Rasayni, Amruth Kumbh, Navi peth pune 30.
E-mail : shivaji_takale@yahoo.co.in

Ayurvedic bhasmas constitute an important class of drugs of mineral origin. Among the different types of *bhasmas*, metal-based ayurvedic *bhasmas* are the supreme drugs due to the extraordinary medicinal properties exhibited by them. Gold, silver, copper, iron, tin, lead and zinc are seven primary metals whose *bhasmas* are well known from ancient times.

These drugs are synthesized by following the traditional ayurvedic processes called as *bhasmikarana* which involves transformation of macrometallic state into micro or nano *bhasma* state. The resultant metallic *bhasmas* are claimed to possess unique and excellent medicinal properties. However the art and science of these *bhasmas* went in dark since past few centuries and attempts are being made at present to reinvestigate this area using modern scientific approach.

We are trying to investigate the origin of the significant medicinal properties ascribed to these *bhasmas* with the help of recent developments in science and technology. Iron based *loha bhasma* is a famous and ancient ayurvedic drug for which different methods of its synthesis are known. While synthesizing *loha bhasma* by some of these methods and characterizing the resultant products through EDAX, XRD and SEM, we have found, two remarkable properties of *loha bhasma*. These are (a) extremely tiny size of the *bhasma* particles tending to nanolevel and (b) attachment of organic component to these nano-particles. In this communication we would like to report the experimental details of synthesis and characterization of *loha bhasma* with the help of EDAX, XRD, SEM and IR spectroscopy.

PCP-08 : Biological Evaluation of Newer Triazoles Clubbed Phenothiazine

Navin B. Patel* and Sabirkhan S. Pathan

Department of Chemistry, Veer Narmad South Gujarat University, Surat
E-mail : drnavin@satyam.net.in

Some newer 10-substituted phenothiazines having a triazoles nucleus have been synthesized by using condensation of 2-chloro-1-phenothiazin-10-yl-ethanone 1 with different 5-(4-methoxy phenyl)-2-amino-1,3,4-oxadiazole 2 followed by addition of various hydrazide in ring structure of oxadiazole. The products 3-[-1-(phenothiazin-10-yl)ethanon-2-yl]amino-4-(N-substituted)amino-5-(4-methoxy phenyl)-4*H*-1,2,4-triazole 4 were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectra and elemental analysis. The synthesized compound were evaluated for their antibacterial and antifungal activity (MIC) against Gram-positive (*S. aureus and B. Substilus*) and Gram-negative (*S. typhi, K. pneumonia, P. aeruginosa and E. coli*) bacteria by broth dilution method was compared with standard drugs gentamycin, ampicillin, chloromphenicol, ciprofloxacin and norfloxacin. An antifungal activity (MIC) against certain fungal species by broth dilution method was compared with standard drugs nystatin and greseofluvin.

PCP-09 : Design and Synthesis of Some Novel Thieno-[2,3-*d*]-pyrimidin-4-(3*H*)-ones as Potent Anti-inflammatory Agents

M. Mahima*, J. Saravanan, S. Mohan and Harshvardhan Mishra

Department of Pharmaceutical Chemistry, PES College of Pharmacy,
Hanumanth Nagar, Bangalore, KTK

A new series of 3-substituted amino-2-methyl thieno [2, 3- *d*] pyrimidin-4-(3*H*)-ones were synthesized from 2-methyl-3-N-amino-5-

methyl-6-acetylthieno[2,3-*d*] pyrimidin-4-one in the present study. Elemental analysis, UV, IR, ^{1}H NMR, and C, H & N analysis confirmed the structure of these newly synthesized compounds. All the compounds were investigated for acute (30mg/kg p.o) and chronic (10mg/kg p.o) anti-inflammatory activity using carrageenan induced rat paw edema model and carrageenan-induced granuloma air pouch model respectively. All the compounds exhibited significant ($P<0.05$) anti-inflammatory activity in acute model while in chronic model only compounds SR-1-7 exhibited significant activity ($P < 0.05$). In addition, the most active compounds were tested for their acute toxicity.

PCP-10 : Synthesis and *In vitro* Anti Microbial Activities of New 3-(4-(6-methylbenzo[d]thiazol-2-yl)phenyl)quinazolin-4(3H)-ones

Navin B. Patel* and Asif R. Shaikh

Department of Chemistry, Veer Narmad South Gujarat University, Surat-395 007
E-mail : drnavin@satyam.net.in, asif_shaikh114@yahoo.co.in

We have synthesized 2-[heterocycles]-3-(4-(6-methylbenzo[d]thiazol-2-yl)phenyl) quinazolin-4(3H)-ones from benzoxazinone. The title compounds were characterized by elemental analysis, IR and ^1H-NMR spectral data. They were screened for antibacterial and antifungal activity at two concentrations and compared with the standard drugs gentamycin, ampicillin, chloramphenicol, ciprofloxacin and norfloxacin. The antitubercular activity of title compounds were evaluated against $H_{37}Rv$ using Lowenstein-Jensen agar method and antimicrobial activity using the broth microdilution method.

PCP-11 : Synthesis and Antimicrobial activity of 4-Thiazolidinones and 2-Azetidinones from Chalcone

Navin B. Patel * and Minesh D. Patel

Department of Chemistry, Veer Narmad South Gujarat University,
Surat 395007, Gujarat
E-mail : drnavin@satyam.net.in

1-(3-Hydroxy-phenyl)-3-thiophene-2-yl-propenone 1 was obtained from the reaction of heterocyclic aldehyde with substituted acetophenone. The treatment of 1 with guanidine nitrate produced 3-(2-amino-6-thiophene-2-ylpyrimidine-4-yl) phenol 2. The synthesis of *N*-substituted benzylidine-4-(3-hydroxyphenyl)-6-(thiophene-2-yl)pyrimidin-2-amines 3a-j was performed by the treatment of compound 2 with the corresponding aromatic aldehydes. The reaction of 3a-j with thioglycolic acid and thiolactic acid formed the corresponding 4-thiazolidinones (4a-j & 5a-j) and with chloroacetylchloride, it gives 2-azetidinones 6a-j. All the synthesised compounds were characterized by IR, ^{1}H NMR, ^{13}C NMR and elemental analysis. The compounds were screened against certain bacterial and fungal strains.

PCP-12 : Synthesis of Some Biologically Active Heterocyclic Combinations via CADD Technique

Amit Bhandari* and Anita Mehta

Synthetic Organic Chemistry Laboratory, Department of Chemistry
M. L. Sukhadia University, Udaipur (Raj.) - 313001
**E-mail : amitbhandari02@gmail.com*

Computer aided drug designing (CADD) has recently attracted attention of synthetic organic chemists. Pharma expert software is a very simple tool for prediction of probable biological activity and toxicity theoretically based on molecular structure. In the present investigation, a series of 3-chlorobenzo[b]thiophene derivatives of N'-(3-(3-chlorobenzo[b]thiophene-2-carbonyl)-4-oxothiazolidine-2-ylidene)-7-methyl-3-oxo-5-phenyl-3,5-dihydro-2*H*-oxazolo [3,2-a]pyrimidine-6-carbohydrazide 5a-d and 3-chloro-N-(5-(7-methyl-3-oxo-5-phenyl-3,5-dihydro-2H-oxazolo[3,2-a]pyrimidine-6-yl)-1,3,4-thiadiazole-2-yl)benzo[b] thiophene-2-carboxamide 8a-d have been designed and synthesized starting from ethyl-6-methyl-2-oxo-4phenyl-1,2,3,4-tetrahydro-pyrimidine-5-carboxylate 1 via a multistep reaction sequence. The structure of all synthesized compounds has been confirmed by different spectral studies. Synthesized compounds have been estimated for probable activities using PASS technique and toxicity of compounds have been estimated using available web-service for prediction of LD_{50} values of rat acute toxicity. This is an attempt to develop CADD and correlate SAR.

PCP-13 : Synthesis and Characterization and Biological Activity of Ethoxyphthalimide Derivatives of 3-{4-[5-(4-substituted phenyl)-4,5-dihydroisoxazol-3-yl]phenyl}-quinazoline-2,4-dione and 3-{4-[5-(4-substituted phenyl)-4,5-dihydro-1H-pyrazol-3-yl]phenyl}-quinazoline-2,4-dione

Monika Kumawat* and G. L. Talesara

Department of Chemistry, M L Sukhadia University, Udaipur (Raj.)
E-mail : glntalesara@yahoo.com, monika.kumawat84@gmail.com

Synthesis of 3-[4-{5-(4substitutedphenyl)-4,5-dihydroisoxazol-3-yl}phenyl]-1-N-ethoxyphthalimido quinazoline-2,4-dione (3.I-Va-d) and 3-[4-{5-(4-substitutedphenyl)-4,5-dihydro-1H-pyrazol-3-yl}phenyl] -1-N-ethoxyphthalimidoquinazoline-2,4-dione are described. Nucleophilic aza substitution on isatoic anhydride with *p*-aminoacetophenone gave 3-(4-acetylphenyl) quinazoline-2,4-dione .This on clasien condensation with various aromatic aldehydes yields the corresponding 3-{4-[3-(4-substitutedphenyl)prop-2-enoyl]phenyl}quinazoline-2,4-dione derivatives. This was condensed by bromoalkoxyphtha-limide to afford -[4-{3-(4-subsitutedphenyl)prop-2-enoyl}phenyl]-1-N-ethoxyphthalimidoquinazoline-2,4-dione. These Compounds were cyclized separately with hydroxylamine hydrochloride and phenyl hydrazine in ethanolic media to give two series of final compounds. Biological activity was evaluated for following compounds.

PCP-14 : Green Route Multi-component Condensation of Barbituric/ Thiobarbituric Acid with Various DNA bases in Water and its Biological Evaluation

Bharat Kumar Z. Dholakiya and Bhavesh Kumar D. Dhorajiya

Department of Applied Chemistry, S.V. National Institute of Technology,
Ichchhanath, Surat-395007, Gujarat
E-mail : bharat281173@gmail.com, bhavesh.orgchem@gmail.com

An efficient and novel multi-component route for the stereochemical selective synthesis using various DNA bases such as (adenine, guanine and cytosine) with formic acid and barbituric acid/ thiobarbituric acid and its substituted derivatives using water as green solvent by conventional thermal heating process was described. In this way, formylation of various DNA bases takes place. The resulted different formamides of DNA undergo Knoevenagel condensation with active methylene group of barbituric acid and thiobarturic acid and its derivatives. The newly synthesized compounds were characterized by spectral analysis (FT-IR, ^{1}H NMR, ^{13}C NMR, HMBC, Mass, UV spectroscopy) and elemental analysis. All Synthesized compounds are biologically evaluated for Anti-Consultants and Anti-Cancer Screening.

PCP-15 : Synthesis and Antibacterial Activity of Quinazolinone Derivatives

R. S. Dave[1], M. T. Machhar* and R. J. Odedara[1]

[1]Department of Chemistry, Arts, Commerce, & Science College,
Pilvai (North Gujarat)
Department of Chemistry, J & J Science College, Nadiad (Gujarat)
**E-mail : rajendradave_63@yahoo.com*

In the present study, the derivatives of novel quinazolinone were synthesized and tested for antibacterial activity against E. Coli MTCC 443, P. Aeruginosa MTCC 1688, S. Aureus MTCC 96 and S. Pyogenus MTCC 442. These derivatives were also tested for antifungal activity against A. Niger MTCC 282. Reaction of 4-chloro anthranilic acid with chloroacetyl chloride followed by 4-fluoro aniline provides 7-chloro-2-(chloromethyl)-3-(4-fluorophenyl) quinazolin-4(3*H*)-one. Treatment of this 2-chloromethyl 4(3*H*)-quinazolinone with 5-nitro indole in the presence of potassium carbonate provides 7-chloro-3-(4-fluorophenyl)-2-(5-nitro indol-1-yl methyl)-quinazolin-4(3*H*)-one which upon reduction provides amino quinazolin-4(3*H*)-one system followed by derivatization of amino quinazolin-4(3*H*)-one into amide & sulfonamide using different aromatic acid chloride & sulfonyl chloride respectively. The new synthesized compounds were characterized using IR, ^{1}H NMR and Mass spectroscopy together with elemental analysis.

PCP-16 : Regioselective Synthesis of Isoxazole-mercaptobenzimidazole Hybrids and Their *In vivo* Analgesic and Anti-inflammatory Activity Studies

Shravankumar Kankala[a,], Srinivas Nerella[a], Ravinder Vadde[a,*] and Chandra Sekhar Vasam[b,*]

[a]*Department of Chemistry, Kakatiya University, Warangal-506009*
[b]*Department of Chemistry, Satavahana University, Karimnagar-505001*
E-mail: ravichemku@yahoo.co.in; csvasamsa@gmail.com

A facile catalytic method for the regioselective synthesis of 3,5-disubstituted isoxazole bound benzimidazole hybrid molecules and their effective analgesic and anti-inflammatory activities and structure-activity relationship (SAR) was demonstrated. These hybrid compounds possessing an electron-withdrawing group displayed higher activity than for compounds containing electron-donating groups and were found to be more potent than the standard pentazocine for analgesic and diclofenac for anti-inflammatory activity.

PCP-17 : Analytical Method Validation of Some Anti Asthamatic Leukotriene Receptor Antagonist Contain Drug for Analytical Application

G. B. Dave* and J. R. Patel[1]

**Department of Chemistry, Government Science College, Idar, Sabarkantha (North Gujarat)*
[1]*Department of Chemistry, Shri Jagdish Prasad Jhabarmal Tibrewala University, Vidhyanahari, Jhunjhunu, Rajasthan*
**E-mail : gunjandave84@yahoo.com*

In this study, a novel rapid analytical HPLC method was developed simultaneous determination of montelukast in bulk and dosage form. Development of an analytical method for the determination of montelukast drug and also validate the method as per the ICH guideline and required acceptance criteria. The method was developed by using symmetry C_{18}(250 × 4.6 mm, 5µm) containing mobile phase methyl phosphate buffer pH 4.5 and Methanol ratio 80:20 was employed. The flow rate was set at 1.0 mL/minute and the injection volume was 10µL. The retention time of montelukast was 4.7min.The linearity of method was 30-180 µg/mL, the correlation coefficient was found to be 0.9999. Eluents were monitored by UV-detector at 280 nm. There was no significant difference in intra-day and inter-day; low coefficient of variation value 0.301% indicates high precision analytical method. The method was validated as per ICH guideline for various parameter like precision, linearity, accuracy, ruggedness and robustness. The validated method will applied for clinical research for BA/BE studies.

PCP-18 : Synthesis, Characterization and Antimicrobial Studies of Nickel(II) Complexes with Amic Acid Derived from 9,10-dihydroanthracene-9,10-α,β-succinic Anhydride

H. B. Gajjar and A. G. Mehta

Department of Chemistry, Sir P. T. Sarvajanik College of Science, Surat (Gujarat)
E-mail : hetal_gajjar2003@yahoo.co.in

Co-ordination chemistry is one of the most recently explored fields of inorganic chemistry. In recent years, the study of metal complexes has been receiving increasing attention. In the last few years, there have been intensive and extensive search of some chelating agents, as a result different classes of chelating agents and their metal complexes have been found.

The present work report a new series of metal chelates of Ni(II) with amic acid ligands derived from 9,10-dihydroanthracene-9,10-α,β-succinic anhydride. The synthesized ligands and their metal complexes were characterized by IR, NMR, TGA etc. Further antibacterial and antifungal activities of these metal chelates have been carried out.

PCP-19 : Polarographic Study of 3-hydroxy-3-phenyl-1-(2,5-dichloro phenyl)triazene

Krishan Kant Kodli and A. K. Goswami*

Department of Chemistry Mohan Lal Sukhadia University,Udaipur (Raj.)
E-mail : akumargoswami@rediffmail.com

Electrochemical study of 3-hydroxy-3-phenyl-1-(2, 5-dichlorophenyl) triazene have been studied by polarography technique at d.m.e in the Britton-Robinson Buffer solution between the pH range 3.5 – 8.0. Verified the electrochemical reduction of the 3-Hydroxy-3-phenyl-1-(2, 5-dichlorophenyl)triazene (HPDCT) is diffusion controlled. Well defined waves are obtained and the half wave potential ($E_{½}$) also measured. The reduction mechanism indicates electron reversible reduction process.

PCP-20 : 2-[(5Z)-5-Benzylidene-4-oxo-2-thioxo-1,3-thiazolidin-3-yl]-N-phenylacetamide based Biologically Active Molecules : Synthesis, Characterization and Biological Evaluation

Aniruddhasinh M. Rana[a], Kishor R. Desai[b] and Smita Jauhari[a]

[a] Applied Chemistry Department, S.V. National Institute of Technology, Surat-395007, Gujarat

[b] Department of Biotechnology, C.G. Bhakta Institute of Biotechnology, Bardoli, Gujarat

E-mail : aniruddha.svnit@gmail.com, smita.jauhari11@gmail.com

In order to explore the antimicrobial effects associated with the 2-thioxo-4-thiazolidinone based framework, several 2-[(5Z)-5-benzylidene-4-oxo-2-thioxo-1,3-thiazolidin-3-yl]-N-phenylacetamide derivatives have been synthesized by an efficient synthetic protocol. Variation in the functional group at 5-benzylidine ring of rhodanine led to set of compounds bearing N-phenyl acetamide accommodated 2-thioxo-4-thiazolidinone moiety. The chemical structures of the final synthesized compounds were confirmed by IR, ^{1}H NMR, ^{13}C NMR spectroscopy, ESI Mass spectrometry and elemental analysis. The antibacterial and antifungal activity were tested at several dilutions of synthesized compounds against gram-positive bacterial strains (*Pseudomonas aeruginosa* ATCC 27853 and *Escherichia coli* ATCC 25922), gram-negative bacterial strains (Staphylococcus aureus ATCC 25923 and Bacillus subtilis ATCC 11774) and fungal strains (*Candida albicans* ATCC 66027 and *Aspergillus niger* ATCC 6275) by using Kirby Bauer disk diffusion technique and Serial broth dilution technique and obtained results were compared with the standard drugs.

PCP-21 : Mass Spectrometric Identification of Supramolecular Assemblies and their Application in Drug Discovery

Naisargee Parikh and Asit K. Chakraborti

National Institute of Pharmaceutical Education and Research (NIPER), S.A.S. Nagar, Punjab - 160062
Email: naisasargiparikh@vahoo.co.in

Thorough understanding of the biological interactions is crucial yet essential for medicinal chemists. This offers insight into various interactions (drug-drug, drug-receptor, drug-transporter and drug-food,) and thus helps into design and synthesis of diversified molecules with better pharmacological profile. In order to understand these interactions, identification of non covalent supramolecular assemblies and its characterization by various analytical techniques has become essential. Among various analytical techniques, mass spectrometry (MS) is gaining priority as an analytical tool to analytical/organic/ pharmaceutical chemists and biologists due to its appealing features like ability to identify short lived non covalent species or ion, ease of sample preparation, operational simplicity and ease of spectral interpretation. Mass spectrometric technique holds the place at the crucial stage of analysis such as structural confirmation, purity determination, hit identification, lead development, PKPD (pharmacokinetic-pharmacodynamic) studies and even in the formulation stage. The MS techniques particularly ESIMS is a solution provider towards this end through 'ion fishing' of charged species as reactive intermediates. However, revealing possible supramolecular assemblies that proceed through noncovalent short lived species remains the challenging task and MALDI and ESI MS techniques are being increasingly used for the purpose that adds a new dimension to analytical techniques. This presentation will summarise about a special application of ESI-MS to 'fish' the noncovalent complex/ion directly from solution phase to gas phase that gives direct insight into the drug interactions and proves it on the basis of trapped reactive intermediate.

PHYSICAL CHEMISTRY SECTION

Sectional President's Address

PIL 01 : An Overview of Nanoparticles Fabrication and Their Catalytic, Electrochemical and Sensor Based Applications

S. K. Mehta

Department of Chemistry and Centre for Advanced Studies in Chemistry,
Panjab University, Chandigarh-160 014, India
E-mail : skmehta@pu.ac.in

The ever increasing area of nanoscience basically nanocatalysis and nanoelectronics requires suitably sized building blocks to design and formulate the devices. Nanoparticles feature unique electronic and chemical properties that arise from their high surface areas and confinement of electronic states. This has encouraged the investigation of different procedures to formulate substances at a nanoscale level. Various facile approaches to nanoparticle fabrication have been explored by our group. These include microwave synthesis of nanoparticles in just over seconds which is a green method. Another method to prepare metal nanoparticles involves the use of metal surfactant complexes which proceeds without any requirement of capping agent or stabilising agent. The nanoparticles formed are capable of displaying fascinating properties owing to their quantum scale dimensions. The catalytic and electronic properties thus originating have been explored in detail. Electrochemical detection of hazardous compounds has been carried out by fabricating some excellent nanoparticle based sensors. NPs have also been used to produce electrochemical sensors for hydrazine and cyanide ion. Some nanoparticles also display excellent catalytic properties for organic reactions i.e. reduction of nitrophenol compounds. The activity of bimetallic particles is much higher than the individual particles and the catalysts have been found to be better than the previous reported results. The versatility of the properties thus offered by these nanoparticles makes them promising as ultimate miniature devices with applications ranging from sensing to catalysis to medicine.

PIL 02 : Development of Catalysts for Hydrogen Production for Fuel Cell Applications : Present Status and Future Perspectives

A Venugopal

Inorganic & Physical Chemistry Division, CSIR-Indian Institute of Chemical Technology, Tarnaka, Hyderabad, Andhra Pradesh
E-mail : akula@iict.res.in

Heterogeneous catalysis plays a pivotal role in the field of energy and environmental research. Depletion of fossil fuel reserves, enhanced oil prices and concern over environmental and security have driven the search for alternative forms of energy, lead to the emergence of what is now known as the “hydrogen economy”. Production of hydrogen for fuel cell applications by reforming processes involves several steps namely steam reforming, water gas shift (WGS) and preferential CO oxidation (PROX). Presence of CO, H_2O, CO_2 and H_2 in the reformate gas mixture allows for the various other possible reactions under the reaction conditions. Hence the CO clean up reactions such as WGS and PROX requires catalysts active at fuel cell operation conditions. The supported Au catalysts are found to be suitable for both WGS and PROX reactions. However, this multi step process seems economically not promising in order to get the fuel cell grade H_2. Recently, the catalytic decomposition of methane (CDM) to produce pure (i.e. COx free) H_2 and carbon of a unique filamentous structure has attracted attention of many researchers. The CDM process is generally carried out over catalysts in the absence of air (or) oxygen atmosphere thus, the process results CO_X free hydrogen and carbon nanofibers as only products selectively. In this investigation the supported Au catalysts were explored for WGS and PROX reactions. Mechanistic studies during WGS reaction and the advantages of supported Au catalysts are described. Simultaneously the associated complications and implications involved in CO clean up reactions are briefly explained. Finally, the results on various Ni catalysts such as Ni-Al-SiO_2, Ni-Cu-Al and Ni-Cu-SiO_2 catalysts screened for CDM process is illustrated.

PIL 03 : Determination of Aspirin Drug at a Novel Graphene Modified Glassy Carbon Electrode and its Applications in Analytical Chemistry

Sharanappa T. Nandibewoor*

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

The voltammetric behaviour of aspirin (acetyl salicylic acid) at graphene modified glassy carbon electrode has been investigated for the first time using cyclic, differential pulse voltammetric techniques. Graphene was synthesized and characterised by using scanning electron microscopy and transmission electron microscopy. The glassy carbon electrode modified with graphene shows an excellent electrocatalytic activity and sensitivity due to its unique properties such as high surface area and large pores volume. The dependence of the current on pH, concentration and scan rate was investigated to optimize the experimental condition for the determination of aspirin. The effect of interferents was studied. The number of electrons transferred in the oxidation process was calculated. In the range of 1.0×10^{-6} to 9.0×10^{-4} M, the current measured by differential pulse voltammetry presents a good linear property as a function of the concentration of the aspirin with a detection limit of 5.22×10^{-8} M with good selectivity and sensitivity. The proposed method was successfully applied to aspirin determination in pharmaceutical samples and for the detection of aspirin in urine as a real sample.

PIL 04 : Surfactant Assisted Preparation of ZnO Nanostructures and their Potential Application for the Removal of Acridine Orange and Coomassie Brilliant Blue R-250 Dyes from Aqueous Solutions

Ganga Ram Chaudhary

Department of Chemistry & Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh - 160014
E-mail : grc22@pu.ac.in

In the present study an attempt has been made to synthesize ZnO nanostructures using cationic surfactant; Cetyltrimethylammonium bromide at relatively low temperature. The prepared nanostructures were characterized by XRD, TEM and SEM measurements. Different morphologies of ZnO nanostructures (rod, flower and spherical) have been attained by varying the reaction conditions. These nanostructures have been used for the adsorption of cationic dye (Acridine orange) and anionic dye (Coomassie Brilliant Blue R-250) from their aqueous solution. Maximum adsorption of the two dyes has been attained by spherical shaped nanoparticles, as its size is relatively smaller than the other morphologies. Batch mode experiments have been performed for both the dyes to study the effect of adsorbent dose, pH, and contact time on different dye concentrations. Langmuir and Freundlich adsorption isotherms have been studied to explain the interaction of the dyes. The Langmuir adsorption capacity was found to be 3688.3 and and 7929.6 mgg^{-1} for Acridine Orange and Coomassie Brilliant

Blue R, respectively. Adsorption kinetic followed pseudo-second-order reaction kinetics for both the dyes. Moreover, the adsorbed dyes were desorbed from ZnO nanoparticles. The identities of recovered nanoparticles as well as both the dyes have found to be same and were reused.

PIL 05 : Ammonium Ionic Liquids as Convenient Co-solvents for the Structure and Stability of Enzyme

Pannur Venkatesu

Department of Chemistry, University of Delhi, Delhi - 110 007
E-mail : venkatesup@hotmail.com; pvenkatesu@chemistry.du.ac.in

We have investigated the biomolecular interactions and related associated structural changes of succinylated con A (S Con A) with new ILs by using several biophysical techniques including circular dichroism (CD) and fluorescence. The ILs studied in the present study includes diethylammonium dihydrogen phosphate $[(CH_3CH_2)_2NH][H_2PO_4]$ (DEAP), diethylammonium hydrogen sulfate $[(CH_3CH_2)_2NH][HSO_4]$ (DEAS), triethylammonium dihydrogen phosphate $[(CH_3CH_2)_3NH][H_2PO_4]$ (TEAP) and triethylammonium hydrogen sulfate $[(CH_3CH_2)_3NH][HSO_4]$ (TEAS). We observed that all ILs have dominant contribution to the stabilization of the native structure of the S Con A. Furthermore, the results reveal that phosphate anions of ILs are strong stabilizers and acted as effective refolding enhancers for thermally denatured enzyme structure, whereas the enzyme was not refolded in the sulfate anions of ILs. These findings suggest a new generation of enzyme stabilizers that can be applied to other protein folding studies and biological systems.

PIL 06 : Photocatalysis : An Eco-friendly Route to Combat Enviromental Pollution and Energy Crisis

Rameshwar Ameta

P. G. Deptt. of Chemistry, S.M.B. Govt. College, Nathdwara (Raj.)

In the present era of energy crisis and environmental pollution, there is pressing demand to find eco-friendly pathways which can put a check on the growing environmental pollution and to solve the problem of energy crisis. Photocatalysis is emerging a green technology in this regard. Details starting from fundamental to applications will be discussed about various photocatalyic processes.

PO-CYSA-01 : Electrochemical Behavior and Determination of Paclitaxel in Pharmaceuticals and Human Biological Fluids at Glassy Carbon Electrode

Jayant I. Gowda and Sharanappa T. Nandibewoor*

P.G. Department of Studies in Chemistry, Karnatak University, Dharwad-580 003
E-mail : stnandibewoor@yahoo.com; jayantgowda4@gmail.com

The electrochemical behavior of paclitaxel drug was studied at a glassy carbon electrode in phosphate buffer solutions using cyclic and differential-pulse voltammetric techniques. The oxidation process was shown to be irreversible over the pH range (4.2–10.4) and was diffusion controlled. Effects of anodic peak potential (E_p), anodic peak current (I_{pa}), scan rate, pH, heterogeneous rate constant (k^0), etc have been discussed. A possible electro-oxidation mechanism was proposed. An analytical method was developed for the determination of paclitaxel in phosphate buffer solution at pH = 7.0 as a supporting electrolyte. The anodic peak current varied linearly with paclitaxel concentration in the range 1.0×10^{-6} M to 1.0×10^{-5} M of paclitaxel with a limit of detection (LOD) of 1.23×10^{-8} M and limit of quantification (LOQ) of 4.10×10^{-8} M. The proposed method was successfully applied to the determination of paclitaxel in pure and real samples.

PO-CYSA-02 : Effect of Structural Variations in Cation of Ionic Liquids on the Coexistence Curve of Isobutyric Acid and Water

Awanish Kumar and Pannuru Venkatesu*

Department of Chemistry, University of Delhi, Delhi-110 007

Interestingly, opposite behavior of the ionic liquids (ILs) having different cation chains with a common anion is observed on the coexisting curve of isobutyric acid-water (IBW). The critical region of IBW was found to increase in the presence of aliphatic chain $[C_6mim][BF_4]$, (IL-1) whereas, the critical region decreases in the presence of aromatic chain $[Bnmim][BF_4]$, (IL-2). The critical exponent (β) increases with IL concentrations, which are fully renormalized critical exponents. Further, dynamic light scattering (DLS) results for binary critical solution of IBW+IL indicate that there exists a fluctuation in the local density that contributes significantly to the fluctuations in the scattered intensity at T_c. This indicates that the IL entangles with the both coexisting phases, thereby the IL strongly interacts with the neighboring solvent molecules. In addition, we report the fluorescence spectroscopy data for the critical mixture of IBW and its mixture with ILs as impurities using Nile red as a fluorescent probe. Noticeable transitions of the two phases were detected at T_c through fluorescence technique. The observed variations in the fluorescence intensities with temperature predict unambiguously the formation of the solvation structure at T_c for the pure critical mixture as well as in presence of ILs.

PO-CYSA-03 : Metal Oxide Nanoparticles as Electrochemical Sensors for Determination of Para-nitrophenol in Neutral Solutions

Kulvinder Singh, S. K. Mehta, G. R. Chaudhary and Sukhjinder Singh

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh-160014
E-mail : kulvinderchem@gmail.com

Metal oxide nanoparticles (NPs) have been prepared by facile simple solution method at low-temperature. The as-synthesized NPs have been characterized by various techniques in terms of their optical as well as structural confirmation. The structural purity and crystallinity have been confirmed by using field emission scanning electron microscopy, electron diffraction spectroscopy, fourier transformation infra red spectroscopy (FT-IR) and X-ray diffraction. The NPs have also been optically characterized by using UV-vis. and Raman spectroscopy. Further these NPs have been found to be efficient for the electrochemical sensing of para-Nitrophenol (PNP). This efficiency of Au electrode modified with metal oxide NPs for PNP sensing has been analyzed using cyclic voltammetry. The fabricated NPs possess high sensitivity and low detection limit in neutral medium.

PO-CYSA-04 : Synthesis and Characterization and Potential Aplication of Novel Metallosurfactants of Nickel and Palladium

Prabjot Singh , G.R. Chaudhary and S.K. Mehta

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh-160014
E-mail : prabjotsinghkk@gmail.com

Double chained metallosurfactants of nickel and palladium were synthesized using dodecylamine and sodium decanoate as ligands. Prepared metallosurfactants were characterized by UV-Visible, FTIR, FTNMR, LCMS, CHN, TGA and DTA analytical techniques. Application part was explored by utilising them in fabrication of metal nanoparticles of size less than 10 nm and formulation of drug delivery vesicles. Antimicrobial studies of synthesized metallosurfactants were also investigated. Synthesized nanoparticles were characterized by UV-Visible, XRD, EDS and TEM.

PO-CYSA-05 : Oxidation of Ketorolac Drug by an Alkaline Copper(III) Periodate Complex in the Presence of Ruthenium(III) as a Homogenous Catalyst

Nagaraj P. Shetti* and Sharanappa T. Nandibewoor

Department of Chemistry, KLE Society's KLE Institute of Technology, Hubli-580030
P.G. Department of Studies in Chemistry, Karnatak University, Dharwad-580003
**E-mail : npshetti@yahoo.com*

The kinetics of oxidation of ketorolac (KET) by diperiodatocuprate(III) (DPC) in aqueous alkaline medium at a constant ionic strength of 0.10 mol·dm^{-3} was studied spectrophotometrically at 298 K in presence of ruthenium(III) as a homogeneous catalyst. The reaction between ketorolac and DPC in alkaline medium in presence of Ru(III) exhibits 1:6 stoichiometry (KET:DPC). The reaction is of first order in [DPC] and has less than unit order in both [KET] and [alkali], and negative fractional order in periodate. The order in Ru(III) was unity. Intervention of free radicals was observed in the reaction. The oxidation reaction in alkaline medium has been shown to proceed *via* a Ru(III)-KET, complex, which reacts with monoperiodatocuprate(III) to decompose in a rate determining step followed by other fast steps to give the products. The main products were identified by spot test, IR and GC-MS spectral studies. The reaction constants involved in the different steps of the mechanism were calculated at different temperatures, which yielded thermodynamic quantities for different steps of the reaction scheme. The activation parameters with respect to the slow step of the mechanism were computed and discussed; thermodynamic quantities were also determined. The active species of catalyst and oxidant have been identified.

PO-CYSA-06 : Kinetics and Mechanism of Cerium(IV) Oxidation of Fosfomycin Disodium Salt – an Antibiotic Drug in Acid Perchlorate Solutions

Laxmi N. Jattinagoudar and Shivamurti A. Chimatadar*

P. G. Department of Studies in Chemistry, Karnatak University,
Pavate Nagar, Dharwad - 580003
**E-mail: schimatadar@gmail.com, laxminj2755@gmail.com*

The kinetics of the oxidation of fosfomycin disodium salt, by cerium(IV) in aqueous perchloric acid medium at constant ionic strength, $I = 1.1$ mol dm^{-3}, has been investigated spectrophotometrically at 25 °C nm. The oxidation products were confirmed and characterized by spectral studies. The reaction is of first order in Ce(IV), fractional order in both fosfomycin disodium salt and H$^+$ ion concentrations. The active species of oxidant is found to be Ce(OH)$^{3+}$. The effect of

ionic strength, added products and dielectric constant of the medium were studied on the rate of reaction. Based on the experimental results a suitable mechanism is proposed. The reaction constants involved in the different steps of the reaction mechanism are calculated. The activation parameters with respect to the slow step of the mechanism are determined and discussed.

PO-CYSA-07 : Surfactant Adsorption and Aggregate Structure at Silica Nanoparticles : A Versatile Stratagem for the Regulation of Particle Size and Surface Modification

Savita Chaudhary and S.K. Mehta

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh 160014
E-mail : chemsavita@gmail.com

The arena of mesoporous silica nanoparticles (MSNs) is phenomenally multilateral. Silica particles have stimulate special consideration in bio-analysis due to its immense improvements in various characteristics such as biocompatibility, distinctive properties of amendable pore size and structure, large surface areas and pore volumes, controllable morphology and adjustable surfaces, lofty chemical and thermal steadiness. These characteristics permit the silica nanoparticles to be extensively employed as the solid-supporting or entrapping matrix. In recent times MSNs play essential function in everyday commercial purposes for instance energy storage, chemical and biological sensors, food processing and catalysis. Herein, the size-dependent interaction of anionic silica nanoparticles with ten different types of cationic surfactants has been studied in terms of the physical chemical aspects of colloid and interface science. The surfactants used consist of the same charges i.e. cationic on the head group and different hydrophobic tails as well as the different counterions. The present investigation aims to explore the comparative effect of different surfactants during the formation of the target composite materials. The nanoparticle size controls, the surface-to-volume ratio and surface curvature with respect to its interaction with surfactant will also be discussed in this work. More importantly, the synthetic strategy developed in this work can be extended to fabricate core-shell nanostructures with functional nanoparticles encapsulated in MSNs, making the strategy useful and widely applicable for preparing advanced mesoporous materials for catalysis and drug delivery.

PO-CYSA-08 : An Insight into Internal Organization of Nonionic Microemulsions

Gurpreet Kaur and S.K. Mehta

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh - 160 014
E-mail : nonie14@gmail.com

Microemulsions are important formulations in cosmetics and pharmaceutics and one peculiarity lies in the so-called “phase inversion” that takes place at a given water-to-oil concentration ratio and where the average curvature of the surfactant film is zero. In that context, we investigated the structural transitions occurring in Brij 96-based microemulsions with the cosmetic oil ethyl oleate and studied the influence of the short chain alcohol butanol on their structure and properties as a function of water addition. The characterization has been carried out by means of transport properties, spectroscopy, DLS, SANS, and electrochemical methods. The results confirm that the nonionic Brij 96 in combination with butanol as cosurfactant forms a U-type microemulsion that upon addition of water undergoes a continuous transition from swollen reverse micelles to oil-in-water (O/W) microemulsion via a bicontinuous region. After determining the structural transition through viscosity and surface tension, the 2D-ROESY studies give an insight into the microstructure, i.e., the oil component ethyl oleate mainly is located at the hydrophobic tails of surfactant while butanol molecules reside preferentially in the interface. SANS experiments show a continuous increase of the size of the structural units with increasing water content. The DLS results are more complex and show the presence of two relaxation modes in these microemulsions for low water content and a single diffusive mode only for the O/W microemulsion droplets. The fast relaxation reflects the size of the structural units while the slower one is attributed to the formation of a network of percolated microemulsion aggregates. Electrochemical studies using ferrocene have been carried out and successfully elucidated the structural transformations with the help of diffusion coefficients. An unusual behavior of ferrocene has been observed in the present microheterogeneous medium, giving a deeper insight into ferrocene electrochemistry. NMR-ROESY experiments give information regarding the internal organization of the microemulsion droplets. In general, one finds a continuous structural transition from a W/O over a bicontinuous to an O/W microemulsion, however with a peculiar network formation over an extended concentration range, which is attributed to the somewhat amphiphilic oil ethyl oleate. The detailed knowledge of the structural behavior of this type of system might be important for their future applications.

PO-CYSA-09 : Formation of Cyclodextrin-stabilized Nanoemulsion/Micromeulsion and Exploiting their Solubilization Behavior

Khushwinder Kaur

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh - 160 014
E-mail : makkarkhushi@gmail.com

This paper exploits the formation and stability of cyclodextrin (CD) encapsulated micromulsion/nanoemulsion by percolation and phase inversion temperature (PIT) emulsification method using AOT and Tween+Lecithin as surfactants. The stability of the formulated system has been checked by UV-VIS absorption spectroscopy and particle size estimations. The results show that the particle size of nanoemulsion increased slightly over a period of one month whereas AOT based microemulsion has been reported to be stable over months. However, it was found that nanoemulsions form a better host for the assimilation of various CD's such as α-CD, β-CD and β-CD-hydrate whereas microemulsions have been reported to host hp-β-CD only. The study of interactions has been carried out using FTIR and fluorescence studies. The structural transitions within the microemulsion and nanoemulsion have also been studied with UV-VIS absorption spectroscopy.

PO-01 : Studies of Ag^I Catalysed Oxidation of L-ascorbic Acid by Cerium(IV) in Perchloric Acid Medium : A Kinetic and Mechanistic Approach

Maheshwar Prasad Sah

Department of Chemistry, S. M. College, Bhagalpur-812001 (Bihar)
E-mail : reach2lecturermps@gmail.com

Kinetics and mechanism of oxidation of L-ascorbic acid by cerium(IV) in perchloric acid medium in presence of Ag^I as catalyst have been investigated. The order of reaction with respect to the oxidant and substrate has been found to be one. The rate of reaction increases with increasing ionic strength of the medium. At constant $[H^+]$ the rate of reaction decreases on increasing sulphate and bisulphate ion concentration. The rate of reaction increases as the $[Ag^+]$ increases. The catalytic ratios have been calculated which show the positive catalytic effect on reaction rate. At constant ionic strength the rate of reaction increases on increasing $[H^+]$ due to the conversion of unreactive species of Ce^{IV} to the reactive species of Ce^{IV}. The thermodynamic parameters have been computed from the rate constants observed at 30-45^0. The fairly high negative values of ΔS and of positive

ΔH suggest the formation of more ordered activated complex and the transition state is highly solvated.

PO-02 : Synthesis and Physico-chemical Study of Multifunctional Cardoepoxy Resin and its Natural Fiber Reinforced Composites

Jignesh P. Patel[1] and P. H. Parsania*

**[1]Polymer Chemistry Division, Department of Chemistry, Saurashtra University, Rajkot-360 005*
E-mail : phparsania22@gmail.com, phparsania@aol.com

Multifunctional epoxy resin (EBCF) has been synthesized by in situ alkali catalyzed condensation of bisphenol-C, formaldehyde and epichlorohydrin and cured using 20% tetrahydrophthalic anhydride at 100°C. Cured resin (EBCF-THPA) is thermally stable up to 255°C and followed single step degradation with 73.3% weight loss and 22% residue at 600°C. Observed kinetic parameters n, E, A and ΔS are 1.4, 136.3 kJmol^{-1}, 9.93 x 10^{-6} s^{-1} and -98.3 J K^{-1} mol^{-1}, respectively. Jute-EBCF and silica filled composites have been fabricated by hand layup technique under 27.58 MPa pressure at 135°C for 4h. Tensile and flexural properties are discussed in light of filler content. Hydrolytic stability of Jute-EBCF composite in water, acid and saline environments has been studied at 35°C and it is observed that it possesses excellent hydrolytic stability even in harsh acid and saline environments.

PO-03 : Rheological Parameters on Laurates of Some Metals in Mixed Organic Solvents

Amit K. Agarwal, M.K. Rawat and Sandhya Agarwal

Department of Chemistry, Agra College, Agra-282002 (U.P.)
Dr. B. R. Ambedkar University, Agra
E-mail : agarwal.chem@yahoo.co.in

The critical micelle concentration of gadolinium, terbium and dysprosium (Laurate) in a mixture of benzene and methanol (50:50 v/v) was determined from conductivity and viscosity measurements. The result shows that the CMC decreases with increasing atomic number of metal ion. The degree of dissociation and dissociation constant data show that the gadolinium, terbium and dysprosium laureates behave as a simple electrolyte in the solution. The results of viscosity measurements have been explained on the basis of the equation proposed by Einstein, Moulik, Vand and Jones-Dole. The values of the molar volume are in close agreement with Vand and Einstein's equation.

PO-04 : Thermodynamics of Dissociation and Micellization of Carboxylates of Dysprosium in Organic Solvent

Sangeeta and M.K. Rawat

Department of Chemistry, Agra College, Agra
E-mail : sangeeta.kumar47@rediffmail.com

Dysprosium laurate and myristate behave as a weak electrolyte in methanol below the critical micelle concentration and conductance data can be explained on the basis of Ostwald's formula and Debye Huckel theory of weak electrolytes. Thermodynamic parameters and dissociation constant for dissociation and micellization of these soaps have also been evaluated. Micellization was spontaneous and predominant over the dissociation process.

PO-05 : Bio-sorption of Basic Dye from Aqueous Medium using a Novel Agricultural Waste Material: *Gossypium Arboreum* Stem

G. H. Sonawane[1] and V. S. Shrivastava[2]

[1] Department of Chemistry, Kisan Arts, Commerce and Science College, Parola, Dist. Jalgaon - 425111 (M.S.)
[2] Department of P.G. Studies and Research in Chemistry, G.T.P. College, Nandurbar - 425412 (M.S.)
E-mail : drvinod_shrivastava@yahoo.com, drgunvantsonawane@gmail.com

The use of cheap, high efficiency and eco-friendly adsorbent has been studied as an alternative to activated carbon for the removal of dyes from wastewater. In this work *Gossypium arboreum* cotton stem (CS), an agricultural solid waste, is proposed as a novel material for the removal of Rhodamine-B from aqueous solutions. A series of experiments were conducted in a batch system to access the effect of system variables like initial pH, initial dye concentration, adsorbent dosage and contact time. The result showed that the adsorption of Rhodamine-B was maximum at pH-4, and at contact time 90 min. As the amount of adsorbent increases the percentage dye removal also increases, but it decreased with increase in initial dye concentration. The adsorption kinetics was found to follow pseudo-second order rate kinetic model with good correlation ($r^2 > 0.9743$) and intraparticle diffusion as one of the rate determining step. The equilibrium data fitted well with the Langmuir model with maximum monolayer adsorption capacity of 2.85 mg/g. The dimension less factor R_L revealed the favorable nature of the isotherm of the dye-CS system. In addition adsorbent was characterized by FTIR, XRD and SEM analysis.

PO-06 : Studies on Some Physico-Chemical Characteristics of Ground Water Analysis in Selected Areas of Agra District

Mitali Sharma* and M.K.Rawat

Department of Chemistry, Agra College, Agra - 282002
E-mail : m.sharma333@yahoo.com

Ground water is one of the most useful water sources. Water is second to oxygen as being essential for life. People can survive days, weeks, or even longer without food but only about four days without water, contamination of such water sources is a big problem creating health hazard. In this study samples were collected from different areas of Agra City.

In this study different parameters like pH, Temperature, Total Dissolved Solid, Alkalinity, Turbidity, Hardness, Suspended solid, dissolved solid, Chloride, and Floride were analyzed. After examination and testing of different physico-chemical and biological parameters (Using WHO and INDIAN STANDARDS), the suitability of ground water for drinking and domestic purposes, was found.

PO-07 : Spectrophotometric Study on Substituent Effect on the Formation of EDA complexes of Aromatic Amines

K.P.Srivastava*

Ganga Singh College, Jai Prakash University, Chapra-841301, Bihar
E-mail: jpukpsrichem@rediffmail.com

The spectrophotometric study was done to understand the effect of substitution on the donor aniline molecule through the formation of EDA complexes with chloranil and bromanil as the acceptors.The shift in CT transition due to substitution, the changes on the ionization energy (I_D) of the differently substituted donor molecules, the changes in the thermodynamic parameter K and the Gibbs free energy of formation (ΔG^0)for chloranil and bromanil systems are reported. A comparison was made between systems performed with the two mentioned acceptors.

PO-08 : DSC Curing Study of Epoxy Resin of 1, 3-bis(4-hydroxy phenyl) prop-2-en-1-one using Diamines and Anhydride

Pooja P. Adroja, Rizwan Y. Ghumara and P. H. Parsania

Polymer Chemistry Division, Department of Chemistry, Saurashtra University, Rajkot- 360 005 (Gujarat)
E-mail : phparsania22@gmail.com, phparsania@aol.com

Epoxy resin of 1, 3-bis(4-hydroxy phenyl) prop-2-en-1-one (ECH) has been synthesized cured using different concentrations of hardeners such as DDE, DDS and PA by DSC at different heating rates in nitrogen atmosphere. Energy of activation and pre-exponential factor have been determined at various degree of curing according to Flyn-Wall Ozawa method. The data are interpreted in light of hardener concentration and nature of hardeners. Isoconversional Flyn-Wall-Ozawa method indicated multistep reactions. The nature and structure of hardeners affected curing kinetics.

PO-09 : Synthesis and Physico-chemical Study of Modified Multifunctional Epoxy Resin of 2, 4, 6-tris (4-hydroxyphenyl)-1-3-5-triazine

Rizwan Y. Ghumara, Pooja P. Adroja and P. H. Parsania

Polymer Chemistry Division, Department of Chemistry, Saurashtra University,
Rajkot-360 005, Gujarat
E-mail : rizwan.yg@gmail.com

Multifunctional epoxy resin of 2, 4, 6-tris (4-hydroxyphenyl)-1-3-5-triazine has been synthesized and modified by reacting it with acrylic acid, methacrylic acid and unsaturated polyester resin. The resultant modified resins have been styrenated and used in making value added jute and glass composites. Both types of composites are characterized for their mechanical and electrical properties and also for their hydrolytic stability in water, acid and saline environments. Fairly good tensile and flexural strengths, electric strength and volume resistivity are found for all the composites fabricated. The data are interpreted in light of the nature of modified resins and nature of fibers as well as effect of environment on hydraulic stability. The composites may find their industrial applications in construction and electronic industries.

PO-10 : Thermodynamic and Transport Properties of Binary Liquid Mixtures of Sulfolane with Methyl Alkanoates at Temperature 308.15K

N. Raghuram and T. Savitha Jyostna*

Department of Chemistry, Kakatiya University, Vidyaranyapuri,
Warangal-506 009, Andhra Pradesh,
Department of Chemistry, Kakatiya University, Warangal – 506 009.
**E-mail : jyostnats@yahoo.co.in*

Volumetric and transport properties of liquid mixtures are required in most of engineering calculations, where fluid flow or mixing is an important factor in many practical problems concerning mass transport applications. The solution properties are utilised in process development, pollution control, environmental protection etc. An understanding of the behavior of liquids is useful to the physical separation process like distillation, extraction and crystallization. Densities, viscosities and speed of sound of binary liquid mixtures of Sulfolane with Methyl ethanoate, Methyl propionate and Methyl butanoate have been determined at 308.15K for the composition range. Excess molar volumes, deviation in viscosity and isentropic compressibility's have been derived from the experimental data. Excess functions of Gibbs free energy of activation of viscous flow ($G^{*}E$), Grunberg - Nissan interaction parameter (d') and intermolecular free length (L_f) and relative association (R_A) are computed from the experimental data.

These quantities are fitted to a Redlich-Kister polynomial type equation to derive binary coefficients and standard deviation. Excess molar volumes (V^E), deviation in viscosity ($\Delta\eta$), deviation in isentropic compressibility ($\Delta\kappa_s$) show negative deviations from the ideal for these systems. The above negative V^E and $\Delta\kappa_s$ values may results from Interstitial accommodation of ester molecules in sulfolane and dipole-dipole interactions that enhance the solvent structure in the mixture, in turn making negative contributions to V^E and $\Delta\kappa_s$.

PO-11 : Density, Viscosity and Excess Thermodynamic Properties of Binary Liquid Mixtures of *o*-Nitrotoluene with Benzene and Toluene at Temperatures 293.15, 298.15 and 303.15 K

Nandini Upadhyay, Anita Gupta and S.C. Goyal*

Department of Chemistry, Agra College, Agra-282002
E-mail : scgoyalorganic@yahoo.com

The extensive information on the thermodynamic properties of binary mixtures is needed not only as their use is increasing in many industrial process as solvent but also for the advancement of theoretical developments through an understanding of the intermolecular interaction between unlike molecules. Densities and viscosities of binary liquid mixtures of *o*-nitrotoluene with benzene, toluene have been determined at 293.15, 298.15 and 303.15 K. From the density viscosity data excess thermodynamic functions viz. viscosity deviation ($\Delta\eta$), excess molar volume (V^E) and Gibbs free energy of activation of viscous flow ($\Delta G^{\#E}$) have been calculated. The results of excess volume (V^E), viscosity deviation ($\Delta\eta$), Gibbs free energy of activation of viscous flow ($\Delta G^{\#E}$) were fitted to Redlich-Kister polynomial relation to derive the coefficients and standard deviations. The result have been interpreted in terms of the interactions between the molecules in the binary mixtures.

PO-12 : Studies on Dynamic Thermogravimetry of Magnesium Salts of α-amino Substituted Fatty Acids

Vinod Kumar Malhotra

Applied Sciences & Humanities N.C.Institute of Technology,
Israna (Panipat), 132103 Haryana

Thermogravimetric curves show that the salts decompose insignificantly upto 200-2600°C, rapidly and finally no change occurs with further increase in temperature above 4000, 5200 and 3200°C, respectively for a-amino barium butyrate, a-amino Magnesium caproate and α-amino iso-caproate. The results of thermogravimetric analysis show that final residue is Magnesium carbonate.

The weights of the residue of these salts are almost equal to theoretically calculated Magnesium carbonate from the molecular formula of salts. Thus barium salts decompose into Magnesium carbonate and the ketone which goes off from the sample.

PO-13 : Kinetics of Formation of Thiazole by Cyclisation

B.H. Zaware[1*] and S.R. Kuchekar[2]

[1]Department of Chemistry, New Arts, Commerce & Science College,
Ahmednagar (MS) 414 001.
[2]Analytical Chemistry Laboratory, Department of Chemistry, A. C. S. College,
Satral, At. Satral, Tal. Rahuri, Dist. Ahmednagar, (MS) 413713.
E-mail : bhaskarzaware@gmail.com, shashi17@gmail.com

The kinetic study of 3-chloroacetyl acetone with various thioureas has been carried out in ethanol. In this study thioureas used are m-methyl phenylthiourea, m-methoxy phenylthiourea, m-ethoxy phenylthiourea and m-chlorophenyl thiourea. The kinetic study reports second order rate constants for these reactions. The rate of reaction is first order with respect to thioureas and first order with respect to 3-chloroacetyl acetone. The effect of substituents on the rate of reaction is also studied. Thermodynamic parameters are used to explain the nature of reactions. The proposed reaction mechanism for reactions is studied and details of kinetics are studied.

PO-14 : A Comparative Study of Differential Thermal Analysis and Differential Thermo Gravimetry of Lithium and Strontium Salts of α-Amino Fatty Acids

Vinod Kumar Malhotra[1], Rita Gahlot[2] and Ira Garg[3]

[1]Applied Sciences & Humanities, NCIT Israna Panipat-132103 (Haryana)
[2]Research Scholar from Karnal
[3]Department of Chemistry, Arya College, Panipat

Chemical analysis of lithium and strontium salts of α-amino fatty acids exhibits that these salts are free from water of crystallization. The nitrogen content of these salts is found by standard analytical methods and the results seem quite similar to their theoretical values. Differential Thermal Analysis (DTA) is one of the techniques in which the heat is produced when the substance undergoes chemical and physical changes. The thermal transition, which a substance undergoes on heating or cooling can be explained with the help of DTA. The main advantage of this technique over TGA is that DTA is capable of finding changes that are not accompanied by change in crystal structure of melting. The peak area is mathematically related to the heat of reaction, hence kinetic information can also be obtained from DTA measurements. This techniques has been extended to heterogeneous kinetics where the variation of peak temperature with heating rate is studied.

PO-15 : Mixed Micellization of Amphiphilic Drug Amitriptyline Hydrochloride and Nonionic Surfactant Triton X-100

Md. Sayem Alam

Council of Scientific and Industrial Research (CSIR) - Central Leather Research Institute (CLRI), Industrial Chemistry Laboratory, Adyar, Chennai
E-mail : sayem@clri.res.in, sayemalam@gmail.com

Herein, we report the surface properties and mixed micellization of an amphiphilic tricyclic antidepressant drug, 3-(10,11-dihydro-*5H*-dibenzo[*a,d*]cycloheptane-5-ylidene)-*N,N*-dimethyl-1-1-propanamine hydrochloride (amitriptyline hydrochloride, AMT) with nonionic surfactant poly(ethylene glycol) *t*-octylphenyl ether (TX-100) using surface tension measurements. The surface properties in aqueous solution of AMT drug in absence and presence of TX-100 are presented. The critical micelle concentration (cmc), maximum surface excess concentration at the air/water interface (Γ_{max}) and the minimum area per surfactant molecule at the air/water interface (A_{min}) parameters are evaluated. Γ_{max} increases and cmc as well as A_{min} decrease with increasing concentration (mole fraction) of the additive (TX-100). Furthermore, for better understanding of the behaviour of drug molecule in water, we also report the thermodynamics of AMT in absence and presence of TX-100 and evaluated Gibbs energies (viz., at air/water interface (G^{s}_{min}), the standard Gibbs energy change of micellization ($\Delta_{mic}G°$), the standard Gibbs energy change of adsorption ($\Delta_{ads}G°$), the excess free energy change of micellization (ΔG^{m}_{ex}). The results have relevance in drug delivery/model drug delivery.

PO-16 : Photodegradation of Methyl Red by Advanced and Homogeneous Photo-Fenton's Processes : A Comparative Study and Kinetic Approach

K. S. Anantha Raju[a, b] **S. Girish Kumar and L. Gomathi Devi** [a, *]

[a]*Department of Chemistry, East West Institute of Technology, Visvesvaraya Technological University, Magadi Main Road, Bangalore-560091, Karnataka*
[b]*Department of Post Graduate Studies in Chemistry, Central College Campus, Dr. B.R. Ambedkar Veedi, Bangalore University, Bangalore-560 001*
E-mail : gomatidevi_naik@yahoo.co.in, ananth.che@gmail.com

The degradation of methyl red (MR), an azo dye, was carried out by the homogeneous photo-Fenton's process (HPFP) and the advanced photo-Fenton's process (APFP) using symmetrical peroxides such as hydrogen peroxide and ammonium persulfate (APS) as oxidants. The APFP showed higher efficiency than their homogeneous counterparts even at high dye concentrations due to the faster reduction of Fe^{3+} to Fe^{2+} ions on the iron surface. H_2O_2 proved to be a better oxidant for both the processes. However, APS efficiently inhibited the precipitation of iron oxy hydroxides at higher dosage of iron powder compared to H_2O_2 by providing excess acidity to the reaction medium. The rate constant for the kinetics of decolorisation by various oxidation processes is of the order: $Fe^0/H_2O_2/UV > Fe^0/H_2O_2/$ dark $> Fe^0/APS/UV > Fe^{2+}/H_2O_2/UV > Fe^0/UV > Fe^0/APS/dark > Fe^0/dark > H_2O_2/UV > Fe^{2+}/APS/UV > APS/UV > Fe^{2+}/H_2O_2/dark > Fe^{2+}/APS/dark > Fe^{2+}/UV$. The degradation reaction was followed by UV-visible and GC-MS spectroscopic techniques. Based on the intermediates obtained, probable degradation mechanisms have been proposed. It was found that the initial mechanism in the APFP involves the reduction of azo groups to amines while in the case of HPFP it leads to the formation of hydroxylated products due to the oxidation of azo groups.

PO-17 : Use of Nano-sized Iron / Zeolite Doped Titanium Oxide for Degradation of Methylene Blue and Erythrosine Blue

Aarti Ameta, Rakshit Ameta and Suresh C. Ameta*

Department of Chemistry, Pacific College of Basic & Applied Sciences, PAHER University, Udaipur (Raj.)
E-mail : rakshit_ameta@yahoo.in; ameta_sc@yahoo.com

We are all aware about ever increasing water pollution problems all over the globe. The water pollution is mainly caused due to the discharge of effluents of different industrial to their nearby water resources without any prior treatment. Various textile, dyeing and printing industries also create water pollution by discharging their colored waste water, which is harmful in nature. Use of a semiconductor as a photocatalyst provides a green chemical, low cost and eco-friendly method for solving the waste water problems. Although titanium oxide TiO_2 is an efficient, low cost commonly used photocatalyst, but its use is limited due to its white color and suspension problem in water. We have attempted to solve both these problems. We have prepared nano-sized iron doped TiO_2 particles, which were colored and also these were loaded on zeolite so that it could not create suspension. Methylene blue and erythrosine B were used as model systems. The effects of different parameters, which affect the rate of the reaction, were observed spectrophotometrically at regular time intervals. Tentative mechanisms were also proposed for photocatalytic degradation of these dyes. XRD and SEM of the prepared sample were also recorded.

PO-18 : Electrical Conductance Studies on the Interaction of γ- Substituted Metal Acetylacetonates with Hetero Cyclic Bases

Shailendra Raghav, Om Kumari* and Surabhi Singh

Department of Chemistry, K.K.P. G. College, Etawah-206001, Uttar Pradesh
E-mail : Omkumari56@yahoo.com

The electrical conductance of M $(NO_2 – acac)_n$ and its molecular complexes with heterocyclic N-Bases have been used to determine equilibrium constant, K_1, rate constant, k, and extent of polarization, p. The conductometric titration technique has indicated 1:1 stoichiometry of these complexes. Kinetic status of the interaction of M $(NO_2 – acac)_n$ with heterocyclic N-bases in different solvents have been also done. Rate constant (k), change in heat content (ΔH) and entropy change (ΔS) for these charge transfer complexes have been calculated.

PO-19 : Dielectric Properties of Pt $(NO_2acac)_2$ with Heterocyclic Bases

Bhoopendra Singh, Azarabegam Afridi and Vikesh Kumar

Department Of Chemistry, K.K.P.G. College, Etawah 206001 Uttar Pradesh
E-mail : vikeshitrc@yahoo.co.in

The dipole moments (μ), of $Pt(NO_2\text{-acac})_2$ and is molecular complexes with heterocyclic N-bases have been studied by refractive index, Guggenheim and dielectric plot methods. The formation of charge transfer complexes $Pt(NO_2\text{-acac})_2$ with heterocylic N-bases is further supported by dipole moment studies. The symmetry of $Pt(acac)_2$ is disturbed when γ-H of this chelate is replaced by the nitro group. An increase in the dipole-moment was observed in these systems after complexation. The maximum dipole moment of Pt(NO_2-acac)$_2$ pyridine complex was observed in pyridine which indicates stronger interaction with pyridine in comparison to other donors. The values are greater for pyridine system at different temperatures. The dielectric titration technique has indicated 1:1 stoichiometry of these charge-transfer complexes. From this study it has been observed that more polar is the solute the larger is the expected increase in its dipole moment values. Hence it may be concluded that the interaction of Pt(NO_2-acac)$_2$ with N-bases is governed by dipole electrostatic attraction.

PO-20 : Thermodynamics of Conductivity Measurements of Nickel Myristate at Different Temperature

M. K. Rawat and Mamta Gautam

Department of Chemistry, Agra College, Agra
E-mail : sangeeta.kumar47@rediffmail.com

Thermodynamic properties for dissociation, micellization and critical micelle concentration (CMC) for mixture of benzene and methanol (50/50 v/v) of varying composition at different temperatures from conductivity measurements were determined. The results showed that this soap behaves as a weak electrolyte in dilute solution and the values of the CMC increase with the increasing temperature. The dissociation and association can satisfactorily be explained in the light of phase separation model and the micellization process is predominant over dissociation process.

PO-21 : Sculpturing Effects of Cetyltrimethyl-ammonium Bromide and Poly(vinyl)alcohol in Shape Transformation of Silver Nanoparticles from Nanorods to Hexagonal Nanoplates

Zoya Zaheer* and Rafiuddin

Department of Chemistry, Aligarh Muslim University, Aligarh-202002, UP
E-mail : zoya.zaheer@gmail.com

The sculpturing effects of cetyltrimethylammonium bromide and poly(vinyl)alcohol on the shape transformation of silver nano-particles are presented. It is a simple process of recent interest for obtaining silver nano-rods, spherical and hexagonal nano-plates in the thiosulphate reduction of Ag^+ ions with or without stabilizers. Formations of silver nanoparticles were observed visually by color change of the reaction mixture from colorless to dark yellow. Interestingly, the reaction mixture remained colorless and no absorption peak due to the Ag-nanoparticles was observed at higher [$S_2O_3^{2-}$] ($\geq 20.0 \times 10^{-4}$ mol dm^{-3}). UV-vis spectroscopy and transmission electron microscopy (TEM) were used to monitor the growth and morphology of Ag-nanoparticles, which reveal to the nano nature of the particles. These studies infer that the particles are mostly spherical in shape and have an average size of 16 nm in absence of CTAB. Selected area electron diffraction (SAED) results indicate that the Ag-nanoparticles grow along the direction.

PO-22 : Removal of Indigo Carmine from Aqueous Solution Using Chitosan Adsorbent

N.S.Rajurkar* and Madhavi Pawar

Department of Chemistry, University of Pune, Pune-411007
E-mail : rajurkar@unipune.ac.in

Indigo carmine is used in textile industries on large scale. When released through effluent it causes water pollution, it is toxic and adversely affects cardiovascular system. Hence removal of this dye before release to the environment is important. Various methods such as physical, chemical and biological are used for its removal. However, adsorption method is found to be effective and environmentally clean. We have used chitosan as an adsorbent. The various parameters such as pH, contact time and dosage were optimized to get maximum removal of this dye. It was observed that maximum removal was found to be 98.67 % at pH 3 with contact time of 1hr by using 0.2 g of adsorbent. The adsorption mechanism was studied using Langmuir and Freundlich model. The data were also analyzed in terms of their kinetic behavior and was found to obey the pseudo second order equation.

PO-23 : Phosphotungsticacid Functionalized MCM-41 : An Efficient Catalyst for Knoevenagel Reaction

M. Nookaraju, I. Ajit Kumar Reddy*, A. Rajini and N. Venkatathri

Department of Chemistry, National Institute of Technology Warangal
Warangal – 506 004, Andhra Pradesh
E-mail : iakreddy@nitw.ac.in, mnraju@nitw.ac.in

Catalysis by mesoporous materials finds wide ranging applications due to their large surface area and tunable pore characteristics. Functionalization of these materials with acidic compounds enables them to efficiently catalyse various industrially important reactions to synthesize fine chemicals and intermediates. Phenyl barbiturates were found to be important intermediates in various pharmaceutical formulations. Phosphotungsticacid functionalized MCM-41 (PWMCM-41) has been synthesized by room temperature impregnation method. It has been characterized by PXRD, SEM-EDAX, FTIR and BET analysis for its morphological and structural characteristics. The material is

found to be porous in nature with regular arrangement of pores. The surface area of the material has been found to be 602 m^2g^{-1}. Presence of phosphorous in the framework has been confirmed by EDAX studies. FTIR spectra showed peaks at 1080 and 984 cm^{-1} corresponding to the stretching vibrations of P-O and W-O bonds.

Catalytic application of PWMCM-41 towards the synthesis of Phenyl barbiturates through Knoevenagel reaction has been investigated in water at room temperature. It has been found that the catalyst gives moderate to excellent yields in shorter reaction times without any side products. The reusability of the catalyst has been investigated.

PP-CYSA-01 : Synthesis of Ruthenium Nanoparticles through Microwave and their Environmental Application in Azo Dye Degradation

Sakshi Gupta[1,2], S. K. Mehta[1], M. Gradzielski[2], and Cristina Giordano[3]

[1]*Department of Chemistry and Centre of Advanced Studies,*
Panjab University, Chandigarh 160014
[2]*Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Berlin 10623, Germany*
[3]*Max-Planck Institut (MPI) für Kolloide und Grenzflächen, Department of Colloid Chemistry, Research Campus Potsdam-Golm, D-14424 Potsdam, Germany*
**E-mail : chem.sakshi@gmail.com*

The properties and applications of nanoparticles greatly depend on their size and shape. Due to the large surface to volume ratio of metallic nanoparticles, they are attractive for catalysis. Especially Pt group metals are used in a large number of reactions as catalyst. In our work we synthesized small and stable Ru nanoparticles using glucose and PEG as reducing and protecting agents, respectively. In order to have an efficient and fast procedure, we have used microwave irradiation as it reduces processing times, increases product yields, and enhances product purity. Effects of concentrations of glucose and PEG, different molecular weights of PEG, microwave power and irradiation time on the size and colloidal stability of the particles have been studied in a systematic fashion. The particles have been characterized by UV-vis absorption spectroscopy, transmission electron microscopy (TEM), X-ray diffraction (XRD) and dynamic light scattering (DLS). The nanoparticles were found to be spherical and of 3-4 nm in diameter. These particles were applied for the removal of a model pollutant from water, for which an azo dye was chosen as a representative major pollutant from the textile industry. The degradation of azo dye can be done by breaking the azo bond which can be catalysed by the metals. The reaction itself was followed by UV-vis spectroscopy. This study of the reaction kinetics was done for varying amounts of catalyst and dye using the synthesized Ru nanoparticles and they were found to be very effective for this catalytic degradation reaction.

PP-CYSA-02 : Facile Synthesis of Water Dispersed Copper Nanoparticles and its use in Organic Reaction

Ravneet Kaur[1,3], Surinder K. Mehta[3], Cristina Giordano[2] and Michael Gradzielski[1]

[1] Stranski-Laboratorium für Physikalische und Theoretische Chemie, Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, Sekr. TC7, D-10623 Berlin, Germany
[2] Max-Planck Institut (MPI) für Kolloide und Grenzflächen, Department of Colloid Chemistry, Research Campus Potsdam-Golm, D-14424 Potsdam, Germany
[3] Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh-160014
E-mail : virgo_ravneet@yahoo.co.in

Cu NPs are favorite candidates for catalyzing many organic reactions due to their cheap availability and mild reaction conditions. But their high reactivity towards oxygen necessiates not only their synthesis but also storage in a strictly inert environment, which is the biggest disadvantage. The present work focuses on two key aspects; firstly Cu NP synthesis using metallosurfactant under atmospheric conditions, with water as the solvent and secondly analysis of the catalytic efficiency of as synthesized metal nanoparticles. Stable, water dispersible Cu NPs were obtained by reducing metal complex in the presence of polyacrylic acid (PAA). Interestingly enough, other protecting agents such as polymers (polymethacrylic acid (PMAA)) or surfactants (dodecylamine, dodecylamine acetate) prove to be less efficient to prevent surface passivation of NPs. Reduction of nitrobenzenes was chosen to test the catalytic effect of the nanoparticles. By employing PAA capped Cu NPs, the catalytic activity was remarkably improved, given the fact that PAA is also efficiently preventing the oxidation of the Cu NPs.

PP-CYSA-03 : Novel Leads for Inhibition of Sulphate/ Thiosulphate ATP Binding Protein Activity

Mounika Badineni, Vasavi Malkhed, Kiran Kumar Mustyala and Uma Vuruputuri*

Department of Chemistry, Nizam College, Osmania University, Basheerbagh, Hyderabad - 500001
E-mail : vuma1957@gmail.com; vuma@osmania.ac.in

Tuberculosis is one of the deadliest threat to public health and a cause of 2 million deaths every year.The emergence of multi-drug resistance in TB is making the treatment more complicated.

Exploration for novel targets and leads is our need. cysA is a one of the four domains of sulphate importer binds to ATP and is required for transportation of sulphate into the cell. Sulphate plays a vital role in the detoxification reactions,responsible for drug resistance in the pathogen. In the present study cysA is treated as novel target for designing new leads against Tuberculosis. The 3D structure of cysA, with 353 amino acid residues, was built by applying comparative homology modeling techniques. The predicted 3D model is refined and validated. Virtual screening studies were applied to identify new leads against the identified putative active site. The leads are projected to be potent novel therapeutics for drug resistance inMtb with cysA antagonistic properties.

PP-CYSA-04 : Highly Sensitive and Selective Cyanide Ion Sensor Based on Modified ZnS Nanoparticles

Khushboo and S. K. Mehta
Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh-160 014
E-mail : kkhushboo2210@gmail.com

Polyethyleneglycol (PEG-2000) modified ZnS nanoparticles (NPs) have been used for the fabrication of a highly sensitive, selective, reproducible and reliable amperometric sensor for cyanide ion in aqueous solutions. The fabricated cyanide ion sensor exhibits a very high and reproducible sensitivity of ~79.7 $\mu A\ cm^{-2}\ nM^{-1}$ with a response time less than 2s and a detection limit of 0.177×10^{-6} mol L^{-1}, which is ~16 times lower than maximum value of cyanide (2.7×10^{-6} mol L^{-1}) permitted by the World Health Organization (WHO) in drinking water. Moreover, various amperometric responses of some common interfering ions (Cl^{-1}, Br^{-1}, NO_3^{-1}, SO_4^{-2} and CO_3^{-2}) have also been recorded which confirm that the fabricated sensor is highly selective. The system has been employed to find out the concentration of cyanide ion in industrial sample, which matches with results obtained from standard method. Hence this sensor is a promising candidate for detecting minute concentrations of cyanide with high sensitivity and specificity.

PP-CYSA-05 : Physicochemical and Spectroscopic Analysis of Lecithin – Tyloxapol Mixed Micellar System for Anti-Tuberculer Drug Delivery

Neha Jindal and S.K. Mehta
Department of Chemistry and Center of Advanced Studies in Chemistry,
Panjab University, Chandigarh – 160 014
E-mail : nehajindalchem@gmail.com

The present study delineates the formulation equimolar mixed micellar system of Lecithin – Tyloxapol using physicochemical and spectroscopic measurements. Thermodynamic and interaction parameters have been computed for the prepared mixed micellar system suggesting synergistic interactions in the mixed systems. The prepared formulation has been explored for the solubilization of anti-tuberculosis drugs (ATD's). Fourier transform infrared spectroscopic and Differential scanning alorimetric studies infer that the drugs are in harmony with the excipients used in the formulation. The entrapment efficiency of the formulation has been evaluated for three ATD's. Micropolarity measurements indicate location of all the three drugs inside the mixed micellar systems. *In vitro* release analyses exhibit sustained and acceptable release of the drugs from the formulation. Comparison of regression coefficients of different kinetic models reveal that release of ATD's from mixed micellar system follows first order exponential decay. It has been established that the fabricated formulation act as good reservoir for continuous delivery of ATD's which may decline the dosing frequency. The formulations will thus improve the drug bioavailability and may create a sound basis for the better management of the disease, making the directly observed treatment (DOT) more viable and affordable.

PP-CYSA-06 : Aggregation Properties of Dioctadecyle-dimethylammonium Chloride (DODAC) and Dodecylethyledimethylammonium Bromide (DDAB) Mixed Binary Cationic Surfactant System

Arun Kumar, S.K. Mehta*, Gurpreet Kaur, Shweta and G.R. Chaudhary

Department of Chemistry and Centre of Advanced Studies in Chemistry, Panjab University, Chandigarh – 160 014
E-mail : arunbisht84@gmail.com

In the present work an attempt has been made for the exact determination of critical vesicle concentration (CVC) and multilamilar vesicles transition of double chain Dioctadecyldimethylammonium chloride (DODAC) surfactant in aqueous media using conductivity, fluorescence, and absorption spectroscopic techniques. To understand the insight of mixed aggregates, thermodynamic free energy, molecular interactions parameter, vesicular and micellization behavior has been studied in presence of single tailed Dodecylethyledimethylammonium bromide (DDAB) surfactant as a function of molar ratio. The total critical micelle concentration, the degree of ionization of the mixed micelle (â), microenvironment and vesicles–micelles transition with different intermediate phase has been experimentally determined. Along with the experimental data, various theoretical models for mixed surfactant systems namely Clint, Rubingh and Motomura have been chequered to predict deviations from ideality. Results of this work support the non-ideal behavior of mixing of these surfactant mixtures and the deviation is mostly related to the difference in the chain length of surfactant.

PP-CYSA-07 : Fabrication and Characterization of Quantum Dots of CuS and their use as Heterogeneous Catalyst in Biginelli Reaction

Pratibha Bansal, G. R. Chaudhary and S. K. Mehta

Department of Chemistry and Centre of Advanced Studies,
Panjab University, Chandigarh, 160014
E-mail : pratibha.bansal25@gmail.com

Nanoparticles exhibit unique physical and chemical properties and have received much attention from scientists and researchers in different areas of science. CuS nanoparticles have quite interesting applications due to their biocompatibility i.e photo catalytic activity ,sensing, ceramics, organic catalyst etc. CuS quantum dots have been synthesized using domestic microwave. It is characterised by UV-visible spectrophotometer, X-ray diffraction (XRD), transmission electron microscopy (TEM), selected area diffraction technique (SAED). Size of nanoparticles is 2-3 nm seen from TEM image and calculated from Debye Scherrer formula. They are the most effective heterogeneous catalyst in one pot synthesis of dihydroprimidone, solvent free reaction, easy work up, very high yield of product, very less amount of catalyst use. Very less reaction time is due to surface to volume ratio of CuS quantum dots.

PP-CYSA-08 : Synthesis and Characterization of γ-Fe_2O_3 Nanoparticles and its Application for the Removal of Coomassie Brilliant Blue R-250 from the Aqueous Solution

Priya Saharan [b], Ganga Ram Chaudhary [a], S.K. Mehta[a] and Suman Mor[c]

[a]*Department of Chemistry and Centre of Advanced Studies in Chemistry,*
Panjab University, Chandigarh
[b]*Department of Environment Studies, Panjab University, Chandigarh*
[c]*Department of Chemistry, Central University of Rajasthan*
E-mail : saharanpriya@yahoo.com

γ-Fe_2O_3 were prepared easily using cationic surfactant cetyltrimethylammonium bromide. The prepared nanoparticles were characterized by XRD and TEM measurements. In the present study the adsorption of an anionic dye, Coomassie Brilliant Blue R-250 onto γ-Fe_2O_3 nanoparticles and its desorption was investigated. The systematic assessments of the parameters such as pH, adsorbent dose and effect of adsorbent on different concentration of dyes *w.r.t* contact time were examined. Adsorption isotherms and kinetics were also applied in order to understand the adsorption mechanism between the synthesized γ-Fe_2O_3 nanoparticles and adsorbate. Moreover, the γ-Fe_2O_3 nanoparticles and the adsorbed dyes were desorbed.

PP-CYSA-09 : Structural and Interactional Behavior of Aqueous Mixture of Choline Lactate

Shafila Bansal,[a,b] Ganga Ram Chaudhary,[a] S. K. Mehta[a] and A. S. Ahluwalia[c]

[a]*Department of Chemistry & Centre of Advanced Studies in Chemistry*
[b]*Department of Environment Studies*
[c]*Department of Botany, Panjab University, Chandigarh - 160014*
E-mail : shafibansal@yahoo.co.in

In order to identify the molecular interactions between green solvent system, water + lactate based room temperature ionic liquid (RTIL), 2-Hydroxyethyl-trimethylammonium L-Lactate ($[(C_2H_4OH)(CH_3)_3N][Lactate]$), thermodynamic *viz.* density ρ, speed of sound *u*, and specific conductivity κ and refractive index n_D have been investigated over the whole composition range, temperature ranging from 293.15 to 323.15 K at atmospheric pressure. The excess molar volume V^E deviations in isentropic compressibility ΔK_S partial molar excess volume V_i^E, deviations in partial molar isentropic compressibility $\Delta K_{S,i}$, deviation in specific conductivity Δκ and deviation in refractive index Δn_D have also been predicted over the whole composition range as a function of RTIL concentration at different temperatures (293.15 - 323.15 K). The results have been fitted into Redlich-Kister polynomial. Thermodynamic parameters shows a large deviation from ideality on mixing of water and $[(C_2H_4OH)(CH_3)_3N][Lactate]$. To have more understanding of the intermolecular interactions occurring in the aqueous mixture of $[(C_2H_4OH)(CH_3)_3N][Lactate]$, spectroscopic properties *viz.* IR, ^1H and ^{13}C NMR of these mixtures have also been examined.

PP-CYSA-10 : Fluoresence Quenching Studies of Salicylalidimine Based Schiff Base for Sensing of Copper in Aqueous Alcoholic Medium

Kamaljot Kaur, S.K. Mehta and Sukhjinder Singh

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh 160014
E-mail : Kamaljot.rajpal@yahoo.com

The study of fluorescence emission by some analytes (Cu^{2+}, Hg^{2+}, $Pb^{2+,}$ etc.) has long been hindering the fabrication of particles in 'turn-on' or ratiometric fluorescent sensors for these analytes. This work reports the synthesis and photophysical properties of a highly photostable Schiff base as receptor. The novel compound was configured as "fluorophore-spacer-receptor" system based on photo induced electron transfer. Photophysical characteristics of the examined compound were investigated in MeOH and water solution. The ability of the new compound to detect cations was evaluated by the changes in its fluorescence intensity in the presence of metal ions (Cu^{2+}, Cd^{2+}, Ni^{2+}, NH_4^+, Na^+, Ba^{2+}, Zn^{2+}). Among the tested metal ions, only Cu^{2+} was efficiently detected. Also, it is clearly shown that the synthesized and characterized Schiff base, considerably improves the sensor's photostability, sensitivity and selectivity.

PP-CYSA-11 : Enhancing the Solublity and Antioxidant Properties of Curcumin in Nanoemulsion

Raj Kumar, K. Kaur and S.K. Mehta

Department of Chemistry and Centre of Advanced Studies in Chemistry,
Panjab University, Chandigarh 160 014
E-mail : Raj.ranote3@gmail.com

Phospholipid-based nanotherapeutics, such as the encapsulation of bioactive compounds in microemulsions and nanoemulsions, are gaining popularity as nutraceutical delivery systems due to their effectiveness in improving the solubility, stability and bioavailability of the loaded food components. Curcumin, a potential component of Indian diet is not only a potential anticancer but also posses remarkable antioxidant properties. The paper exploits the formulation of curcumin loaded o/w nanoemulsions by sonication method where ethyl oleate act as oil phase and Tween 80, soy lecithin act as emulsifiers. The particle size and stability of nanoemulsion has been characterized by dynamic light scattering and UV-visible studies. Attempts have also been made to understand the morphology of loaded nanoemulsion. Efforts have also been made to understand *invitro* digestive release and loading studies. Also, the radical scavenging activity in this nanoemulsion has been found to be 90%. The protein interaction (protein oxidation) with curcumin loaded nanoemulsion has been characterized by fluorescence and FTIR technique.

PP-CYSA-12: Spectroscopic Investigation and Reactivities of Ruthenium(III) Catalyzed Oxidation of Anticholinergic Drug Atropine Sulfate Monohydrate by Hexacyanoferrate(III) in Aqueous Alkaline Media : A Mechanistic Approach

Manjunath D. Meti and S. A. Chimatadar*

P. G. Department of studies in chemistry, Karnatak University, Dharwad 580003
E-mail : schimatadar@gmail.com, manjunathmeti4@gmail.com

The kinetics of oxidation of an anticholinergic drug atropine

sulfate monohydrate by hexacyanoferrate(III) has been investigated spectrophotometrically in presence of ruthenium(III) catalyst in aqueous alkaline medium at 25°C and at constant ionic strength of 1.0 mol dm^{-3} . The stoichiometry is 1: 2, i.e., one mole of atropine sulfate requires two moles of hexacyanoferrate(III). The oxidation products, tropine and benzaldehyde were identified and confirmed by IR, GCMS, and ^1H NMR. The order with respect to hexacyanoferrate(III) and ruthenium(III) concentrations were found to be unity, while the order with respect to the atropine sulfate and OH^- concentrations were less than unity over the concentration range studied. The effect of ionic strength and dielectric constants were studied on the rate of reaction. The active species of oxidant and catalyst are $Fe(CN)_6^{3-}$ and $[Ru(H_2O)_5(OH)]^{2+}$ respectively. Based on the kinetic data and product analysis, a suitable mechanism involving complex formation has been proposed and the rate law is derived. The catalytic constant (K_C) was also calculated for catalyzed reaction at different temperatures. The activation parameters with respect to the slow step of the mechanism and thermodynamic quantities are also determined and discussed.

PP-CYSA-13 : A Study on the Effect of Thiophene on the Polymerization of Acrylonitrile Initiated by Benzoyl Peroxide

Ritesh Gupta, Akash Dev and R.K.S. Dhakarey*

**University Department of Chemistry, Institute of Basic Sciences, Khandari, Agra*
E-mail : riteshgpt99@gmail.com, iccrajkot2012@gmail.com

Polyacrylonitrile (PAN) 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 thiophene on the polymerization of acrylonitrile initiated by benzoyl peroxide has been studied. The different techniques like NMR, 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 thiophene. The FT-IR study proves the successful interaction of polyacrylonitrile with thiophene.

PP-CYSA-14 : Synthesis and Characterization of Polythiophene and its Composites with Calcium Carbonate Nanoparticles

Faizan Akbar and R.K.S. Dhakarey

Department of Chemistry, I.B.S., Khandari, Agra
E-mail : bondfaizan@gmail.com, iccrajkot2012@gmail.com

Polymer nanocomposites represent a new alternative to conventionally filled polymers. Because of their nanometer sizes, filler dispersion nanocomposites exhibit markedly improved properties when compared to the pure polymers or their traditional composites. These include increased modulus and strength, outstanding barrier properties, improved solvent and heat resistance and decreased flammability. The present study involves the synthesis of polythiophene (PTP) composites of calcium carbonate via insitu oxidative polymerization procedure. These composites were characterized by UV-VIS, FT-IR and XRD which proves the successful chemical synthesis of PTP and its composites. FTIR absorption peaks confirms the insertion of $CaCO_3$ in the backbone of polythiophene and also justifies the strong interaction of $CaCO_3$ with PTP. UV-VIS studies showed that UV absorption increases in nanocomposite as compared to pure polythiophene. The detailed studies will be presented.

PP-01 : Kinetics and Mechanism of Photo-catalytic Degradation of Bromothymol Blue with Ruthenium Doped TiO_2 Nano Particles

Raviraj M. Kulkarni[1*], Ramesh S. Malladi[1],
Manjunath S. Hanagadakar[1], Manjunath B. Bellakki[2],
Bhaskar Devu Mukri[2] and Sharanappa T. Nandibewoor[3]

[1]Department of Chemistry, Gogte Institute of Technology, Udyambag, Belgaum – 590008, Karnataka
[2]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, Karnataka
[3]PG department of studies in Chemistry, Karnatak University, Dharwad – 580003, Karnataka
E-mail : ravirajmk@git.edu

Photocatalytic degradation of Bromothymol blue in aqueous solution by Ru-TiO_2 under UVC (254 nm) irradiation was studied. The 0.2%, 0.4%, 0.8% ruthenium doped TiO_2 (Ag-TiO_2) nano particles were synthesized, by using the Liquid Impregnation (LI) method. The resulting nano particles were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM) and FTIR analysis. Scherrer equation was used to determine the size of the synthesized nanoparticles. The crystallite size of undoped TiO_2 was found to be 17.00 nm, while the crystallite sizes of 0.2%, 0.4% and 0.8% Ru-TiO_2 were 16.67 nm, 15.70 nm and 14.40 nm respectively. The pseudo-first

order rate constants of Bromothymol blue photodegradation by Ru-TiO_2 under UVC (254 nm) radiation at pH values in the range 3.0 to 6.0 were determined. Langmuir-Hinshelwood mechanism was used to determine the pseudo-first order rate constants. The pseudo-first order rate constants were found to decrease with increase in pH. Effect of UV intensity, catalyst dosage and initial concentration of Bromothymol blue on the degradation rate constant were also studied and discussed.

PP-02 : Synthesis, Characterization and Photo-catalytic Properties of Ruthenium Doped ZnO Nano Structures

Deepti R. Kulkarni[1]*, Raviraj M. Kulkarni[2] and
Sharanappa T. Nandibewoor[3]

[1]Department of Physics, KLS Gogte Science College, Tilakwadi, Belgaum-590006, Karnataka
[2]Department of Chemistry, Gogte Institute of Technology, Udyambag, Belgaum-590008, Karnataka
[3]PG Department of Studies in Chemistry, Karnatak University, Dharwad-580003, Karnataka
E-mail : deeptinadagouda@gmail.com, ravirajmk@git.edu

ZnO nano structures were prepared by both solution combustion technique and precipitation technique. In solution combustion technique $Zn(NO_3)_2$ is used as precursor and urea as a fuel. In precipitation technique $Zn(NO_3)_2$ and NaOH were used as raw materials. The resulting ZnO nanostructures were doped with 0.2%, 0.4%, 0.6% and 0.8% ruthenium, by using the Liquid Impregnation (LI) method. The doped as well as undoped nano structures were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM) and FTIR analysis. Scherrer equation was used to determine the size of the synthesized nanoparticles. The photocatalytic properties of ruthenium doped ZnO nanostructures prepared by both solution combustion and precipitation techniques were evaluated by measuring the degradation of methyl orange in water under the UV region and compared.

PP-03 : Kinetics and Mechanism of Silver (I) Catalyzed Reaction of Levofloxacin with Aqueous Chlorine

Raviraj M Kulkarni[1], Manjunath S Hanagadakar[1*],
Mahadev S. Gudaganatti[1], Ramesh S. Malladi[1] and
Sharanappa T. Nandibewoor[2]

[1]Department of Chemistry, Gogte Institute of Technology, Belgaum-590 008, Karnataka
[2]PG Department of studies in Chemistry, Karnatak University, Dharwad-580 003, Karnataka
**E-mail : manju.hanagadakar@gmail.com, ravirajmk@git.edu*

The kinetics and mechanism of the Ag(I) ion catalyzed reaction of levofloxacin (LFC) by free available chlorine (FAC) during water chlorination processes was investigated for the first time between the pH values 4.2 and 8.2. The pH dependent second order rate constants were found to decrease with increase in pH (e.g. Apparent second order rate constant; $k''_{app.LFC}$ = 149.72L mol^{-1} sec^{-1} at pH 4.2 and $k''_{app.LFC}$ = 2.234 L mol^{-1} sec^{-1} at pH 8.2 and at 25 !). The reaction rates revealed that Ag(I) catalyzed reaction was about eight-fold faster than the uncatalyzed reaction. The products of the reaction were determined by Liquid chromatography and high resolution mass spectrometry. The reaction proceeds via formation of intermediate complex between Ag(I) ion and levofloxacin, then HOCl reacts with the complex to form chlorinated product. The effect of catalyst, effect of initially added product, effect dielectric constant and effect ionic strength on the rate of reaction was also studied. The effect of temperature on the rate of the reaction was studied at four different temperatures and rate constants were found to increase with increase in temperature and the thermodynamic activation parameters E_a, $\Delta H^{\#}$, $\Delta S^{\#}$ and $\Delta G^{\#}$ were evaluated for the reaction and discussed.

PP-04 : Photocatalytic Degradation of lomefloxacin using Ag-TiO_2 Nano Particles

Raviraj M. Kulkarni[1], Ramesh S. Malladi[1*], Manjunath S. Hanagadakar[1], Manjunath B. Bellakki[2], Bhaskar Devu Mukri[2] and Sharanappa T. Nandibewoor[3]

[1]Department of Chemistry, Gogte Institute of Technology, Udyambag, Belgaum – 590 008, Karnataka
[2]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore – 560 012, Karnataka
[3]PG Department of studies in Chemistry, Karnatak University, Dharwad-580 003, Karnataka
**E-mail : rammesh_malladi@rediffmail.com, ravirajmk@git.edu*

Photocatalytic degradation of lomefloxacin in aqueous solution by Ag-TiO_2 under UVA (365 nm) irradiation was studied. The 1% and 2% silver doped TiO_2 (Ag-TiO_2) nano particles were synthesized, by using the Liquid Impregnation (LI) method. The resulting nano particles were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM) and FTIR analysis. Scherrer equation was used to determine the size of the synthesized nanoparticles. The crystallite size of undoped TiO_2 was found to be 17.00 nm while the crystallite sizes of 1% and 2% Ag-TiO_2 were 14.50 nm and 14.11 nm respectively. The pseudo-first order rate constants of lomefloxacin photodegradation by Ag-TiO_2 under UVA (365 nm) radiation at pH values in the range 4.0 to 8.0 were determined. The pseudo-first order rate constants were found to decrease with increase in pH. Effect of UV intensity was studied by varying the lamp distance from the target and the intensity was measured using an optical power meter (2936 C optical power meter, Newport). The rate constants were found to increase with increase in UV intensity. Effect of catalyst dosage and initial concentration of lomefloxacin on the degradation rate constant were also studied and discussed.

PP-05 : Effect of Anionic Gemini Surfactant on Aggregation Energies of Amphiphilic Drug

Sahar Noori, Andleeb Z. Naqvi, Wajid H. Ansari and Kabir-ud-Din

Department of Chemistry, Aligarh Muslim University, Aligarh, 202002
E-mail : sahar.noori@gmail.com

Micellization of an amphiphilic phenothiazine drug amitriptyline hydrochloride (AMT) in presence of anionic gemini surfactants has been studied by tensiometric measurements at different stoichiometric mole fractions of the gemini surfactants. Various parameters like critical micelle concentration (CMC), surface excess concentration (Γ_{max}), minimum area per molecule (A_{min}), interaction parameter of mixed micelle and adsorption monolayer (β^m, β^σ) as well as thermodynamic and micellar properties have been determined using Clint, Rubingh, Rosen and Motomura approach. The strong interaction showing very low CMC and large negative interaction parameter β were due to weakening of the electrostatic head group repulsion which favors the mixed micelle formation. The drug bind tightly with the anionic gemini surfactant by electrostatic, hydrophobic and ion–dipole interactions. Thermodynamic parameters for all three drug–geminis mixed systems were evaluated. From excess free energy of micellization we can conclude that thermodynamically stable micelles are formed with strong synergistic interaction.

PP-06 : Mixed Micellar Properties and Related Interaction Parameters of Butanediyl-1, 4-bis(dodecyldimethylammonium bromide) Gemini Surfactant with Pharmaceutically Important Amphiphiles

Gaurav Sharma[a], P. Ajmal Koya[b] and Kabir-ud-Din[a]

[a]Department of Chemistry, Aligarh Muslim University, Aligarh-202 002
[b]Department of Chemistry, National Institute of Technology-Mizoram, Chaltlang, Aizawl-796 012
E-mail : gauravsharma122007@gmail.com

Mixed micellization of cationic gemini surfactant butanediyl-1,4-bis(dimethyldodecyl-ammonium bromide) with pharmaceutically important amphiphiles, viz. nonionic surfactants (Brij-56, Brij-58) and triblock polymers (P-85 and F-108) has been studied tensiometrically.

Various physicochemical parameters of the studied systems including ideal *cmc* values, experimental and ideal micellar compositions, interaction parameters (both in mixed micelles and at monolayers), activity coefficients of the components, etc. have been evaluated by considering theoretical models of Clint, Rubingh, Rosen and Maeda. The critical micelle concentration (*cmc*) of the mixed micelles was lower than the *cmc*s of the individual components and showed a negative deviation from ideal cmc (cmc^*) values. The analysis reveals that the mole fractions of gemini (both in mixed micelles and in monolayers) are less compared to the nonionic surfactants/triblock polymers and the values of ΔG^0_{m}, ΔG^0_{ad}, G_{min} and $\Delta G^{\mathrm{m}}_{\mathrm{ex}}$ show that the stability of the studied mixed micelles decreases as the content of the gemini in the bulk phase increases.

PP-07 : Acoustic Behaviour of Trifluoperazine Drug in Different Co-solvents at 308K

Usha Wasnik* Ravi Jumle[a] and P.R. Rajput[b]

**Department of Chemistry, Arts Science and Commerce College, Chikhaldara Dist : Amravati (M.S.) 444807*
[a]Department of Chemistry , Shivaji Science College, Akot Dist : Akola (M.S.)
[b]Department of Chemistry, VBMV, Amravati (M.S.)
**E-mail : us.wasnik@gmail.com*

Measurements of ultrasonic velocity, density and viscosity at different concentrations of Trifluoperazine hydrochloride in 20% methanol and 20% dioxane have been carried at 308K using ultrasonic interferometer at frequency 2MHz. The derived acoustic parameters namely adiabatic compressibility (β_s), specific acoustic impendence (Z), intermolecular free length (L_f), apparent molar compressibility (ϕ_κ), apparent molar volume (f_v) were evaluated with a view of identification of the molecular interaction occurs in these solutions.

PP-08 : Role of Nickel Containing Polytungstometalate in Removal of Methyl Violet

Mamta Ordia[a], Daksha Sharma[b] and Rakshit Ameta*[c]

[a]Central Academy School, Sardarpura, Udaipur (Raj.)
[b]Department of Chemistry, Vidya Bhawan Rural Institute, Udaipur (Raj.)
[c]Department of Chemistry, Pacific College of Basic & Applied Sciences, PAHER University, Udaipur (Raj.)
E-mail : rakshit_ameta@yahoo.in; mamtakashvi@gmail.com

Advanced Oxidation Processes (AOPs) are considered as promising technology for waste water treatment. Photochemistry, which is a part of AOPs plays an important role in solving the removal of various organic pollutants from effluents of various industries. In the present work, the photocatalytic degradation of methyl violet has been investigated in aqueous solution using nickel containing polytungstometalate under different conditions. The progress of reaction was monitored spectrophotometrically. The effect of different parameters, which affect the rate of degradation of dye; such as effect of pH, dye concentration, concentration of polytungstometalate and light intensity were studied. A tentative mechanism involving hydroxyl radicals as an active oxidizing species has also been proposed.

PP-09 : Volumetric Parameters of N-P-chlorophenyl-4 Chlorobenzohydroxamic Acid at 303.15 and 313.15K

Shakuntla Raj and Rama Pande*

School of Studies in Chemistry, Pt. Ravishankar Shukla University,
Raipur-492010, Chhattisgarh
E-mail : shakun.raj2@gmail.com, rama.pande11@gmail.com

N-p-chlorophenyl-4-chlorobenzohydroxamic acid shows anti-tumor activity as studied in this laboratory. Its volumetric parameters, viz., molar molar volume (V), specific molar volume (V^S), excess molar volume (V^E), apparent molar volume (ϕ_v), apparent molar volume at infinite dilution (ϕ^0_v) and the values of experimental slope (S^*_v) at temperatures 303.15 and 313.15 K in dimethyl sulfoxide (DMSO). These data have been further used to explain the intermolecular interactions and are also applicable in QSAR analysis as molar volume is one of the important characteristic of steric parameters.

PP-10 : Enhanced Photocatalytic Activity of Manganese Doped TiO_2 Deposited with Metallic Silver Nanoparticles : A Charge Transfer Mechanistic View

B. Nagaraj and L. Gomathi Devi*

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

Silver was deposited on manganese doped titanates (Mn-TiO_2) by photoinduced deposition method. These samples were characterized by Powder X-ray diffraction (PXRD), UV-visible absorbance spectroscopy (UV-vis), Fourier Transformed Infrared Spectroscopy (FTIR), Photoluminescence (PL) and Scanning Electron Microscope (SEM). Manganese doped TiO_2 shows bicrystalline framework of both anatase and rutile phases. The catalyst shows enhanced photocatalytic activity due to the synergistic effect of bicrystalline framework of anatase and rutile structures with high intimate contact due to the similarity in their crystallite sizes. The deposited metal nanostructures help in the formation of resonant surface plasmons in response to a photon flux, localizing the electromagnetic energy close to their surfaces. Better charge separation is achieved near the semiconductor surface due to the localized field enhancing the photocatalytic activity. Different percentage of silver ranging from (0.1 - 1.5%) was deposited on the surface of Mn-TiO_2. The photocatalytic activity of the prepared catalyst was evaluated by using resorcinol as model compound along with oxidants like H_2O_2 and Ammonium per sulfate under UV/Solar light illumination. Optimum deposition was found to be 0.1% of silver. The electronic level of the dopant, high intimate contact between the anatase and rutile phases along with efficient electron trapping by silver nanoparticles plays significant roles in photocatalytic process.

PP-11 : Study of Rh(III) Catalysed Oxidation of Lactose in Presence of Some Oxidizing Agents- A Comparative Kinetic Study in Acidic Medium

Manoj Kumar Ghosh* and Surendra K Rajput

Department of Chemistry, Govt. Nagarjuna PG College of Science, Raipur (CG)
**E-mail : mkghosh01@yahoo.co.in*

The kinetics of Rh(III) catalysed oxidation of lactose by cerium (IV), potassium bromate and hexacyanoferrate(III) have been studied. In a particular kinetic run the order of reaction of Oxidant is found to be unity. Zero order dependence of rate with respect to Lactose was observed in cerium(IV) and bromated oxidation, compared to first order dependence in Lactose observed in hexacyanoferrate oxidation. The order of reaction with respect to $[H^+]$ is inverse fractional, nearly 1.5 and zero for cerium(IV), $KBrO_3$ and $Fe(CN)_6^{3-}$ oxidation respectively. The rates follow first order kinetics in [Rh(III)] in all the three oxidation reaction. The effect of $[KHSO_4]$ have also observed. Mechanism consistent with observed results under different conditions have also been proposed.

PP-12 : Synthesis and Study of Ester Mesogenic Homologous Series : Bis-(4-n-alkoxybenzoyloxy) 2,2-diphenyl Propanes

Mita D. Khunt and U.C. Bhoya

Department of Chemistry, Saurashtra University, Rajkot-360 005, Gujarat
E-mail : drucbhoya@gmail.com

Homologous Series Bis-(4-n-alkoxybenzoyloxy)2,2-diphenyl propanes have been synthesized and studied with a view to understand mesomorphic characteristics of the molecule. Mesomorphic property commences from sixth member of the series as polymesomorphism. Polymesomorphism is exhibited from hexyl to octyl derivative enantiotropically. Decyl derivative is exhibited from hexyl to octyl derivative enatiotropically. Decyl derivative is missing smectogenic mesophase but passes only nematogenic mesophase. The series is of high melting type with considerable mesomorphic range. Transition temperatures are determined by hot stage polarizing microscope.

PP13 : Study of Thermodynamics of Hydrochloric Acid in Glycine-Water Mixture by EMF Measurement Method

***Sanjay Ghosh, [1]Manoj K. Ghosh and [2]Ashish K. Ghosh**

**Department of Chemistry, Govt Nagarjuna PG College of Science, Raipur-492010,(C.G)*
[1]Department of Engineering Chemistry, Parthivi College of Engineering and Management, Bhilai-3
[2]Department of Physical Chemistry, Science College, Patna University,Patna-800005
E-mail : mkghosh01@yahoo.co.in

The present investigations have been carried out to determine the activity coefficients of hydrochloric acid in aqueous glycine solutions under various conditions to study on the ion solvent interactions in different temperatures. The study on the ion- solvent interactions in dioxin-water mixture are reported the number of mono and dicarboxylic acids. We can use HCl-NaCl and HCl–KCl as an electrolyte. The standard molar potential (E_m^0) of the cell; Pt;H_2(g)/HCl(m) x% Glycine; Hg_2Cl_2(S)/Hg have been determined in 05%,10%, 15%, 20%, 25% 30%, 35% and 40% (w/w) of Glycine-Water media at six different temperature range from 303 to 333K and molality range from 0.005 to 0.1 mol Kg^{-1}. The mean molal activity coefficients of HCl in the same media and temperature range are also computed. The primary and secondary ion-solvent effects are also reported.

PP-14 : Volumetric and Acoustic Properties of Ionic Liquid with Toluene and Isomeric Chlorotoluenes at Different Temperatures

K. Sreenivasulu[a], V. Govinda[b], P. Vasundhara[a], P. Venkateswarlu[b] and K. Siva Kumar[a]

[a]Department of Chemistry, S.V. Arts U.G and P.G College (TTD'S), Tirupati-517502, A.P.
[b]Department of Chemistry, S.V. University, Tirupati-517502, A.P.
E-mail : Sivakumark78@gmail.com

To understand the molecular interactions between ionic liquid (IL) with Toluene and isomeric chlorotoluenes, we have measured thermophysical properties such as densities (ρ) and ultrasonic sound velocities (u), at (298.15–308.15) K under atmospheric pressure for the binary mixtures of 1-Butyl-3-methylimidazolium Chloride–([BMIM][Cl]) (IL) with toluene and isomeric chlorotoluenes. The

experimental Densities and ultrasonic sound velocities values were obtained by using Rudolph Research Analytical densitometer (DDH-2991 model) and multi frequency ultrasonic interferometer over the entire composition range. Excess molar volumes (V^E), apparent molar volume ($V_{\phi,i}$), isentropic compressibility (k_s), excess isentropic compressibilities (κ_S^E) specific acoustic impedance (Z), and excess specific acoustic impedance (Z^E), intermolecular free length (L_f), Excess intermolecular free length(L_f^E), have been computed for these systems. The results were compared with those predicted by empirical equations proposed by Hwang et al. and Redlich-Kister.

PP-15 : Synthesis and Study of New Homologous Series : 4-n-alkoxy Benzyl Benzoates

Chintan M. Pandit and U.C. Bhoya

Department of Chemistry, Saurashtra University, Rajkot-360 005, Gujarat
E-mail : drucbhoya@gmail.com

A new homologous series of 4-n-alkoxy benzyl benzoates have been synthesized with a view to understand the relation between liquid crystal properties and molecular structure. Transition temperatures of the members of the homologous series are observed under Leitz Labourlux 12 POL-polarizing microscope with heating stage. The homologues of the series show variation in texture and transition temperatures. Series consist of twelve homologues in which butyl to octyl derivatives are enantiotropically nematogenic only. Decyl, dodecyl, tetradecyl and hexadecyl derivatives are enantiotropic smectic in addition to nematogenic character.

PP-16 : Thermodynamic Properties of Binary Mixtures of Aniline with Toluene's and Chloro Toluene at Different Temperatures

P. Vasundhara[a], K. Srinivasulu[a], P. Venkateswarlu[b] and M. Subbalakshmammaa

[a]Department of Chemistry, S.V. Arts U.G and P.G College (TTD'S), Tirupati-517502, A.P.
[b]Department of Chemistry, S.V. University, Tirupati-517502, A.P.
E-mail : sivakumark78@gmail.com

The densities(ρ) of pure liquids and their mixtures have been measured at 298.15 to 318.15 K and atmospheric pressure for five binary mixtures of aniline with toluene, ortho chloro toluene, meta chloro toluene and para chloro toluene by using Rudolph Research Analytical densitometer (DDH-2991 model) over the entire composition range. Further, ultrasonic sound velocities of all these mixtures at 303.15and 313.05 K. From these measurements, the excess molar volumes (V^E_m), apparent molar volumes ($V_{\phi i}$), isentropic compressibilities (K_S), and excess isentropic compressibilities (K_S^E), have been calculated. The measured excess molar volumes have been correlated with Redlich-Kister and Hwang equations and experimental sound velocities were analysed in terms of various theoretical models namely Collision factor theory (CFT), free length theory (FLT), Nomoto's relation (NO). The experimental results were discussed in terms of intermolecular interactions between component molecules.

PP-17 : Molecular Interactions between Benzyl Alcohol with Benzene and Substituted Benzenes

L.Venkatramana[1], K. Sreenivasulu[2] ,V. Govindu[3], P. Venkateswarulu[3] and K. Dayananda Reddy[*1]

[1]Department of Chemistry, P.V.K.N. Govt. Degree & P.G. College, Chittoor-517001, A.P.*
[2]Department of Chemistry, S.V. Arts Degree & P.G. College (T.T.D'S), Tirupati-517502, A.P.
[3]Department of Chemistry, S.V. University, Tirupati-517502, A.P.
E-mail : kollureddy@yahoo.com

Densities (ρ) of pure liquids and their mixtures have been measured at 298.15 K to 313.15 K and atmospheric pressure for the binary mixtures of benzyl alcohol with benzene, toluene, chlorobenzene, bromobenzene and nitrobenzene over the entire composition range by using Rudolph Research Analytical Digital densitometer (DDH-2911 model). Further, the Ultrasonic sound velocities for the above said mixtures were measured at303.15 K and 313.15 K. isentropic compressibility (k_S) have been measured.The measured excess molar volumes have been correlated with Redlich-Kister and Hwang equations, and experimental sound velocities were analyses in terms of various theoretical models namely collision factor theory(CFT), free length theory(FLT), Nomoto's relation(NO) binary liquid mixers, excess volumes (V^E) and excess isentropic compressibility (k_S^E) were calculated. The experimental results have been analysed in terms of intermolecular interactions between component molecules.

PP-18 : Studies on Some of the Acoustic Properties of Binary Liquid Mixtures of Benzene and Carbon Tetrachloride with Cumene and Pseudocumene

K. Yadav* and Anita Kumari#

Deptt. of Chemistry (P.G Centre), Samastipur College, Samastipur-848134, LNMU-DBG
#Research Scholar, LNMU-Darbhanga.
E-mail : yadav.kusheshwar@yahoo.com, yadavkspj@gmail.com

The study of equilibrium properties of benzene+carbontetrachloride have been measured as a function of mole fraction by using ultrasonic interferometer of frequency 2M Hz at 303.15K and 298.15K to understand the nature of molecular interactions. In this study the theoretical ultrasonic velocities were derived on the basis of Nomoto's relation and ideal mixture relation due to Van Deal and the percentage deviation of ultrasonic velocity from Nomoto's relation. Percentage deviation of Rao's constant, percentage deviation of Wada's constant, molecular interaction (available volume of Rao's constant (R) have also been calculated. Since excess functions are better measure of the extent of interaction present between the component molecules of any system. It is used in several fields of scientific researches e.g in physics, chemistry, biology, medicine and industry.

PP-19 : Mixed Micelles-to-Vesicles Transition in Zwitterionic/Anionic Surfactant System : Soy Lecithin/bis(2-ethylhexyl) Sulfosuccinate Sodium (AOT)/Water- a Prelim Investigation Towards Effective Encapsulation

Shweta

Institute of Forensic Science & Criminology, Panjab University, Chandigarh-160 014
E-mail : 25shweta@pu.ac.in

A mixed surfactant system consisting of double tailed anionic, bis(2-ethylhexyl) sulfosuccinate sodium (AOT) and zwitterionic, phosphatidycholine (LC) has been investigated in the aqueous media for spontaneous formation of microaggregates and their co-existence with micellar assemblies. The concentration of monomer-to-microaggregate transition (cac) as well as the concentration at which microaggregates exist with the vesicles (cvc) have been determined from conductivity and surface tension experiments at complete range of mixing ratio of two components. Molecular interactions have been elaborated through parameter, which reflects the difference in surfactant-surfactant interaction before and after mixing. The obtained cac and cvc values depict that the aggregates are formed at ease in the middle range of mole fraction (X_1=0.3-0.7). The implied physico-chemical study allows the analysis of aggregational behavior of the mixed formulation from molecular point of view.

PP-20 : Conductometric, Rheological and Acoustic Studies on Potassium Soaps

M.K. Rawat and Yadvendra Sharma

Department of Chemistry, Faculty of Engineering and Technology,
Agra College, Agra (282002)

The conductivity, density, viscosity and molar volume measurements have been made on the soap solutions of potassium (caproate, caprylate and caprate) with a view to determine nature, critical micellar concentration (C.M.C.) and interaction parameters. The results confirm that the soaps behave as a simple electrolytes and the CMC of these soaps decrease with increasing chain length of fatty acid constituent of the soap molecules. The values of CMC for these soaps obtained from conductivity and viscosity measurements are in agreement with the results obtained from ultrasonic measurements. The results show that the soap-soap interactions are weaker than soap-solvent interactions.

PP-21 : Use *N*'-(3,4-dimethoxybenzylidene) Pyridine-3-carbohydrazide as Corrosion Inhibitor for Mild Steel Corrosion in Acidic Medium Acid

Sangita Sharma[*] **and Naveen Kumar**

Department of Chemistry, Hemchandracharya North Gujarat University,
Patan -384 265 (Gujarat)
E-mail : smridhee2000@yahoo.co.in

The Schiff base *N*'-(3,4-dimethoxybenzylidene)pyridine-3-carbohydrazide was synthesized and characterized using various analytical tools like IR, NMR, ^{1}H, elemental analysis and TGA. It is studied as corrosion inhibitor for mild steel in 0.5M trichloroacetic acid by weight loss method and polarization method. The study was carried out at various temperatures ranging from 35-55± 0.1°C and different concentrations of *N*'-(3, 4-dimethoxybenzylidene) pyridine-3-carbohydrazide. The studied Schiff base is found to be an efficient inhibitor with percentage efficiency of 80-90%. Adsorption characteristics are explored for the inhibitor and the inhibition follows the Fredulisch's adsorption isotherm. A mechanism is proposed for this adsorption phenomenon.

PP-22 : Hydrolysis of Mono-3-chloro-2-methyl Aniline Phosphate Ester in Acidic Medium

Bhawana Bairagi and S.A. Bhoite*

School of Studies in Chemistry, Pt. Ravishankar Shukla University, Raipur,
Chhattisgarh 492010
E-mail : bhawana2005@gmail.com

Kinetic study of the hydrolysis of mono-3-chloro-2-methyl nitroaniline phosphate has been carried out in 0.1 to 7.0 M HCl at 50^{o}C. The rate of hydrolysis increases with increase in acid molarity up to 4 M HCl and after that it decreases. The lowering of rates after 4 M HCl has been attributed to the effect of water activity. Hydrolysis has been shown to be governed by both neutral and conjugate acid species. Hydrolysis of the monoester via conjugate acid species has been assigned bimolecularity of the reaction on the basis of Arrhenius parameters, Zucker- Hammett hypothesis and Bunnett&Bunnett – Olsen's parameters. Specific nature of the acid catalysis has been supported by pseudo-first kinetic order and solvent isotope effect. Solvent effect has been found to indicate the formation of a transition state in which charge dispersion occurs. Comparative kinetic rate data and isokinetic relationship have been used to propose the probable bond fission.

PP-23 : Viscosity, Density and Ultrasonic Velocity Studies of Binary Liquid Solutions of Isoamyl Alcohol and Isobutyl Alcohol in Benzyl Amine

M.G. Patil[a], **S.R. Patil**[a] **and A.U. Borse**[b*]
[a]*Arts, Science and Commerce. College, Chopda- 425107, (Jalgaon), M.S.*
[b*]*School of Chemical Sciences, N.M.U. Jalgaon, M.S.*
E-mail : manoharpatil.2011@rediffmail.com

Viscosity(η), density(ρ) and Ultrasonic velocities(U) are reported for binary mixtures of of isoamyl alcohol and isobutyl alcohol with benzyl amine over entered range of mole fractions at 303.15 and 313.15 K and atmospheric pressure. The viscosity deviation($\Delta\eta$), excess molar volume(V^E) and isentropic compressibility(K_s) have been calculated. These values were fitted with Redlich-Kister type polynomial equation.

PP-24 : Conductometric and Spectroscopic Studies of Various Surfactants in Aqueous Media in Presence of Organic Chalcogen

Rajeev Kumar
Department of Environment Studies, Panjab University Chandigarh-160014

Organochalcogen compounds represent an important class of compounds that contain direct C-E (E=S,Se,Te) bond. Despite a great deal of similarity organosulfur, organoselenium and organotellurium compounds exhibit certain characteristic differences in their properties. The growing importance of organoselenides as reagents and intermediate in organic synthesis, biochemistry, material and physical chemistry has stimulated interest in developing cheap and convenient methods for their preparation. The study of solubilization of the water-insoluble organic derivative of diselenide compounds in the surfactant micellar media. These chalcogenides are rigid nonplanar moieties having bulky selenium bridge and find potential applications in synthesis of various Se compounds. The pronounced consequences of organochalcogen compounds have been phrased in terms of alternation in the physicochemical behavior of the micellar media in the presence of these additives. The thermodynamic parameters, $\Delta G^o_{m,}$ ΔH^o_m and

ΔS^{o}_{m} have also been calculated and analyzed for the two different concentrations of the additive in the surfactant aqueous media. The system was monitored spectrophotometrically on a UV-Vis spectrophotometer as the function of additive as well as the surfactant concentrations. Insights into the dynamics of additive association with surfactant were carried out using FTIR and ^{1}H NMR studies.

PP-25 : Viscosities and Excess Molar Volumes of Binary Liquid Mixtures of 1,4-Dioxane with Organic Solvents at 298.15, 303.15 and 308.15 K

Prashant Pachauri, M.K. Rawat and Rita Dixit

Department of Chemistry, Agra College, Agra-282002

The excess molar volume V^{E}, viscosity deviation $\Delta\eta$ and excess Gibbs free energy of activation of viscous flow $\Delta G^{\#E}$ have been derived for binary liquid mixture of 1,4-dioxane with benzene, toluene, cyclohexane, n-hexane, chloroform and carbon tetrachloride from experimentally determined viscosity (η) and density (ρ) at temperature 298.15, 303.15 and 308.15 K over the entire composition range. These derived excess functions have been further fitted to the Redlich-Kister equation using a multiparametric nonlinear regression analysis. The viscosity data have been correlated with the various viscosity models such as Grunberg and Nissan, Tamura and Kurata, and Hind et al. to calculate the several intereaction parameters.

PP-26 : Study of Thermodynamics Property and Acoustical Function of Binary Liquid Mixture in Dimethylsulphoxide(DMSO) at 303.15K

A. K. Ghosh and R. Gunjan

Department of Chemistry, Patna University, Patna
E-mail : raman_gunjan2001@yahoo.com

Intermolecular interaction, acoustical and thermodynamics properties like ultrasonic velocity,viscocity, have been measured for the binary liquid mixture of some of the aromatic hydrocarbons such as toluene,benzene and chlorobenzene with dimethylsulphoxide(DMSO) at 303.15K. Thermodynamic parameter such as adiabatic compressibility (K_s), free length (L_f), free volume (V_f), internal pressure (P_i) and impedance (Z). The excess values of (V_E) some of the above parameters are also evaluated and discussed with reference to intermolecular interaction of the liquid mixture. It is eventually concluded that a weak intermolecular interaction is noticed. Such interactions are primarily due to weak vander Waals' forces, basically London dispersion force, dipole-dipole interaction, dipole- induced dipole interaction,sigma-pie, pie-pie interaction and H-bonding. The results studied indicates that among all the component the molecular interactions are more pronounced in the component System-II(DMSO+benzene).

PP-27 : Studies on Periodic Precipitation of Lead Carbonate in Agar Gel Medium

N. S. Rajurkar and Babita Ambekar

Department of Chemistry, University of Pune, Pune-411007
E-mail : rajurkar@unipune.ac.in

The present work deals with the studies on periodic precipitation of lead carbonate in agar gel medium. For this purpose lead nitrate was used as an outer electrolyte and sodium carbonate as an inner electrolyte and the reaction is carried out in 1% agar gel. The effect of inner (0.025 M and 0.05 M) and outer electrolyte (0.5 M and 1 M) concentrations was studied on the morphological characteristics of periodic precipitation. These include size of the rings, spacing between rings and number of rings per day. The concentration of reacting ions in the ring and in between the rings was estimated by Atomic Absorption Spectroscopy technique. The obtained results were verified on the basis spacing law, time law and width law.

PP-28 : Determination of Activation Energy for the Diffusion of Fe^{3+} Ions in Agar Gel Medium Containing Zinc Sulfate

N. S. Rajurkar*[1] and M. M. Kute[2]

[1]Department of Chemistry, University of Pune, Pune-411007
[2]Department of Chemistry, Modern College of Arts, Science and Commerce, Ganeshkhind, Pune-411053
E-mail : rajurkar@unipune.ac.in

The present paper deals with studies on the diffusion of ferric ions in agar gel medium containing zinc sulfate. The effect of gel concentration, electrolyte concentration and temperature on the diffusion of Fe^{3+} ions in zinc sulfate was studied with a view to verify Wang's model of diffusion and the applicability of transition state theory to diffusion in a gel medium. The diffusion coefficients were measured using the zone diffusion technique. The activation energy (*E)* is found to decrease with increasing electrolyte concentration in agreement with Wang's model. This observation is explained on the basis of the distortion in the water structure caused by ions and agar molecules. For a given electrolyte concentration activation energy is found to decrease with $W^{1/3}$ and D_0 with $W^{-2/3}$, where w is weight percentage of agar. This observation is accounted on the basis of transition state theory of diffusion.

PP-29 : Oxidation of Lysine by Chromium(VI) in Acid Perchlorate Medium : A Kinetic Study

Shanu Mathur[1], M.B. Yadav[2], Naveen Mittal[3] and Vijay Devra[4]

[1]Maa Bharati P. G. College, Kota-324007
[2]P. G. Department of Chemistry, Govt. College Kota , Kota-324001
[3]P. G. Department of Chemistry, Govt. J. D. B. Girls College, Kota-324001
[4]P. G. Department of Chemistry, Govt. J. D. B. Girls College, Kota-324001
E-mail : vdevra1@rediff.com

The kinetics of oxidation of lysine with chromium (VI) has been studied in perchloric acid medium. The oxidation product was identified as chromium(III) and 5-aminopentanaldehyde. The reaction is first order with respect to chromium (VI) and less than unit order in lysine concentration. Increase in acid concentration accelerates the reaction rate. Ionic strength and added products did not have any significant effect on the reaction. A suitable mechanism is proposed and reaction constants have been evaluated. Activation parameters have also been calculated.

PP-30 : Modifying Properties of Aqueous Gemini Surfactants with External Additives : Ionic Liquids 1-Hexyl-3-methylimidazolium Bromide at 303.15 K

Naved I Malek* and Utkarsh More

Applied Chemistry Department, S. V. National Institute of Technology, Surat-395 007, Gujarat
E-mail : utkarshumore@gmail.com

The critical micelle concentration (CMC) of cationic Gemini surfactant 1, 6- hexanediyl-a,ro-bis(dimethyltetradecylamminium bromide; C_{14}-C_6-C_{14}) with and without additives (I-Hexyl-3-methylimidazolium Bromide; [Hmim] [Br] is measured by surface tension, refractive index, electrical conductance and spectral change of dye by UV-Vis measurement at 303.15 K. The surfactant concentration required to reduce the surface tension of the solvent by 20 mN/m, C20, ratio of C20 and CMC, maximum surface excess, Γ_{max}, and minimum surface area per molecule, Λ_{min}, were evaluated from surface tension versus log Ct(Ct is the total surfactant concentration) plots. The CMC, degree of counterion binding (β), the standard Gibbs energy of aggregation (ΔG_m^0), the limiting molar conductivities (Λ_m^0) for the of aqueous C_{14}-C_6-C_{14} with and without addition of the ILs have been used for elucidation of aggregation characteristics of the studied Gemini surfactants. The dependence of the CAC, ΔG_m^0 and Λ_m^0 on the length of the alkyl chain of the cations and anions has been discussed.

PP-31 : Molecular Interaction Studies of Quinoline with Cresols at Temperatures 303.15, 308.15, 313.15, 318.15 K

**Chagarlamudi Kavitha*[1], Abbineni Ratnakar[1],
Mopidevi Durga Bhavani[2] and Kolla Narendra[2]**

[1]Department of Chemistry, V. R. Siddhartha Engineering College, Vijayawada-07
[2]Department of Physics, V. R. Siddhartha Engineering College, Vijayawada-07
**E-mail : chkavitha.chem@gmail.com*

Densities, ultrasonic velocities and viscosities of ternary mixtures of quinoline with cresols were measured at 303.15, 308.15, 313.15 and 318.15 K over the entire range of composition. Using these experimental data, various thermo acoustical parameters and some of their excess values such of adiabatic compressibility (β^E), molar volume ($V_m{}^E$), deviation in viscosity ($\Delta\eta$)) and excess Gibb's free energy of activation for viscous flow (ΔG^{*E}) were also calculated and the results were fitted to Redlich-Kister polynomial equation. The observed variation of these parameters, with composition and temperature were explained on the basis of intermolecular interactions present in these mixtures.

PP-32 : Theoretical Evaluation of Ultrasonic Velocity in Binary Liquid Mixtures at Different Temperatures

**Narendra Kolla*[1], Fakruddin Shaik[1], Bhavani Mopidevi[2],
Kavitha Chagarlamudi[2], Ratnakar Abbineni[2] and
Srinivasu Chintalapati[3]**

[1]Department of Physics, Velagapudi Ramakrishna Siddhartha Engineering College, Vijayawada, Andhra Pradesh -520007
[2]Department of Chemistry, Velagapudi Ramakrishna Siddhartha Engineering College, Vijayawada, Andhra Pradesh -520007
[3]Department of Physics, Andhra Loyola College, Vijayawada, Andhra Pradesh -520008
**E-mail : narenk75@gmail.com*

Theoretical values of ultrasonic velocity in binary liquid mixtures of n-heptanol, n-octanol and n-nonanol with anisaldehyde have been evaluated using Nomoto's relation, Junjie's theory, Rao's specific velocity, Van Deal-Vangeel ideal mixing relation. Theoretical values are compared with experimental values. Further, the molecular interaction parameter (α) was computed by using the experimental and the theoretical ultrasonic velocity values. The theoretical values are in better agreement with experimental values of ultrasonic velocity for alcohols + anisaldehyde mixtures. The results are discussed in terms of self association in the alcohols.

PP-33 : Excess Thermodynamic Properties of the Binary Mixture Aniline + Anisole between 293.15 to 323.15 K

Zubin R. Master and Naved I. Malek

Applied Chemistry Department, S. V. National Institute of Technology, Surat- 395007
E-mail : zrm17979@yahoo.com

The density (ρ), viscosity (η), refractive index (n_D) and speeds of sound (u) of the binary mixture Aniline + Anisole have been measured over the entire range of composition and at temperatures ranging from 293.15 to 323.15 K and at atmospheric pressure. The experimental values were used to determine the excess molar volume (V_m^E), excess ultrasonic velocity (u^E), isentropic compressibilities (Ks), excess isentropic compressibilities (k_S^E), Rao's molar volume (R), thermal expansion coefficients α_p, specific acoustic impedance (Z), excess acoustic impedance (Z^E), excess viscosities (η^E), excess refractive index (Δn_D), molar refraction (R_m) and excess molar refraction (ΔR_m). Results were fitted to Redlich-Kister polynomial equation.