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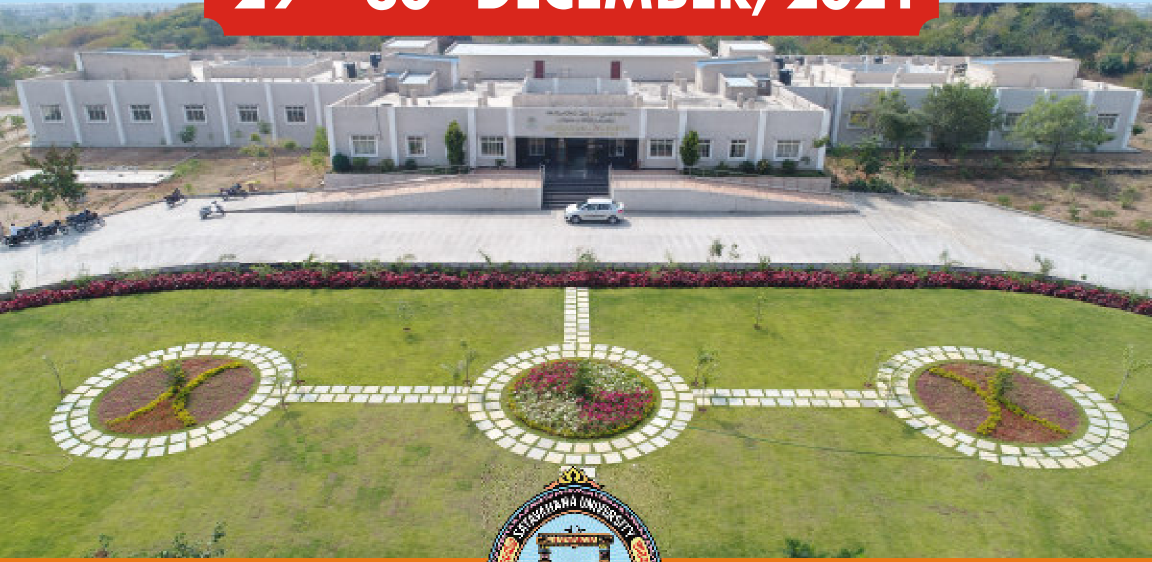
ANNUAL CONFERENCE
INDIAN COUNCIL OF CHEMISTS

29th - 30th DECEMBER, 2021



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ANNUAL CONFERENCE 2021

ABSTRACTS BOOK

Satavahana University
Department of Chemistry, Karimnagar (T.S.)

29th - 30th DECEMBER, 2021

Editor : Prof. R.K.S. Dhakarey

Welcome

Dear Fellow Researchers & Scientists

On behalf of the Indian Council of Chemists, it is my pleasure and honour to welcome you all to the XXXX Annual Online Conference to be held on 29th - 30th December, 2021 at Satavahana University Department of Chemistry, Karimnagar (T.S.).

As we all are facing difficult time due to spread of COVID pandemic, this Virtual Conference will give us opportunity to share our scientific chemical knowledge in online mode. In this Confernece we are giving opportunity to young researchers & other academician for oral presentations.

We are very much thankful to invited speakers and other senior researchers who contributed abstracts of their research work for this ICC Confernce.

I am thankful to all for your participation.

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

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Acknowledgements

The Indian Council of Chemists is going to hold its XXXX Annual Conference at Department of Chemistry, Satavahana University, Karimnagar (T.S.). in online/virtual mode on 29th-30th December, 2021 and the abstract book containing the abstracts of papers selected for presentation in the Conference is in your hands. The Council justifiably feels proud of its achievements during the past 40 years of its existence.

The Council is grateful to Prof. Sankasala Mallesh, Dr. M. Vara Prasad, Dr. Vannala Ramesh, Dr. Madderla Sarasija, Dr. A. Jeyanthi, Dr. V. Namratha, Staff Members and Students of Satavahana University Department of Chemistry, Karimnagar (T.S.) for their utmost cooperation in organizing the Conference.

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

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

Prof. R.K.S. Dhakarey
Editor

CONTENTS

ABBREVIATIONS

AIL - Analytical Invited Lecture
AO - Analytical Oral
IIL - Inorganic Invited Lecture
IO - Inorganic Oral
OIL - Organic Invited Lecture
OO - Organic Oral
PIL - Physical Invited Lecture
PO - Physical Oral
CYSA - Contestent for Young Scientist Award

KEY NOTE ADDRESS

New Tool Kits for Molecular Carpentry

V. Chandrasekhar[1,2]

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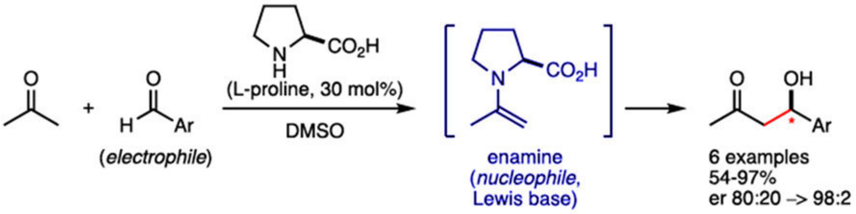
This year’s Nobel Prize in Chemistry has been awarded jointly to Benjamin List, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany and David W. C. MacMillan, Princeton University, Princeton, NJ, USA, “for the development of asymmetric organocatalysis”[1]. In this talk we will discuss the key works of the Laureates (Figure).



1. The Nobel Prize in Chemistry 2021. NobelPrize.org. Nobel Prize Outreach AB 2021. Wed. 17 Nov 2021. <https://www.nobelprize.org/prizes/chemistry/2021/summary/

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY SECTION

Sectional President's Address

Role of Analytical Techniques in Materials Characterization : An Overview

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Current research is focused on synthesizing material of vast variety. Analytical techniques and instruments play a crucial role in characterization of such materials. On applying such techniques one can get valuable information of materials synthesized for a range of applications. Various techniques such as TG-DTA-DTG analysis, FT-IR spectroscopy, Raman spectroscopy, UV-Visible Spectrophotometer, X-ray powder diffraction, X-ray Photoemission Spectrophotometer (XPS), Photoluminescence (PL), Scanning Electron Microscopy (SEM), EDX, Transmission Electron Microscopy (TEM), BET measurement for surface area, etc. are routinely used in characterization of inorganic materials. In addition to these techniques, spin properties are studied using ESR/EPR, magnetic studies using VSM, electrochemical studies by CV are done e.g. in tuned graphene, spin properties are monitored using ESR and VSM. Similarly, Second Harmonic Generation (SHG) by Kurtz-Perry powder technique and dielectric measurements by LCR meter for non-linear optical material are carried. While,^{1}H NMR, ^{13}C NMR spectroscopy and various chromatographic techniques are extremely useful for purification and characterization of organic materials. X-ray single crystal structure analysis gives unambiguous high-end characterization of organic and organometallic complex compounds especially for configurational confirmations. In the present topic, an overview with respect to Synthesis of pure / modified/ substituted material done by different methods and their characterization by various methods is taken.

AIL-01 : Development of Visible Active Metal Oxide Based Nanocomposites for Dye Degradation

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Inorganic and g -C_3N_4 nanoparticles hybrid materials tend to show better chemical, physical and mechanical properties than their component. Thus, their attractive applications in hybrid materials are more and more interesting to scientists in various fields. The inorganic nanoparticles with interesting and useful properties are uniquely associated with g -C_3N_4 nanoparticles. A consequence of their design and synthesis of hybrid photocatalyst have been focused on the combination of inorganic constituents likeZnO, TiO_2 with g -C_3N_4. As a result of the development in nanotechnology, the design/discovery and fabrication of surface modification of the hybrid have gained attraction to many researchers, particularly metal free crystalline materials empathize unique and beneficial properties of the hybrid such as photocatalytic, antimicrobial, antibacterial and self-cleaning properties.

Metal oxides face some problems like limited light absorption in visible light,To tackle these shortcomings a combination withsemiconductors like TiO_2 gives solid support making good absorption in visible light. In this, the green, eco-friendly synthesis of metal oxide nanocomposites were obtained from melamine powder and metal oxides. The photocatalytic degradation of MO inthe presence of UV-Vis. light is described over here. It is found that 98 % degradation takesplace which is two times greater than bare TiO_2 (46 %) under UV-Vis. light. Its reusability waschecked and found to be stable after 5 runs. The current study gives rise to a conclusion that. Many catalyst are also active in sunlight and shown better performance.

AIL-02 : A Plenty of Scope in the Field of Graphene Supported Nanocatalysts

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In the present time, as a consequence of indiscriminate industrialization, humankind is recognizing the solemnity of environmental contamination which induces precarious by-products that affect the surroundings. As a result, climes all over the globe have been disturbed leading to multiple awful weather conditions.

The prime approach to deal with it is to procure benefits by employing catalysts. Catalysts possess a crucial role to save energy for the majority of manufacturing units consuming higher inputs of energy, eventually conserving the environment. However, important issues associated with catalysts are excessive price, passable activity, agglomeration issues, moderate recyclability; which can be addressed by fabricating the catalysts on various solid supports; ultimately reducing the cost and obtaining greater competence. This provides ease of separation and recycling, minimizing agglomeration, declining the scrap, leading to the reduction of adverse environmental footprint.

Numerous solid supports are available to work as support for catalysts and enhance their catalytic proficiency. However, we emphasize the attention on carbonaceous materials especially graphite; a novel lightweight porous nanocarbon consisting of phenomenal properties like higher surface area, fascinating mechanical and thermal strengths, the ease of functionalization which serve as an excellent candidate to work as a support. The present talk is aimed to highlight the research carried out in my laboratory on graphene supported heterogeneous catalysts and their most pertinent results will be discussed.

AIL-03 : Toxicological Assessment of Environmental Bio-contaminants in Indoor Air of Pune and their Effective Mitigation by Natural Polymer-based Nanofibers

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Indoor particulate matter pollution is one of the leading global concern of our millennium with adverse outcomes on people's health. Degradation of indoor air quality in terms of biological components of particulate matter (known as bioaerosols) recently emerged as a pivotal cause of public health emergency owing to their highly diverse and dynamic nature. Present study is an interdisciplinary work aimed at investigating the level of bacteria and fungi associated with PM in indoor residential settings of Pune city with examining their toxicological profileand further inactivatethese bioaerosols by developing an antimicrobial Chitosan based nano-fibers. Highest concentration of bacterial (2016 ± 215 $CFUm^{-3}$) and fungal aerosols(1651 ± 298 $CFUm^{-3}$) were observed to be associated with PM_{10} size fraction. Commonly isolated bacteria and fungi identified in the indoor environments were Staphylococcus Aureus, Bacillus Sp., Pseudomonas Aeruginosa, E.coli., and Aspergillus sp., Cladosporium sp., Penicillium sp., Fusarium sp. respectively reveal a significant health risk due to their association with various respiratory tract infections.The cytotoxic profile of indoor PM and their biological constituents determined by MTT assay on A549 cells exhibited a significant decrease in cell viability (42.8% for PM_{10} and 48.6% and $PM_{2.5}$ samples) indicating the cytotoxic behavior of particles. In order to determine the route of mitigating these airborne pathogenic microbes for clean air management, biodegradable natural-polymer (Chitosan) based nanofibers were developed by electrospinning method due to its inherent antimicrobial nature and cost efficiency. Morphological examination revealed the uniform bead-free structure of the scaffolds with an average diameter varied from 82.1-285.6 nm.Different weight ratio of fibers exhibited an adequate surface area (16-36 m^2g^{-1}) for releasing the essential functional groups in order to prevent the microbial growth. No evidence of cytotoxicity of these scaffolds was observed in cell-viability test, suggested their biocompatible nature.Results of antibacterial efficiency of these fibers demonstrated their promising antibacterial action against the predominant airborne pathogens in indoor environments, and fibers embedded with maximum content of chitosan showed maximum inhibition on microbial growth. Results derived from the current study demonstrated that the indoor air of Pune is contaminated in terms of microbial load which can be effectively mitigated by the developed antimicrobial Chitosan scaffolds. Moreover, small diameter, low cost and minimal toxicity of these fibers made them useful to the level of industrial (bacterial filtration) and commercial applications (protective clothing) which will motivate future innovation in this area.

AIL-04 : Air Quality Determinants : Importance of Including Indoor Settings

Ajay Taneja

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Pollution is regarded as one of the great existential challenges of the Anthropocene epoch causing the largest category of welfare damage. Nine out of 10 people in the world breathe polluted air, causing more than 7 million premature deaths every year — double the number of people dying from HIV, malaria and tick-borne encephalitis combined. What remains partially unknown, however, is that while 3 million of these premature deaths are caused by outdoor air pollution-related diseases, more than 4 million are caused by indoor air pollution; yet the former covers the headlines that circuitously lead to ignorance of the air quality that people breathe. The study of Indoor air quality can be henceforth regarded as a dome in lieu of merely a discipline as the researcher's approach initially begins with addressing the concern related questions latterly followed by identification of suitable tools/techniques needed for solving the related 'purpose'. The effects of indoor air pollutants range from short term effects including eye and throat irritation to respiratory diseases and cancer abiding in the fullness of time.

In this work, a selection of datasets of studies done on indoor air quality at North Central part of India (Agra) region in homes and buildings located in different microenvironments during last fifteen years is presented. Sampling was undergone to monitor PM concentration with its diurnal, seasonal and annual trends assessed with identification of spatial-temporal trends in different microenvironments viz. roadside, rural and urban areas. Chemical composition of PM including metals and ions were identified. Source apportionment through PCA explained 76-88% of source contribution. Recent studies undergone elaborated the issue of size fractionated chemical composition of PM including ultrafine particles collected through deployment of impactors. Bioavailability index further calculated showed the importance of smaller size particles in simulated lung environment that further varied with element and size elucidating increase in aerosol enrichment to finest particle. In view of size segregated aerosol, q-UF particles were found to govern indoor (37%) and outdoor (28%) concentration levels; accounting as major health concern. Through regression model, the infiltration capacity of varied particle size modes in different housing conditions was found. Shifting of particles towards q-UF range in indoors of roadside homes impacted resident exposure to toxic particles. The work too includes the emerging issue with and future scenarios of the current pollution status in Indian context. It concludes with various remediation strategies and policy abatement by different governmental agencies in pollution control methods and technologies. The mainstay of control is henceforth trusted upon the education and awareness of the masses to pollution free 'cleaner' indoor environment.

AO-CYSA-01: Applications of TiO_2-CdS/Pt Composites Toward Solar Water Splitting and Hydrogen Generation

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Sunlight is an excellent source of clean energy and it can be stored for its use upon demand. For this purpose among the various approaches, Quasi Artificial Leaf or solar water splitting over semiconductor materials is the best option for harvesting and store abundant solar energy as clean and easily transportable hydrogen fuel. TiO_2 has been extensively studied as one of the typical photocatalysts over last few decades because of its low cost, nontoxicity, and high chemical stability. Recent studies have demonstrated that combining a wide band-gap photocatalyst with smaller band-gap semiconductors such as metal chalcogenides would be an effective way to harvests visible light and promote charge separation, leading to high efficiency for H_2generation. Herein, we present the preparation of TiO_2-CdS/Pt composites on Fluorine doped Tin Oxide (FTO) plates. The titania electrodes were sensitized with CdS growing by successive ionic layer adsorption and reaction (SILAR) method. The as synthesized materials were characterized by using different analytical technique. Like powder X-ray diffraction (PXRD) patterns, XPS, FT-IR, PL, DRS etc. The morphology and microstructure of the TiO_2-CdS/Pt composites were examined by scanning electron microscope (SEM). As synthesized FTO coated with TiO_2-CdS/Pt composites were used for water splitting and hydrogen generation under natural solar light. Gas analysis was carried out by regular sampling every hour, and gas chromatograph (GC) equipped with a TCD detector was employed for quantitative analysis. FTO coated with TiO_2-CdS/Pt composite shows excellent activity towards hydrogen generation. The activity was found to depend on number of SILAR cycle and dipping time

AO-CYSA-02 : Concentration of Pollutants in Schools of Agra during Online Classes after COVID Second Wave

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Indoor air pollution is 2-3 times harmful than that of ambient and among the top five environmental health risks to public health ranked by environmental pollution agency. The concern increases when the exposed population is delicate i.e. children as they have still developing organs, more physical activities and breathe more air as compared to their body weights which lead pollutants to become more concentrated in their systems. They spend second highest time in schools after homes. Owing to improper ventilation, filtering systems, high population density, proximity to outdoor particle source and challenging maintenance of building schools; schools represent a critical microenvironment for exposure to indoor air pollution to children. Both PM and indoor dust are crucial pathway of heavy metal exposure (inhalation, ingestion and dermal contact) to children in schools. Sampling was carried out in residential and on road schools located in urban and semi-urban areas of Agra in month of July when schools were closed due to COVID. SKC Cascade Impactor was used for PM sample collection ($PM_{2.5}$ and $PM_{1.0}$) on filter papers which were further extracted for metals concentration determination while settled dust was collected from tables, floor and windows of classrooms using soft paint brush and dustpan. The metals concentrations in PM and settled dust were determined by ICP-OES. $PM_{2.5}$ dominated over $PM_{1.0}$ in roadside school of semi-urban region while $PM_{2.5}$ and $PM_{1.0}$ were found in similar concentration in residential school of semi-urban area and roadside & residential school of urban region. In semi urban region, Ba was found in highest concentration in both sized PM in classrooms of roadside school while Al was highest in residential school. In $PM_{2.5}$ and $PM_{1.0}$, Zn and Al was highest in roadside school and residential school of urban region respectively. Al was highest while Se had lowest concentration in settled dust samples of residential and on roadside school of urban and semi-urban regions.

AO-CYSA-03 : Analysis of Trace Metals Content and Physicochemical Properties in *Caricapapaya* near Jhunjhunu, Rajasthan India

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Papaya (*Carica Papaya*) also called ‘pawpaw’, succulent fruit of a large plant of family caricaceae. *Carica Papaya*seeds ripe, leaves and unripe fruit are used as traditional medicine, also considered as Nutraceutical fruit due to its multifaceted medicinal properties. It has high content of Vitamin A, B and C. The plant of *Carica Papaya* has versatile biological function and pharmacological activity such as anti-inflammatory antioxidant, diuretic, hypoglycemic, anthelminthicactivity. The papain present in latex of *Carica Papaya*was found to be an enzyme for industrial use and of high research interest. Other, Chymopapain having antiviral, antifungal properties. Samples of *Carica Papaya* seed oil cultivated nearby industrial areas of khetri Jhunjhunu Rajasthan were collected and on digestion of oil for trace metals. MP-AES (Microwave Plasma Atomic Emission Spectrometers) technique was used for determination of trace metals (Cd, Cr, Co, Zn, Fe, Ni and Pb) accumulated in seed oil of *Carica Papaya.*The following trace metals concentration were obtained (mg/100g) Cr (2.78), Fe (1.91), Pb (1.43), Cd (0.82), Cu (1.48), Ni (1.23), Co (0.99), and Zn (0.79).Trace metals are among the major environmental contaminants and pose a severe threat to human and animal health by their long-term persistence. On HPLC (High Performance Liquid Chromatography) analysis, Oleic (55.38%), Linoleic acid (34.12%), Palmitic acid (5.80%), Stearic acid (3.20%), were found to be present in *Carica Papaya*seed oil. Oleic acid was also found as major fatty acid.*Carica Papaya* is one of the naturally gifted plants which in turn prevent and alleviate various disease & illness.

AO-CYSA-04 : Reduction of 2-Nitroaniline in Presence of Copper Ferrite

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The noble-metal nanocatalyst are widely used, but ferrite-based magnetic catalyst are rarely used. The magnetic metal ferrite MFe_2O_4 (M= Cu, Ni, Co and Zn) catalysts were synthesized by a hydrothermal method and used to reduce some nitroaromatic compound in presence of sodium borohydride. The metal ferrite quantum dots was analysed by X-ray diffraction spectroscopy (XRD), Energy-dispersive X-ray spectroscopy (EDX), and Scanning Electron Microscopy (SEM) to confirm morphology and size of particles. The reduction of 2-nitroaniline was observed in presence of metal ferrites as catalyst and sodium borohydride as the reductant. The conversion of 2-nitroaniline to o-phenylenediamine monitored by UV-Visible spectrophotometer. The effect of various parameters such as pH, concentration of nitro compound, and amount of catalyst were studied. The reaction was completed in 10 min in the presence of copper ferrite. It was observed that metal ferrite can be reused again without any significant loss of activity.

AO-CYSA-05 : Role of Tungsten Doped Bismuth Vanadate as Photocatalyst for Degradation of Toluidine Blue

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Advanced oxidation process (AOPs) have been used as an alternative and effective option for treatment of industrial wastewater, especially in case of non biodegradable compounds.It is well known

that bismuth-vanadate shows photocatalytic active property. In present work, it is doped with tungsten and used for degradation of toluidine blue dye. Doped and undoped bismuth vanadate were synthesised and characterised. These synthesized photocatalyst was characterized by using techniques such as FESEM, EDX and XRD.Effect of different operational parameters like pH, concentration, amount of bismuth vanadate, dose of dopants, light intensity, etc. was studied on the rate of reaction. On the basis of observations suitable mechanism for the photocatalytic degradation of toluidine blue dye has been purposed.

AO-CYSA-06 : Electro-Catalytic behavior and determination of Cardio Vascular β-blocking Agent, Acebutolol in Biological Fluids by Voltammetric Techniques

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In this research paper, different voltammetric tools such as cyclic, linear sweep, and square wave voltammetry were used to investigate acebutolol, β -blocker type of drug which is treated for a variety of ailments, including cardiovascular disease, using a carbon paste electrode under physiological environment. Under various phosphate buffer solutions, the voltammetric behavior of acebutolol displays two oxidation peaks and a reduction peak in the potential range of -0.2 to 1.4 V, with the optimum pH 7.0. The electrode reaction was diffusion controlled, accompanied by transfer of two protons and two electrons. The probable mechanisms were proposed. The square wave voltammetric technique (SWV) was used to perform quantitative analysis of acebutolol. The linearity range was found to be between 0.06 -10μM. The LOD and LOQ were measured to be 2.06 nM and 6.88 nM, respectively. Furthermore, the new approach was used to determine the amounts of acebutolol in physiological samples.The developed method is useful in pharmacokinetics and clinical laboratories.

AO-01 : Photocatalytic H_2 Production Over Ce/ZnO from Aqueous Methanol Solution

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

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Continual use of fossil fuel causes serious environmental problems.

H_2 is an excellent alternative for fossil fuel because its use does not result in the emission of carbon dioxide. The most eco-friendly H_2 production method is the photochemical water splitting over semiconductor materials. Photocatalysis using semiconductor materials, such as ZnO, allows the H_2 evolution with the aqueous 10 vol % methanol solution when it is irradiated by UV or solar light.In the present work the nanoparticles of ZnO with different amounts (0.5, 1, 2 and 3 mol %) of Ce were synthesized using the solution free mechanochemical method. It was determined the effect of the heat treatment on ZnO nanoparticles from 500 to 700 °C. The materials were characterized by powder XRD, HR-TEM, SEM, EDX, XPS, UV–visible and Photoluminescence (PL) spectra.The effects of Ce doping on the adsorption ability of ZnO, band gap, surface area, separation of electron-hole pairs, and photocatalytic activity of ZnO were investigated.The hexagonal wurtzite structure for Ce incorporated ZnO crystallites is supported by X-ray diffraction data. According to the PL spectra, the intensity of the green emission band increases as Ce ions are inserted into ZnO, which shows the low recombination rate of photogenerated charge carriers, which is responsible for greater photo-catalytic H2 production.When the dopant precursor concentration is too high, cerium oxide aggregates form around the nanorods, diminishing photocatalytic activity. 2 mol % Ce incorporated ZnO calcined at 600°C produces $43\mu molh^{-1}g^{-1}$ of hydrogen.

AO-02 : Treatment of Dyes from Synthetic Wastewater by using Plant Material as an Adsorbent

Anjali Bohra and Kailash Daga

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Environmental is compose of biotic (living) and abiotic (non-living) factors.it surround us and protect us but because of human activities it is degrading day- by- day and the substances which are polluting are-dyes, heavymetals, sulphidesetc. Dyes are used by many industries and the dye bearing waste water is discharged in rivers result in to waterpollution. These dye effluents are toxic and difficult to be remove by conventional waste water treatments. The removal of colour and dyes by adsorption using low-cost adsorbent has recently become the subject of considerable interest[1]

In the present work we have taken the seeds of ziziphusmauritianaplant to make charcoal and removal of dyes from waste water and the results were studied on FT-IR and UV-spectroscopy.

AO-03 : A Brief Overview of Heavy Metal Detection by Biosensors

Dharmendra Pratap Singh and Neerja Sharma

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Biosensors are a powerful alternative to traditional analysis methods not only to control the quality of natural water, but also to process water used by the industries in the production process, as well as to discharge wastewater into natural water sources. The aim is to provide the required quality and water safety from the perspective of heavy metal contamination. Biosensors have a dynamic trend for detecting heavy metal contamination and largely applied for improving the ground water quality. Biosensors have basic and most important features such as high sensitivity, low response time, specificity and relatively low production cost. Biosensors can detect and analyze the presence of various toxic heavy metals in water. Biosensors can be used for direct and continuous monitoring the water quality by measuring specific analyzes. This chapter provides an overview of the development and application of biosensors to control water quality and safety in view of the presence of heavy metals.

AO-04 : Dicarboxylate Assisted Fabrication of CuO Catalysts for Lowering Thermal Breakdown Temperature of Ammonium Perchlorate

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Amid various transition metal oxides, CuO is noteworthy due to its wide applications in heterogeneous catalysis, gas sensors, high-Tc superconductivity, electrochemical cells, field emission (FE) emitters etc. Ammonium perchlorate (AP) is a widely used oxidizer in composite solid rocket propellants. In an ideal manner, for a better performance of propellants, it is essential to reduce the thermal decomposition temperature (TDT) of AP. The cupric oxide (CuO), when used in catalytic amount exerts a remarkable effect on the decomposition of perchlorates by lowering its TDT. The crystal structure, particle size distribution, morphology, surface area and nanostructure of the CuO are imperative factors in controlling the AP thermal decomposition parameters. In our attempt, we have synthesized the different CuO nanocrystallites by calcinations of their dicarboxylate complex

precursors. The prepared oxide materials are thoroughly characterized by various instrumental techniques like IR, XRD spectroscopy, and the morphology of the materials was explored by SEM-EDS analysis. The nanocrystallite CuO materials are further employed as a catalyst for lowering down the TDT of AP. The use of 1 wt. % CuO catalyst obtained from its pure oxalate complex has shown a significant decrease in TDT from 396°C to 300˚C and may find application in propellant systems.

AO-05 : A Study on Removal of Fluoride Ions by Low- Cost Natural Adsorbent

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Increased concentrations of fluoride ions in drinking water can cause various diseases, such as rachitis, neurological disorders, tendon and ligament ossification and dental diseases. Very high concentrations can cause disorders of kidneys, thyroid, liver and testicles. With prolonged exposure at higher fluoride concentrations, dental fluorosis progresses to skeletal fluorosis. The Low Cost Natural Plant Adsorbent was investigated as an inexpensive and effective adsorbent for the adsorption of Fluoride ion from aqueous solution. The effects of initial Fluoride concentration, initial solution pH, and phases contact time, and adsorbent dose on the adsorption of Fluoride on Plant Leaves were investigated. The amount of fluoride adsorbed was found to vary with initial solution pH, Adsorbent dose, Fluoride concentration, and phases contact time. The Langmuir and Freundlich adsorption models were evaluated using the experimental data and the experimental results showed that the Langmuir model fits better than the Freundlich model. The adsorption rate data were analyzed according to the pseudo-first order kinetic and pseudo-second order kinetic models. It was found that kinetic followed a pseudo-second order model.

AO-06: Corrosion and Corrosion Protection of Calciferous Animals by Effluents

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Industries are discharged their effluents in rivers. Most of industries are established at the bank of rivers all over world and they released their effluents without charged in water sources. Effluents have possessed several types of impurities but acidic materials generated ambient environments for calciferous animals.

Freshwater contains unio, spire, gastropod, tortoise etc. and these species are maintained biodiversities water. Their outer parts are made of calcium carbonate ($CaCO_3$). When these species are come in contact of acidic water, chemical reaction starts their outer surface. The acidic medium produces galvanic, pitting, stress and crevice corrosion with calciferous animals. Acids deteriorate calciferous parts in this way their life is destroyed. Effluents are decreased the concentration of water in rivers thus the deficiency of oxygen occurs inside and outside of calciferous animals which accelerate corrosion reaction. Effluents are also developed microorganisms or macroorganisms in water. The Calciferous animals are surrounded by these organisms and they secrete acids which create hostile environment for them. It observes that most rivers these species are disappeared. Sulphur enters in fresh water through industrials, hospital, households, agricultural, food, animals and humans wastes which are oxidized to produce sulpuric acid. This acid corrodes calciferous animals. The oxides of carbon, nitrogen, sulphur are absorbed water to form carbonic, nitric and sulphuric acids. They develop corrosive medium for calciferous animals. Human and animals body are decomposed into river to release methylthiol and hydrogen sulphide and these substances are oxidized with BOD to form sulphuric acid which corrodes calciferous animals. The acid rain also develop unfriendly atmosphere for freshwater calciferous species. The corrosion rate was determined by weight loss experiment. The protection of calciferous animals in above mentioned acidic environment by the use of Aloe Vera as inhibitor and Turmeric as filler.

AO-07: Biosynthesis, Characterization and Antifungal Study of MgO/ZnO Nanocomposite using Azadirachta indica Leaf Extract

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The present study focuses on a green route for the synthesis of MgO/ZnO nanocomposites (MZ NCs) using Azadirachta indica aqueous leaf extract. The formation of biosynthesized MZ NCs was confirmed by different physico-chemical techniques viz. UV-vis, FT-IR, XRD, SEM, TEM, XPS and EDS with elemental mapping. Absorption peaks at 866.90cm-1 and 556.56 cm-1 in the FT-IR spectrum of MZ NCs may be assigned to Mg-O and Zn-O stretching and disappearance of some peaks in the spectrum of NCs confirms the involvement of phytochemicals for capping and stabilization of MZ NCs. Higher magnification studies with SEM analysis revealed the particles were

poly-dispersed, spherical and have the size range from 25 to 50 nm with some agglomeration. EDS analysis and element mapping showed the presence and uniform distribution of Mg and Zn in the prepared composites. Powder XRD study showed sharp peaks assigning to crystalline nature of the composites. Purity and presence of oxides of magnesium and zinc in the product had been investigated by X-ray Photoelectron spectroscopy (XPS). The obtained nanocomposites were tested for growth inhibitory activity on different fungus species, showed potential inhibitory activity. This study concludes that the plant Azadirachta indica was an excellent and reliable green source for production of potential antifungal MgO/ZnO NCs.

AO-08 : Treatment of Heavy Metals from Synthetic Wastewater by using Plant Material as an Adsorbent

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Pollution is affecting our environment in a negative way and it results in to environmental pollution and these substances which are polluting is called pollutant. These are of many types like organic (dyes) waste and inorganic (heavy metal) waste. Heavy metals play a vital role in environmental pollution and has created a problem all over the world. More and more countries have signed treaties to monitor and reduce heavy metal pollution [1] to solve we have lots of technique among them one adsorption. We can use many plant parts such as seeds,leaves,flower and stem.in the present work we have use leaves of calotropisprocera to make charcoal and absorb metals from wastewater and the results are calculated first by FT-IR and then by UV-spectroscopy and we obtained that this charcoal is having a good absorbing power.

AO-09 : Solar & Visible Light Induced Photocatalytic degradation of Acid Alizarin Violet N over Nano TiO_2 based Catalysts

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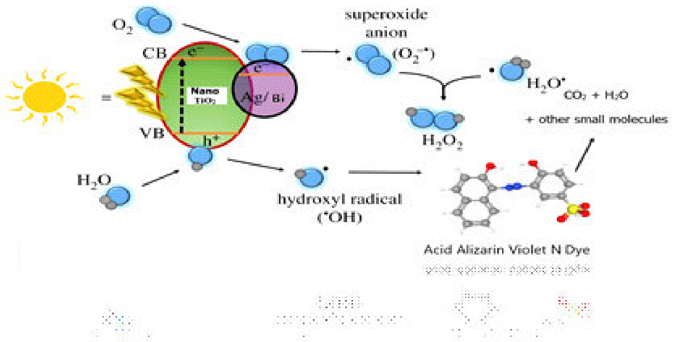
Photocatalytic degradation is today recognized as one of the efficient, economical and eco-friendly combating technologies to treat waste waters in the effective removal of the pollutants. TiO_2 based catalysts are inexpensive, simple and efficient to degrade the organic dyes. But the wide band gap and low rate of charge separation in TiO_2 (3.2 eV) hampers its efficacy with low visible light utilization. This can be overcome by doping in 3 ways: (i).O atom sites with N, P, S etc., and defects (ii). Ti atom sites with Cu, Zn, Ni, Fe etc., and (iii). Interstitial doping.

The present study thus is focussed on the doping of nano TiO_2 with Ag and Bi to widen its visible light absorption window that can enhance its photocatalytic activity. The Ag and Bi doped nano TiO_2 catalysts were synthesized by sol-gel method with 5wt% of the cation doping. These photocatalysts were then characterized by BET-SA measurements, XRD, UV-DRS, FT-IR, SEM-EDAX, XPS and PL techniques. The photocatalytic activity studies were studied by measuring the absorption intensities from time to time by UV-visible spectrophotometer and TOC measurements. Further the effect of scavengers on the photocatalytic activity of catalysts was also studied using both hydroxyl ion radical and peroxide ion radical/hole scavengers such as isopropanol, benzoquinone, ammonium oxalate and formic acid.

The photocatalytic activity of the catalysts studied both in visible and solar light clearly demonstrated a very high efficiency of the catalyst in degrading acid alizarin violet N (AAVN) dye to an extent of more than 98% on Ag doped TiO_2 followed by Bi modified TiO_2 to an extent of 96% and bare TiO_2 upto 90% with 50 ppm of dye. However, the doped catalysts maintained a nearly 80-90% degradation activity with higher concentrations of dye upto 150 ppm also unlike bare TiO_2 which degraded the AAVN dye only to 70% at higher concentrations. The good catalytic activity exhibited by the doped TiO_2 catalysts may be attributed to the well-formed nanoparticles of the photo catalysts as observed from XRD and SEM analysis and from the red shift observed from UV-DRS and PL spectra that clearly indicate the enhanced absorption of these catalysts in the visible region. The studies on reuse of the catalysts indicate them to retain the activity upto a min. of 4 cycles.



Photocatalytic Degradation of AAVN over doped Nano TiO_2 catalyst

INORGANIC SECTION

Sectional President's Address

Zero Field Splitting of Some Ni(II) Complexes

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Under the influence of crystal field perturbation, the degeneracy of d-orbitals or a spectroscopic term gets resolved by the electrostatic interaction, but the spin degeneracy of the term remains intact until a magnetic field is applied. When the complex contains more than one unpaired electron, the spin degeneracy, however may also be resolved by the crystal field and spin levels may undergo splitting even in the absence of magnetic field. This phenomenon is broadly known as Zero field splitting. For an even number of unpaired electrons the spin degeneracy may entirely be removed by crystal field. Ni(II) is a d^8-system having two unpaired electron with S = 1 and $m_S = +1, 0$ and -1. Zero field splitting removes that degeneracy of m_S and esr spectroscopy deals with such system specially, however UV/Visible spectra may also be adopted for the derivation of zero field splitting in Ni(II) complexes with D_{4h}-symmetry. The axial distortion parameter 'D_t' may be calculated by Wentworth and Piper formula. Zero field splitting parameter 'D' could be derived using the expression–

$$D = \frac{9.K_1}{\alpha^2}\left\{\frac{\mu_{eff}}{\mu_0} - 1\right\}^2$$

Since for d^8-system in O_h-crystal field the ground static cubic field terms is $^3A_{2g}$ which is orbitally non degenerate and subsequently no orbital contribution is expected to the magnetic moment of O_h-Ni(II) complexes. However several papers have been reported on six coordinate Ni(II) complexes with magnetic moment higher than 2.828 corresponding to two unpaired electron. Such abnormal magnetic moment may arise due to mixing of several terms because of the lowering of symmetry. According to Ballhausen the combined effects of a non cubic field and the spin orbit coupling in the six coordinate Ni(II) complexes lead to the zero field splitting of the ground state cubic filled term $^3A_{2g}$ which is three fold degenerate spin level. Its next excited state is $^3A_{2g}$ which is triply degenerate and hence under the perturbation of tetragonal field splits into a two-fold orbitally degenerate level and a singly degenerate one. Now spin orbit coupling comes in the action causing a coupling of a ground state together with the excited state subsequently the spin multiplate of the ground state experiences the splitting of the excited state. Subsequently the triplet spin level of $^3A_{2g}$ undergo a small splitting that is called zero field splitting, which ultimately explains the abnormal magnetic moment of Ni(II) complexes.

IIL-01 : Synthesis and Characterization of Some Biological Relevant Lanthanide(III) Complexes of Thiosemicarbazone and Pentamethylene Sulfoxide

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Coordination compounds are a class of substances with chemical structures in which central metal is surrounded by non-metal atoms or groups of atoms joined to it by chemical bonds. Coordination compounds include such substances in vitamin B12, hemoglobin, chlorophyll, dyes and pigments, and catalysts used in preparing organic compounds. Perhaps the earliest known coordination compound is the bright red alizarin dye first used in India and known to the ancient Persians and Egyptians, The first synthesis of a complex is available in literature by German physicist and alchemist Andres Libravius (1549-1615). Around the year 1600 he obtained blue $[Cu(NH_3)_4]^{2+}$ from NH_4Cl, $Ca(OH)_2$ and brass in water. The modern theory of coordination chemistry is based on the work of Alfred Werner (1866-1919, Nobel prize in Chemistry in 1913). The application of coordination compounds are of great importance and play important functions in the area of analytical chemistry, metallurgy, biological function system, industries and medicines. Medicinal inorganic chemistry is a discipline of growing significance in both therapeutic and diagnostic medicine. The discovery and development of the antitumour compound cisplatin cis$[Pt(NH_3)_2Cl_2]$ played a profound role in establishing in the field of medicinal inorganic chemistry.

Thiosemicarbazones and their metal complexes are a broad class of biologically active compounds. Mixed ligand complexes of transition metal containing ligands with N,S and N,S,O donors are known to exhibit interesting stereochemical, electrochemical and electronic properties. The real impetus towards developing their coordination chemistry was due to their physic-chemical properties and significant biological activities. 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 derivatives possess significant importance. In present studies some mixed ligand complexes of lanthanides (III) derived from 4[N(2',4'-dichlorobenzalidene) amino] antipyrine thiosemicarbazone (DCBAAPTS) and pentamethylene sulfoxide (PMSO) with the general composition LnX_3.n(DCBAAPTS).PMSO (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 DCBAAPTS behaves as neutral tridentate (N,N,S-donor) while PMSO acts as unidentate O-donor. The ligand and the corresponding Ln(III) complexes were simultaneously screened for their antibacterial and antifungal activities.

IIL-02 : Copper(II) Mono- and Binuclear Complexes with different Nuclearities and Geometries: X-ray Structures, Recurrent Supramolecular Motifs, Hirshfeld Surface Analysis, DFT Calculations and Superoxide Dismutase Activity

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The synthesis, characterization, DFT calculations and superoxide dismutase (SOD) mimetic activity of four new copper(II) mono- and binuclear complexes with formulas $[Cu(HL)(ClO_4)(H_2O)]CH_3OH$ (**1**), $[Cu(HL)(DMF)](ClO_4)CH_3OH$ (**2**), $[Cu_2(HL)_2(pyrazine)](ClO_4)_2$ (**3**) and $[Cu_2(HL)_2(4,4\text{-bipy})(ClO_4)_2]2H_2O$ (**4**) (HL = 4-bromo-2-(pyridine-2-ylhydrazonomethyl)-phenol, 4,4-bipy = 4,4-bipyridyl) have been synthesized and characterized by elemental analysis, FTIR, UV-vis and electron paramagnetic resonance (Epr) spectroscopy. Molecular structures of all complexes have been obtained using single crystal X-ray analysis. The geometry of copper(II) in **1** is distorted square pyramidal and distorted square planar in **2**. In binuclear complexes each copper(II) centre has distorted square planar and distorted square pyramidal geometry in **3** and **4**, respectively. The complexes **1-4** possess the self-assembled supramolecular structures *via* different molecular interactions (hydrogen bondings, $CH\cdots\pi$ and $\pi\cdots\pi$ stacking interactions). The possible intermolecular interactions were explored using 3D Hirshfeld surface and related 2D fingerprint plots, spectroscopic properties were studied using UV-visible and electron paramagnetic resonance techniques. Optimized geometry, frontier molecular orbital (FMO) and natural bond order (NBO) analysis were performed using density functional theory (DFT) calculations. To predict the chemical reactivity of complexes some global reactivity descriptors (chemical potential μ, electronegativity χ, hardness η and electrophilicity index ω) have been evaluated using DFT. The low temperature magnetic susceptibility measurements of binuclear complexes have been obtained predicts the magnetic exchange coupling value (J) by variable temperature measurements. The magnetic exchange coupling value (J) obtained are -8.1 and -2.4 cm^{-1} for **3** and **4**, respectively. The superoxide dismutases (SOD) of all complexes were measured using NBT assay method. The complexes show moderate superoxide dismutase (SOD) mimetic activity.

IIL-03 : Metal Chelates as Anti-hyperglycemic Agents: Synthesis and Studies of some Vanadium Compounds

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The interfacial studies overlapping Inorganic chemistry and Biomedical sciences , have attracted the attention of bioinorganic scientists in search of novel pharmacophores and metallodrugs. Inorganic chemistry applied to biology and medical sciences, has emerged as a recent offshoot of bioinorganic/medicinal-inorganic chemistry, which includes also, the metal-based drugs, metal sequestering or mobilizing agents, metal containing diagnostic aids and the medicinal recruitment of endogenous metal ions. There are references in indigenous Indian medicinal system Ayurveda , on the same. The metal complexes are amenable to combinatorial synthetic methods and an immense diversity of structural scaffolds can be achieved. Metal centers are capable of organizing surrounding molecules to achieve pharmacophoric geometries that are not readily achieved by other means. Understanding these interactions can lead the way towards rational design of metallopharmaceuticals implementations of new co-therapies. The design and synthesis of a suitable ligand perhaps is the key step in the development of coordination complexes with unique properties and novel reactivity. Principle of Reverse Pharmacology may help substantially in restoring the concept and therapeutic use practices of Traditional Medicinal systems, on issues to prevent and minimize the prevalent attacks of mutating and resisting microbes including viruses and fungi.

Metal complexes derived from Schiff bases and its derivatives have been studied extensively due to their facile synthesis, unusual configurations, and structural labiality. The insertion of designed Schiff bases as ligands in metal coordination sphere produces specific functionalities and exciting features with interesting theoretical and practical applications. Related issues shall be discussed in this lecture.

IIL-04 : Synthesis and Characterization of Complexes of Oxovanadium (IV) and Oxomolybdenum (V) with BIS (Isatinyl) Thiocarbohydrazone

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Isatine and its various derivative are an important class of heterocyclic compound and has privilege pharmacological activities. Its basic molecule indole derivatives are of plant origin and occurs in root and leafs of isatis tinctoria, couroupita guianesis, strobilanthes cusia and melochia tomentosa etc. Isatin is also found in human as it is a metabolic derivative of adrenaline. The presence of several reaction centers in isatine derivatives render them capable of participating in a large number of reactions and medicinal activities, like - antiviral, anticonvulsant, antioxidant, antitubercular, antidepressant, antiepileptic, transthyretin fibrillogenesis inhibitory, analgesic and spermicidal activities.

In present investigation we have prepared characterised and investigated antifungal behaviour of oxovanadium (IV) and oxomolybdenum (V) complexes with bis (isatinyl) thiocarbohydrazone.

Bis(isatinyl)thiocarbohydrazone has strong complexing property acting as multiple donor sites and forms strong stable complexes with most of the transition metal ions. Oxovanadium (IV) and Oxomolybdenum (V) forms insoluble products with bis(isatinyl) thiocarbohydrazone (HBisttch) of composition $VO(HBisttch)SO_4$, $MoO(HBistth)Cl_3$, $VO(Bisttch)_2$. $2H_2O$, $Mo_2O_4(Bisttch)_2$.$2H_2O$ and $Mo(HBisttch)Br_3$. These complexes are almost insoluble in aqueous medium but dissolve appreciably in organic solvents.

Mo_2O_4 $(Bisttch)_2$. $2H_2O$ is diamagnetic and other MoO^{3+} and VO^{2+} complexes are paramagnetic and show magnetic moment value in the range (1.70 – 1.78 BM) for one unpaired spin supporting oxidation state (IV) for VO^{2+} and (V) for MoO^{3+}. The anti-fungal screening with five fungi was performed by radial growth technique. It was found that the ligand and its complexes show strong antifungal properties in alcoholic DMF solution. The infrared and electronic absorption spectrum of complexes have been recorded and spectral bands of complexes have been assigned.

IIL-05 : Study of Some Tetragonally Distorted Octahedral Complexes of Cu(II)

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Cu(I) is a d^9 system having ^2D as its spectroscopic term which undergoes splitting under the influence of Octahedral Crystal field perturbation into ^2Eg and ^2T_2g Cubic terms. Obviously only one transitional band is expected in the electronic spectra of complexes of Cu(II) corresponding to only one spin allowed transition, i.e., $^2Eg \rightarrow {}^2T_2g$. But in the present study, the six coordinate complex of Cu(II) are found to have displayed three bands in their electronic spectra. It unambiguously indicates the further splitting of both the ground state cubic term ^2Eg and the excited state cubic term ^2T_2g under the influence of tetragonally distortion due to lowering of symmetry from perfect octahedron. As the ground state cubic term of Cu(II) under octahedral crystal field, i.e ^2Eg is doubly degenate and hence it is very prone to John Teller distortion effect to lift the degeneracy of ^2Eg by lowering of the symmetry. In term, the excited state cubic field term, ^2T_2g also suffers splitting. On the basis of three electronic bands the crystal field parameters $Dq_{(xy)}$ and $Dq_{(z)}$ have been derived along with the tetragonally distortion parameters, or Ds and Dt. The positive values of Ds and Dt and the less value of $Dq_{(z)}$ than Dq(xy) conspicuously suggest tetragonally distorted octahedral (D_{4h}) symmetry of these Cu(II) complexes with elongation along z-axis.

IIL-06 : Synthesis, characterization of Transition Metal Nanoferrites and their Catalytic Applications in MCR's Organic Reactions

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During the recent years ferrite nanoparticles have been found very interesting due to their unique characteristics which make them suitable for different applications. Among the different kinds of nanoparticles, metal ferrite nanoparticles field is one of the most widely studied and utilized. The easy preparation, higher stability and unique properties make the ferrite particle as the material of choice in many applications. Moreover, structural , magnetic and optical environments in spinel ferrites can be quite different, due to the distribution of iron and the divalent metal ions among the tetrahedral and octahedral sites of the spinel lattice.The metal ferrite nanoparticles [MFe_2O_4, M (II) = Co, Cu, Mg, Ni and Zn] were prepared by solution combustion method. The process was convenient, environmentally-friendly, inexpensive and efficient. The structure of the spinel compounds prepared by this method was confirmed by XRD and FT-IR studies. The surface morphology was observed by scanning electron microscopy. Due to its diverse properties, metal ferrites can be utilized as a catalyst in various organic reactions. The catalytic activity study of transition metal ferrites nanoparticles towards the synthesis of 3,4 dihydropyrimidin 2(1*H*) ones/thiones, 2-3 dihydroquanozolin 4(1*H*) one, Hantzch 1,4-dihydropyridine, tetrahydrodipyrazolopyridine and benzoxazin-ones/thiones derivatives with varied substitution have been described. The advantages of these protocols are its greenness with respect to mild reaction conditions, short reaction time, operational simplicity and high yields. Ferrite nanocatalysts can be easily recovered from reaction systems and reused up to several runs almost without loss of catalytic activity, thus they are considered as attractive catalysts for multicomponent reactions. The synthesized compounds were confirmed by using FT-IR, ^{1}H & ^{13}C NMR spectroscopic data and melting points compared with reported values.

IIL-07 : Chemical Implication of Metal-sulfur Cubanes in Term of Molybdenum and Sulfur

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Metal-sulfur cubanes play a very crucial role in biology as iron-sulfur protein especially ferridoxin available in hydroxylase and aconitase enzyme, iron-molybednum co-factor in nitrogenase enzyme and also in super-conductor as Chevral's phase compounds. The chemistry of molybdenum-sulfur and also related tungsten-sulfur cubanes are highly interesting.

Early 4d and 5d metals in lower oxidation status have virtually no simple aqueous chemistry comparable with that of the 3d-series elements. With 3d transition metals, readily available aqua species like $[M(H_2O)_6]^{n+}$ (n= 2,3), have no counter part in there higher congeners. Attempts have been made to study the chemistry of such aqua complex ion in term of higher congeners 4d and 5d transition metals.

Molybdenum and tungsten belong to the same group in periodic table and they show parallel behaviours in most of their chemical reactions, yet their chemistry differ in some of the aspect that will be presented in the present talk.

IIL-08 : Spectroscopic Study of Complexes of 2-(4-pyridyl) Benzothiazole

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2-(4-pyridyl) benzothiazole is prepared by reflucing the suspension of Sulphur, N-picoline and freshely distilled aniline. It has three potential donor site,i.e. the two endocyclic nitrogen atoms and one endocyclic sulphur atom. It is used for the synthesis of complexes with Co(II),Ni(II) and Cu(II) metal ions. The percentage composition of complexes obtained from their element analysis and their molar conduction lead to formation of the complexes as $[ML_2x_2]$where M stands for Co(II),Ni(II) and Cu(II),L for 2-(4-pyridyl) benzothiazole and X is $cl-$ .The comparative study of FTIR spectra of the free legand as well complexes helps trace of coordinating sites of the legands in complexes. The magnetic moment values of complexes predict their paramagnetic nature with magnetically dilute properties .Co(II) complexes display three legands due to three spin allowed transitions from which the different crystal field parameters are calculated leading to octahedral geometry of co(II) complexes. The UV/visible spectra of Ni(II) and Cu(II) complexes predict their octahedral geometry with a slight distortion.

IO-CYSA-01 : Synthesis and Characterization of Metal-Based Cellulose Film towards Fruits and Vegetable Packaging

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This paper presents a perspective on the research trends and solutions from recent years in the domain of antimicrobial packaging materials. The antibacterial, antifungal, and antioxidant activities can be induced by the main polymer used for packaging or by addition of various components from natural agents (bacteriocins, essential oils, natural extracts, etc.) to synthetic agents, both organic and inorganic (Zn, Ag, Ca) nanoparticles, synthetic antibiotics etc.). The general trend for the packaging evolution is from the inert and polluting plastic waste to the antimicrobial active, biodegradable or edible, biopolymer film packaging. Like in many domains this transitionsan evolution rather than a revolution, and changes are coming in small steps. Changing the public perception and industry focus on the antimicrobial packaging solutions will enhance the shelf life and provide healthier food, thus diminishing the waste of agricultural resources, but will also reduce the plastic pollution generated by humankind as most new polymers used for packaging are from renewable sources and are biodegradable. Polysaccharides (like chitosan, cellulose and derivatives, starch etc.), lipids and proteins (from vegetal or animal origin), and some other specific biopolymers (like polylactic acid or polyvinyl alcohol) have been used as single component origin blends to obtain antimicrobial packaging materials. Where the package's antimicrobial andantioxidant activities need a larger spectrum or a boost, certain active substances are embedded, encapsulated, coated, and grafted into or onto the polymeric film. This paper tries to cover the latestupdates on the antimicrobial packaging, edible or not, using as support traditional and new polymers, with emphasis on natural compounds.

IO-CYSA-02 : Spectroscopic and Biological Evaluation of Some Metal Chelates

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Glycine has found a good potential of biological activities. When it is condensed with a heterocyclic based aldehyde the resulting Schiff"s base may show enhanced antimicrobial activity. This ligand has several potential donor sites and hence capable of undergoing chelation with transition metal ions. In the present study the heterocyclic based aldehyde which 5-methyl 3- formyl pyrazole-3-yl has been condensed with glycine to produce 5-methyl pyrazole-3-yl-3-formal glycine (MLPF). This Schiff's base was used for chelation with Ni (II), Cu (II) and Zn (II) metal. The secondary ligand pyridine and á-picoline were used to occupy the axial position. The FTIR spectra revel the chelation from azomethyl nitrogen and dehydrogenated carboxylic oxygen. Thus, Five membered metal chelates are formed consisting of two heterocyclic five membered rings. The different crystal field parameters were derived from the UV visible spectral bands which predicts Oh or D_{4h} symmetry around the metal ion. The ligand as well as all the complexes were screened against gram -ve bacteria E.coli, K.pneumoniae and P.mirabilis as well as gram +ve bacteria like S.aureus, B.subtilis and M.luteus. The ligands as well as its complexes are found to be active against all the bacteria. The complexes have been found to be more biological active than the ligand. The inhanced microbial activity may be explained by chelation effect theory.

IO-CYSA-03 : Effect of Sr substitution on Structural, Electrical and Optical properties of $LaFe_{1-x}Sr_xO_3$ Perovskite Oxides

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The pure $LaFeO_3$ and Sr (0, 0.2, 0.4, 0.6, 0.8) substituted $LaFeO_3$ were successfully synthesized by citrate gel auto combustion method. These synthesized materials were characterized by TG-DTA, UV-DRS, FTIR, XRD spectroscopic techniques. As the amount of strontium (Sr) increased, electrical conductivity also increased at temperature up to 673K. The thermogravimetry and differential thermal analysis (TG-DTA) was used to identify the combustion temperature and the weight loss regime. The spherical morphology and elemental composition of the catalytic materials was ascertained by SEM-EDS analysis. X-ray diffraction (XRD) results were used to calculate the crystallite size and phase composition of the compound. The well intense peaks in the XRD pattern confirmed the perfect doping of strontium (Sr) in the $LaFeO_3$ lattice structure. The energy band gap (Eg) of the synthesized materials were calculated from the UV-DRS spectra using Tauc's relation. The band gap was observed to significantly decrease with increase in content of Sr in $LaFeO_3$.

IO-CYSA-04 : Surfactant Assisted Fabrication of ZnO Nanocrystallites for Catalytic Green Synthesis of 3-Substituted Indoles

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Medical applications of indole derivatives are promising against tuberculosis, malaria, diabetes, cancer, migraines, convulsions, hypertension, bacterial infections of methicillin-resistant Staphylococcus aureus and even viruses.

In present work, we have synthesized several ZnO nanocrystallites by surfactant assisted hydrothermal synthesis using several surfactants like SDS, Triton X-100, C-TAB and PVP. All the ZnO nanocrystallites were characterized by IR, XRD, FE-SEM and UV-DRS techniques. The XRD spectra showed the hexagonal wurtzite crystal structure of ZnO with crystallites size of 23-30 nm. The SEM images revealed different morphologies of synthesized ZnO nanocrystallites like spindle, Djembe shaped, nano flake and nano flower. The UV-DRS spectra exhibited the band gap of the ZnO materials from 2.90 eV- 3.10 eV.

The catalytic application of C-TAB assisted synthesized ZnO nanocrystallites is explored towards the synthesis of 3-[(arylthio)(aryl)methyl]-1H-indole derivatives through one-pot reaction in green solvent water at ambient conditions. All the indole derivatives were thoroughly characterized by IR, ^1H NMR, ^{13}C NMR and Mass spectroscopy. The key highlights of the established reaction protocol are green solvent, mild reaction conditions, moderate to good yields, ease of work up, inexpensive catalyst and no formation of dithioacetal by products.

IO-01 : Studies on DNA Binding, Cleavage, Molecular Docking, Antimicrobial and Anticancer Activities of Cr(III), Fe(III), Co(II) & Cu(II) Complexes of o-Vanillin and Fluorobenzamine Schiff Base Ligand

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The ligand [2-((2-fluorophenylimino)methyl)-6-methoxyphenol] and its metal complexes $[Cr(HL)_2]$ (1), $[Fe(HL)_2]$ (2), $[Co(HL)_2]$ (3) and $[Cu(HL)_2]$ (4) are synthesized. Characterisation of the complexes by sophisticated analytical techniques revealed the geometry around central metal ion to be octahedral for 1, 2 and 3 complexes and complex 4 with square planar geometry. Kinetic parameters of the complexes were estimated by Coats – Redfern method and the complexes were found to be thermally stable. DNA binding affinity of these metal complexes was explored by means of fluorescence, UV-visible and viscosity studies and the studies suggested intercalative mode. K_b and K_{SV} values were determined from the absorption and fluorescence studies for the synthesized complexes. Nuclease studies in the presence of H_2O_2 were performed using pUC19 supercoiled DNA. Docking studies were done using human DNA topoisomerase - I (DNA topo I) receptor protein. Biological studies revealed higher activity for complexes than the ligand and in vitro anti-tumour studies showed that complexes 3 and 4 possess potential inhibitory efficiency with an IC_{50} of 48.79±0.7 ìg/mL and 39.74±1.6 ìg/mL respectively. Molecular docking studies were carried out using Argus labs and geometry optimization is performed. Molecular orbital calculations of the ligand and complexes are computed using the reasonably accurate parametric model PM3 method 16 – 19.

IO-02 : Procurement Methods of Taro Starch : A Boon in Food Industry

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Taro, an eminent member of *Araceae* family, is frequently produced in developing countries by small-scale farmers. It belongs to the genus ***Colocasia*** and species ***esculenta***. Taro root contains a speciality starch ultimately known as resistant starch. People have been using it as a staple food for over 9000 years. It is midst the second most cultivated crops full-grown in tropical and sub-tropical zones. Taro is known for its edible corms, tubers and fibrous roots which contain a vast amount of micro- and macronutrients.

The starches have become a great matter of attention worldwide over the past few decades due to their complex structure consisting of polymeric glucose units. These units consist of linear (amylose) and branched (amylopectin) structures linked together. Basically, the starches present in root crops and seeds of cereals are quintessential food source. Carbohydrate content present in taro keeps on varying, reliant upon the different locations for its cultivation but remain unaffected by its respective corm size. High content of speciality starch explores its wide variety of applications in food industry as an emulsifier, binding agent and in pharmaceutical industry as a tablet-disintegrating agent. The present paper gives an overview to the various techniques implemented for the procurement of Taro starch in order to attain tailored properties and also explores its wide applications in food industry.

IO-03 : Spectroscopic Characterization of Coordination Compounds of 3-(m-nitrobenzylidene) amino-2-methylquinazoline-4-one (NMQ)

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By refluxing 0.01 mole of 1, 3-benzoxazine-4-one with hydrazine hydrate gives 3-mino-2-methylquinazoline-4-one which on condensation with 3-nitrobenzaldehyde produces 3-(m-nitrobenzylidene) amino-2-methylquinazoline-4-one (NMQ) as a Schiff base it has various coordination sites and easily produces metal chelates with Co(II), Ni(II) and Cu(II) from FTIR Spectra of complexes. The azomethine group and carbonyl oxygen are involved in coordination with metal ion. Both Co(II) and Ni(II) complexes display three bands each in their electronic spectra which were assigned to ${}^4T_{1g} \rightarrow {}^4T_{2g}$, ${}^4T_{1g} \rightarrow {}^4A_{2g}$ and ${}^4T_{1g} \rightarrow {}^4T_{1g}(P)$. For Co(II) complexes while ${}^3A_{2g} \rightarrow {}^3T_{2g}$, ${}^3A_{2g} \rightarrow {}^3A_{1g}(F)$ and ${}^3A_{2g} \rightarrow {}^3T_{1g}(P)$ electronic transitions. On the basis of these electronic spectral bands their crystal field parameters like 10 Dq, Racah Parameter (B), Nephelauxetic effect (β_{35}) were calculated and have been found in the good agreement with the values reported for octahedral complexes Cu(II) complexes display a broad band in their electronic spectra which is a good que for distorted octahedral geometry of Cu(II) complexes.

IO-04 : Spectral Study of Some Metal Chelates

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The reaction of para substituted acetophenone benzoate at zero degree celcious produces 1-phenyl-3-(p-substituted anisyl)-1,3-dione which has two coordinating sites and thus capable of forming metal chelates with transition metal ions this ligand has been used for chelation with Co(ii) and Ni(ii) metal ions using á-Picoline, â-Picoline and Y-Picoline as auxiliary ligand. The FTIR Spectra confirms the Keto-enol isomerism in the ligand which chelates metal ions in enolic form. The metal chelates have been characterised by various physical methods like molar conductivity, magnetic susceptibility and electronic spectra. The electronic spectral bonds and the values of different parameters derived from electronic spectral bonds predicts octahedral with a bit tetragonal distortion in the geometry of these complexes.

IO-05 : Study of Chelation Behaviour of 2-furfuraldehyde Semicarbazone to Fe(II), Co(II), Ni(II) and Cu(II)

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2-furfuralsemicarbazone is a multidentate ligand having several potential donor sites. It may act as monodentate coordinating through any potential donor site or it may also act as bidentate coordinating through two sites resulting in the formation of metal chelates. This Schiff base ligand could be prepared by the condensation of 2-furfuraldehyde and semicarbazide. It was used for complexation with Fe(II), Co(II), Ni(II) and Cu(II) transition metal ions. On the basis of percentage composition derived from element analysis of complexes they have been formulated as $[ML_2X_2]$, where M = Fe(II), Co(II), Ni(II) and Cu(II), L = 2-furfuralsemicarbazone and X = $\alpha - \text{picoline}$. The comparison of FTIR spectra of complexes with that of free ligand reveals the coordination sites azomethine nitrogen and enolic oxygen and thus five membered ring is formed. The very low value of their molar conductivity in DMF solution of 10^{-3} M concentration predict their non-electrolytic nature. The magnetic moment values, their electronic spectra and values of various Crystal Field Parameters provided strong evidence in the favor of their octahedral geometry.

IO-06 : Non-isothermal Kinetic Parameters Evaluation and Geometry Optimization of Binary Complexes of Schiff Base Derived from 2,4-Dihydroxy Acetophenone (Resacetophenone) and 3-Hydrazino Benzoxazine-2-one

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Thermogravimetric analysis is the technique which provides information about the stability of complexes from a thermogram. Thermal stabilities of Co (II), Ni (II), Cu (II) and Zn (II) complexes of DPE-HBO derived from resacetophenone and 3-hydrazino benzoxazine-2-one were measured by TGA analysis. In the current study, the following Kinetic parameters- (E_a) activation energy, (ΔH) enthalpy, (ΔS) entropy and (ΔG) free energy changes, were determined by the thermogravimetric data obtained. The kinetic and thermodynamic parameters for the degradation of the above binary metal complexes were calculated using Coats-Redfern (CR) integration method which involves thirteen various kinetic models.

In this study, geometry optimization was also performed and the stabilities of the metal complexes were evaluated from the molecular orbital structures from which the quantum chemical parameters were calculated with the help of HOMO and LUMO energies.

IO-07 : Spectroscopic Studies of some Complexes of Mn(ll) and Fe(ll) with Derivative of the Amino Acid and Glycine

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High importance significance of protein complexes invited our attention in the field of Coordination chemistry of first series transition metal complexes with derivative of the amino acid glycine. N-acetyl glycine has been taken as the main ligand and it's complexes with Mn(II) and Fe(ll) have been prepared. The micro analytical data and molar conductivity value led to the formation of the complexes as ML2X2.

Where L is N-acetyl glycine and X is H_2O, pyridine and alpha picoline. The comparison of Infrared spectra of complexes with that of free ligand revealed that the main ligand Co-ordinate through Amino nitrogen and deprotonated carboxylic acid oxygen. The magnetic moment of Fe(ll) complexes has been found 4.90-4.92 BM which corresponds to four unpaired electrons in the complexes. It indicates the spin free octahedra geometry of the complexes which is further confirm by appearance of one broad band in their electronic spectra. The magnetic moment value around 5.87BM shows the presence of five unpaired electrons in Mn(ll) complexes. It is d5 system for which the ground state is 6s which is single degenerate and gets transformed into 6A1g in octahedral crystal field penetration. The other higher states has different spin multiplicity hence Mn(ll) complexes displays four bands of very low intensity which have been assigned to spin forbidden transition. On the basis of electronic spectra band value of racah parameters B and C.

IO-08 : Bio-Mediated Production of Nanoparticles

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Nanoparticles are often defined as those that measure to the size of nanometers (10^{-9}) and they often posses properties like uniformity in shape, size, conductance, physical and chemical properties enabling them to draw the attention of investigator from various fields. They can be prepared using physical, chemical and also by green synthesis methods.Synthetically prepared nanoparticles can be in different shapes like nanotubes, wires, spheres etc. The physical and chemical properties are mostly determined by shape, size and composition. The applicability of properties of single component nanoparticles is restricted. Hence to overcome these limitation bimetallic nanoparticles, which consists of two distinct metals can be synthesized. These Bimetallic nanoparticles' composites exhibit fascinating properties that can be different from their corresponding single component particle. The study of interaction of nanoparticles with the living system is the need of this hour, as they are providing promising results against diseases. However, the rapidly developing field of nanotechnology is likely to become yet another source for disease through inhalation, skin uptake etc. Therefore information about safety and the hazards that are caused by them is urgently required, as indiscriminate use can cause toxic effects. The ease of preparation is drawing attention due to their physical and chemical properties. The Biosynthesis of nanoparticles has been proposed as a cost effective, environmental friendly alternative to the chemical and physical methods. Novel methods are thought to be used to synthesize the nanoparticles at ambient temperature, p^H. Thus, this biological reduction process is gaining popularity over the chemical reduction process.

IO-09 : Synthesis, Spectroscopy, X-ray Crystallography and Anticancer Activity of some Transition Metal Ion Complexes of a New Pyrazole-based Schiff base Ligand

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A new pyrazole containing ‘NN’ bidentate Schiff base ligand, (MPAFA), and its Co^{II} [{$Co(MPAFA)_3$}.2Br.$2H_2O$ & {$Co(MPAFA)_3$}.$2ClO_4$] and Ni^{II} [{$Ni(MPAFA)_2(H_2O)_2$}.2Cl.$2H_2O$ & {$Ni(MPAFA)_3$}.$2ClO_4$] complexes have been synthesized and characterized by various physico-chemical and spectral parameters. X-ray data of the complexes have revealed that all the four complexes reported here are octahedral in nature. The ligand contains in its structure the coordination function of the tertiary nitrogen atom of pyrazole ring and the azomethine nitrogen, suitably spaced for chelation with the metal ions. The reported ligand and its metal ion complexes have been screened for anticancer activities. The details of the structural characteristics and the anticancer activities of the compounds shall be discussed.

IO-10 : Synthesis, Spectroscopic and Structural Characterization of a Copper (II) Complex with 5-methyl-3-formylpyrazole-N(4)-Dihexylthiosemicarbazone (HMP_zNHex_2): Catalytic Activity for Chemical Fixation of CO_2 into Cyclic Carbonates

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A new dinuclear Cu(II) complex ($C_{36}H_{66}Cl_4Cu_2N_{10}O_2S_2$) was constructed by the reaction of Cu(II) chloride with 5-methyl-3-

formylpyrazole-N(4)-dihexylthiosemicarbazone (HMP_zNHex_2). The reported complex was characterized by single crystal X-ray diffraction studies along with several physico-chemical and spectral parameters. Single crystal X-ray diffraction studies on the Cu(II) complex exhibited that the complex crystallized in monoclinic $P2_1/c$ space group. The ligand (HMP_zNHex_2) was bonded to the Cu(II) ion in bidentate fashion, through the pyrazolyl (tertiary) ring nitrogen atom and nitrogen atom in the thiodiazole ring. Cyclic voltammogram of Cu(II) complex showed a quasireversible Cu^{II}/Cu^{III} couple with irreversible Cu^{II}/Cu^{I} couple. The synthesized Cu(II) complex acted as catalyst for the chemical fixation of CO_2 into cyclic carbonates using epoxides in the presence of Bu_4NBr as a co-catalyst at atmospheric pressure.

IO-11 : Coordination Chemistry of the Copper(II) Complexes of 3,5-Di-tert-butyl-2-hydroxybenzoylhydrazones of Heterocyclic Aldehydes and their Antimicrobial and Antitubercular Activity Studies

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The heterocyclic aroylhydrazones L1H, L2H & L3H were synthesized by condensing 3,5-Di-tert-butyl-2-hydroxybenzoylhydrazide with furan-2-aldehyde, pyrole-2-aldehyde and thiophene-2-aldehyde respectively. The ligands were complexed with the copper(II) ions with varying counter ions. However, only four distinct copper complexes were obtained, even though all the three ligands were reacted with copper(II) salts with chloride, perchlorate, acetate and nitrate counter ions. The various physico-chemical and spectral analysis like molar conductance, elemental analysis, FTIR, C^{13} and H^1NMR, UV-Visible, EPR, and single crystal XRD analysis were used in the characterization of the compounds. The metal to ligand i.e. M:L ratio as 1:2; for all the complexes with the molecular formulae as $[Cu(L1H)(L^7)Cl]$ C1, $[Cu(L1)_2]$ C2, $[Cu(L2)_2(H_2O)]$ C3 and $[Cu(L3)_2(H_2O)_2]$ C4 respectively, were assigned based on the analyses. The complexes C1 and C3 were assigned with the square pyramidal and C4 with the octahedral geometries. Whereas the complex C2 was square planar as found in its single crystal XRD studies. All the synthesized compounds were evaluated for the antimicrobial and antitubercular activities. The antimicrobial activity of all the compounds against S. aureus microorganism were found to be very active with low MIC values of

0.4µg/mL, except for C1 and L3H with 1.6µg/mL, and were much better than the control Ciprofloxacin (2µg/mL). The complexes C1, C2 and C3 exhibited quite promising low MIC values ranging from 3.12 – 1.6µg/mL and were much better than their parent ligands L1H and L2H. Whereas the both the ligand L3H and its complex C4 were active with low MIC values of 1.6µg/mL. The antitubercular activity studies indicated that the complexes C1, C2 & C3 exhibited the low MIC ranging from 3.12 – 1.6µg/mL than that of their ligands'. Whereas the both the ligand L3H and its complex C4 were active with low MIC values of 1.6µg/mL.

IO-12 : Ternary Complex of Cr(III) with Isatin Derivative and 8- Hydroxyquinoline : Synthesis and Characterization

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Schiff bases are versatile compounds for the design of ternary complex. An experiment has been made to synthesize novel complex of Cr(III) by the reaction of two ligands: The primary ligand ,L_1 which was prepared by condensation reaction of Isatin and 2- aminopyridine and the secondary ligand was 8-Hydroxyquinoline. The reaction was performed through conventional reflux method. Isatin has great biological diversity in medicinal and pharmaceutical field. Along with Isatin, pyridine derivatives also have antibacterial, antifungal activities. The synthesized ligand and complex were characterized by elemental analysis, molecular weight determination, magnetic moment measurement, melting point determination and spectral analysis (IR, UV, ^{1}H NMR, etc.). The synthesized compounds will be further evaluated for biological studies against selected bacterial and fungal strains.

IO-13 : Synthesis, Characterization and Biological Activity of Semicarbazone and Thiosemicarbazone Ligands

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Semicarbazones and thiosemicarbazones are multidenate ligands with N, O and S donor atoms. Semicarbazones and thiosemicarbazones are schiff bases which are prepared by the condensation of an aldehyde or a ketones with semicarbazide and thiosemicarbazide. For the present study 2-acetylfluorenesemicarbazone has been synthesized by the condensation of 2-acetylfuorene and semicarbazide and 2-

acetylfluorenethiosemicarbazide has been synthesized by the condensation of 2-acetylfluorene and thiosemicarbazide. The ligands have been used for complexation with Fe(II), Co(II) and Ni(II). The characterization of the ligand and metal complexes were done by various spectroscopic technique like FTIR, Electronic spectra, Elemental analysis, Molar conductivity and Molar susceptibility. The percentage composition and molar conductivity predict the formulation of complexes. The FTIR spectra of complexes and ligand indicates the coordination of the ligand from carbonyl oxygen and azomethine nitrogen. The NH and NH_2 group of the ligands don't participate in coordination. Thus the ligand act as neutral bidentate and forming five membered ring with metal ions. The magnetic moment of these complexes are well in accordance with the number of unpaired electrons. The electronic spectra of the complexes have been studied leading to structural elucidation of complexes. The number of electronic bands and deviation of various crystal field parameters clearly predict the distorted octahedral geometry around metal ions. Semicarbazones and thiosemicarbazones and their derivatives found wide medicinal application due to their potentially beneficial biological activities like antibacterial , antimalarial, antiviral and antitumors.

IO-14 : Study Of Schiff-base Complexes Hiff-base Complexes of Co (II), Ni(II) And Cu (II)

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Study of shiff-bases are known as the versatile ligands for complextaons with transiton metal ions.

In the present-Paper be report the prepatation a shiff-Base viz, 3hydroxy. 4-Methoxy Benzaldehyde, 4-phenyl semi carbozone (HMBPS) buy the reacton of 3-Hydroxy, 4-Methoxy Benzaldehyde and 4-Phenyl semi carbazide. This shiff- Base has varios donar sites which has been used for compelxation with Co(ll), Ni(ll), And Cull). The FTIR spectra of complexes reveal that azomethyne group and carbonyl group absorption frequency of the free ligand under go considerable change in complexes. From this it could be bidentate ligand co-ordinating through Azomethyne Nitrozen and corbonyl oxgen.

The megnetic sueaptibility and UV / visible spectra of complexex conspicuously show the octa hedral geometry of this complexex.

IO-15 : Ruthenium-Carbon(Aryl) Bond Cleavage and Change in the Ligand Coordination Mode in a Four-Membered Ortho-Metalated Ruthenium(II) Organometallics Promoted by Thiolato Ligands

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The reaction of Ru(η^2-RL)(PPh_3)$_2$(CO)Cl [η^2-RL is C_6H_2O-2-$CHNHC_6H_4$R(p)-3-Me-5 and R= Me, OMe, Cl] with excess sodium p-chlorothiophenolate (p-ClC_6H_4SNa) in dichloromethane-tetrahydrofuran medium afforded the binuclear complexes of the type [Ru(PPh_3)(η^2-RL)(CO)(p-ClC_6H_4S)]2 [η^2-RL is C_6H_3O-2-$CHNC_6H_4$R(p)-3-Me-5] in excellent yield. The binding of the thiolato ligands is attended with the cleavage of the Ru-C(aryl) and Ru-Cl bonds in Ru(η^2-RL)(PPh_3)$_2$(CO)Cl and the RL ligands are now coordinated with the metals in [Ru(PPh_3)(η^2-RL)(CO)(p-ClC_6H_4S)]$_2$ via the imine nitrogen and the phenolato oxygen atoms. The CO ligand in [Ru(PPh_3)(η^2-RL)(CO)(p-ClC_6H_4S)]$_2$ lies trans to the phenolato function as in Ru(η^2-RL)(PPh_3)$_2$(CO)Cl. The spectral (UV-vis, IR, NMR, mass) and electrochemical data of the complexes will be presented. In dichloromethane solution the complexes display two successive one-electron oxidation waves. The comproportionation constants (KC) as calculated by the $\Delta E_{1/2}$ values of the complexes are in the order of 10^5 indicating that the two metal centers in [Ru(PPh_3)(η^2-RL)(CO)(p-ClC_6H_4S)]$_2$ are only weakly coupled by the bridging thiolato liagnds. Structure determinations of [Ru(PPh_3)(η^2-RL)(CO)(p-ClC_6H_4S)]$_2$ (R=Me, OMe) have revealed a distorted octahedral $RuCONPS_2$ coordination sphere with the pairs (P, S), (C, O), and (N, S) defining the three trans directions. The Ru····Ru distances in the complexes are clearly outside of the range for a Ru-Ru single bond. The electronic structures and the absorption spectra of the complexes are also scrutinized by the densityfunctional theory (DFT) and Time-dependent DFT analysis and will be presented.

IO-16 : Study of Some Complexes of First Transition Metal Series

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Transition metal ions particularly of 3d.series are very good accepters of lone pair of electrons and hence they are capable of forming of complexes with ligands having good donar sites. Pyridene dithiocabamate yeasts with sodium monochloacetate which on treatment with hydrazine hydrate produces pyridine thiocabamite. Now this carbamite on tratment with salicilaldehyde produces salicyilidene pyridine this semicabazone. This ligand has been used for complexatation with Cu(ll) metal ion. The megnatic moment of these complexes shows all these Culll) complexes are magnatically defute. The FTIR spectra helps trace the co-ordination sites of the ligand. The clectronic speactra of these compexes predicts the distorted octahedral (D4h) geometry of complexes.

IO-17 : Studay of Some Complexes of Cr(III), Ti(III) and V(III)

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3-Hydroxy-4-methoxybenzaldehyde on condensation with thiosemicarbazide produced vanillinethiosemicarbazone having several potential donar sites. It was used for multiple chelation with Ti(III), V(III) and Cr(III) transition metal ion. The chelation behavior of multidentate vanillinethiosemicarbazone was traced but by the comparison of FTIR spectra of the metal chelates with that of the free ligand which unveiled the chelation point of the ligand as azomethine nitrogen and thionyl sulphur. The molar conductivity of these metal chelates fail in the range of 165-190 22-1 cm mol1 which was suggestive of their electrolytic nature with 1 : 3 ionic ratio in DMF solution. The magnetic susceptibility and electronic spectra of all these metal chelates lead to their octahedral symmetry. The The paramagnetic nature of these metal chelates predicted their high spin nature. The value of nephelauxetic effect clearly indicated some covalent nature of M-L bond in these chelates.

IO-18 : Spectroscopic Characterization of Ferrous Metal Ions Complexes

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A Schiff-base ligand; phenyl(2-hydroxy phenylomethyle) azane was prepared by the reaction of saliaylaldehyde and aniline taken in 1:1 molar iatio and it was used for the synthesis of complexes with ferrous metal ions, i.e. Fe(II), Co(II) and Ni(II). The ligand absorbs at 3590 (m^{-1} in its FTIR spectrum due to n_{O-H} (phenolic group) stretching vibration which disappeared in the FTIR spectra complexes. It indicates the deprotonation of phenolic –OH group and coordination through deprotonated oxygen. The azomethine group of the free ligand strongly absorbs at 1675 cm^{-} which undergoes red shift by 30-40 cm^{-1} in the FTIR spectra of complexes. It is indicative of coordination through azomethine nitrogen to ferrous metal ions in complexes. Thus the ligand in joined to Fe(II), Co(II) and Ni(II) through depostonated phenolic oxygen and azomethine nitrogen. The electronic spectra of complexes were taken into account to predict the geometry of complexes.

IO-19 : Study of some Tetragonally Compressed Complexes

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The correlation between the term splitting and bond linglt changes resulting from the Jahn Teller effect may be established when the octahedronis regular. But when there is tetragonal compression of the octahedron, the situation is somewhat different. It demands the derivation of distortion parameters D_S and D_t. In the present a ligand, benzaldehyde-phenyl semicarbazone has been prepared and it was used for complexation with Fe(II), Co(II) and Ni(II) metal ions. The mode of coordination of the semicarbazone ligand has been establisled by the perusal of IR spectra of complexes. The electronic spectral bands of the complexes were used for the derivation of the distortion pentameters D_S and D_t. The negative values of D_S and D_t clearly predicts their tetrogonally distort octahedral symmetry with compression along z-axis.

IO-20 : Fe Based MOFs for Photocatalytic Degradation of Pollutants from Waste Water

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The global population has grown 7.9 billion in 2020 and to get safe drinking water to the larger growing population is one of the biggest problem around the world. Pollution produced from different industries causes serious damage to the aquatic system as well as our human health because of high toxicity of chemicals, carcinogenicity and solubility. Large amounts of organic contaminants such as pharmaceuticals, synthetic waste, pesticides and dyes are released into waters. A new source of sustainable energy is essential to fulfill our future demand due to the limited availability of sources. Various techniques have been discovered in the past to remove the hazardous chemical compounds from polluted water but photocatalysis is a very promising and cost effective way to remove organic pollutants where an electron-hole pair is generated on exposing to light of proper energy. Metal-organic frameworks (MOFs) are organic-inorganic hybrid crystalline porous materials which have great potential in the field of photocatalysis due to their large surface area, tunable porosity. In the present study a Fe based MOF has been used for the degradation of dye. The structural and optical properties of the as-prepared photocatalyst material were also characterized and the catalytic reaction mechanism has been investigated.

IO-21 : Nickel Substituted Calcium Ferrites ($Ca_{1-x}Ni_xFe_2O_4$; x=0.00, 0.04, 0.08, 0.12, 0.16); Magnetically Separable Nano Catalyst for the Efficient Reduction of 2-Nitrophenol

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This study deals with the scrutiny of mixed metal oxide of calcium ferrite $Ca_{1-x}Ni_xFe_2O_4$ (x=0.00, 0.04, 0.08, 0.12, 0.16) as catalysts for the reduction of 2-nitrophenol. The ferrite samples with uniform particle size are synthesized using the citric acid auto combustion technique. Calcium nickel iron citrate precursors by TG-DTA, revealed the calcination temperature 700°C. FT-IR spectra confirmed the spinel phase formation. The Powder X-ray diffraction patterns demonstrated the orthorhombic single-phase formation of synthesized catalysts. UVDRS spectra revealed the decreasing trend in band gap energy. The catalytic activity of synthesized ferrites is used for reduction of 2-nitrophenol to 2-aminophenol by using $NaBH_4$ as reducing agent. The effect of varying ratio of amount of catalyst, amount of $NaBH_4$, effect of solvents and reuse of catalysts is scrutinized. The reduction reaction followed pseudo first order kinetic equation. The enhanced reduction efficacy was observed with the introduction of Ni^{2+} in to the calcium ferrite lattice due to catalytically active octahedral site preference of Ni^{2+} ion and exertion of synergistic effect is observed due to the formation of Ni-Ca and Ni-Fe ion pairs. All synthesized catalysts exhibited inherent magnetic properties with excellent catalytic activity and can be easily separated by external magnet for next cycle use.

Sectional President's Address

Synthesis of Newer Fused Qunoline Heterocycles of Biological Interest

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Quinoline is a versatile scaffold with immense therapeutic potential and frequently used in new drug design development process. Additionally, they found in numerous natural product and pharmacologically active substances displaying a broad range of biological activities. Synthesis of fused heterocyclic compounds through the combination of different pharmacophores in a molecular framework is of considerable interest due to a wide variety of such molecules showing promising biological activities. Particularly, the hybrid compounds containing quinoline motif constitute an privileged class of compounds for new drug development Therefore, development of new and efficient methodologies to access these molecules of medicinal utility have attracted much of the attention

We have developed the methodologies for the construction of novel quinoline fused triazolo-azepines/oxepines (2), tetrahydrobenzo[b][1,6] naphthyridines (4) and benzofuroquinolines (6) via the palladium catalyzed transformations.

OIL-01 : Cascade Reactions of Propargylic Alcohols and Propiolamides

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Propargylic alcohols and N-substituted propiolamides have received ample attention as handy substrates for the construction of complex structures, particularly via cascade reactions. Propargylic alcohols have been used as propargylating agents to numerous propargylated compounds, followed by their cyclisation to several heterocyclic or aromatic compounds with the assistance of alkyne functionality. We established the cascade reactions of propargylic alcohols and their derivatives to access the diverse heterocyclic compounds. Further, N-arylpropiolamides were found suitable precursors towards alkyne-assisted ipso-cyclisatoin reactions. The present lecture will highlight the recent accomplishments with regard to development of cascade reactions involving propargylic alcohols and N-arylpropiolamides towards natural product frameworks and spirocyclic compounds.

OIL-02 : β-Iodovinyl Sulfones : A Versatile Building Block in Organic Synthesis

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Organosulfur compounds are ubiquitously found in natural products, pharmaceuticals, agrochemicals, and organic electronic materials. The direct construction of carbon-sulfur and sulfur-sulfur bonds are continuously occupied a special place in contemporary organic synthesis. The b-iodovinyl sulfones are a privileged class of multifunctional compounds, and they serve as a powerful building block in organic synthesis.

In this talk, the unprecedented reactivity of β-iodovinyl sulfones will be discussed as shown in Scheme 1. (i) Highly efficient palladium-catalyzed annulation between b-iodovinyl sulfones and 2-halophenols is presented for the synthesis of 3-sulfonyl benzofurans. (ii) Metal-free synthesis of β-keto sulfones and β-keto thiosulfones using β-iodovinyl sulfones, which acted as indirect enolate in the presence of NaOAc. (iii) A unique vicinal bisthiolation of (E)-b-iodovinyl sulfones with thiols under the influence of K_2CO_3/DMSO at room temperature for quick assembly of (E)-1,2-dithio-1-alkenes is demonstrated. (iv) A novel cycloannulation between β-iodovinyl sulfones and N-tosylaminopyridines was also successfully developed for the synthesis of 3-sulfonylpyrazolo[1,5-a]pyridines.

OIL-03 : Nanocomposites and Mixed oxides as Reusable Catalysts for Organic Synthesis

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New-generation materials, such as nanocomposites, have wide-ranging applications as adsorbents, catalysts, membranes, etc. These materials possess excellent thermal stability and other advantages: their crystalline structure, shape selectivity, and scope to modify their structure and surface properties. The combination of heterogeneous catalysts with potential for recyclability and multi-component reactions (MCRs) deliver excellent yields of various value-added organic moieties, with remarkable selectivity and atom efficiency in green solvents at moderate conditions in short reaction times.

The scope of various mixed oxides and nanocomposites as recyclable catalysts for synthesising different heterocyclic moieties will be described in the talk.

OIL-04 : Oxidative Coupling and Annulation Strategies for the Construction of Privileged N-Heterocycles

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The development of efficient methods for construction of C-C and C-X (X = N, O, S, etc) bonds under mild conditions is one of the great challenges in organic chemistry. Transition-metal catalyzed classical coupling reactions have been proven to be powerful tools for the construction of various C-C and C-X bonds, and reactions of this type have been widely applied in the areas of pharmaceuticals, agriculture, food industries, and so on. Generally, in those classical coupling reactions, bond formations occur between an electrophile and a nucleophile in the presence of a transition-metal catalyst. Both the electrophiles and the organometallic nucleophiles are usually obtained from pre-functionalization of their corresponding hydrocarbons. However, with the development of modern synthetic methodology and the urgent demand for green and economical synthesis, traditional couplings face big challenges on account of their inevitable drawbacks such as low atom economy and considerable generation of harmful by-products. At this point, direct bond formation between two or more nucleophiles, especially hydrocarbons, would be an ideal alternative. As for the coupling between two nucleophiles requires an extra oxidant to promote bond formation, this type of reactions are designated as oxidative couplings.

We have recently investigated several oxidative annulation reactions for the construction of nitrogen heterocycles such as quinoxalines, quinazolines, bis(indolyl)methanes, 2,4,6-triarylpyridines, 3 alkylideneindolin 2 ones, and 1,3-benazoles using amines as reaction partners. Sustainable metal catalysts such as iron or copper salts, and abundant oxidants viz., air or molecular oxygen were used for conducting the oxidative annulation reactions. The results of these studies will be presented in the conference.

OO-CYSA-01 : Comparison of the Physico-Chemical and Catalytic Properties of Co and Ti based Magnetic Layered Double Hydroxides in Oxidative Aromatization of 1,4-DHPs and Oxidative Deprotection of Oximes

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Considering the unique properties of Layered double hydroxides (LDHs), such as tunability of the types of metal cations, high adsorption capacity, tunable basicity, the M^{2+}/M^{3+} molar ratios, and the high ion-exchange nature of interlayer anions, herein we have synthesized four Co and Ti based magnetic LDHs (Fe_3O_4-CoTiMgAlLDH, Fe_3O_4-CoTiMgLDH, Fe_3O_4-CoTiAlLDH and Fe_3O_4-CoTiLDH) using urea hydrolysis method. Herein, the main point of interest was to evaluate the effect of substituting Mg and Al with Co and Ti on the physico-chemical properties as well as studying the catalytic activity of the synthesized catalysts in oxidative transformations such as oxidative aromatization of 1,4- dihydropyridines and oxidative deprotection of oximes. Among all catalysts, Fe_3O_4-CoTiLDH exhibited the highest catalytic activity for both the transformations. The enhanced catalytic performance using Fe_3O_4-CoTiLDH was combinedly attributed to the successful fabrication of Fe_3O_4-CoTiLDH nano-composite (XRD & FTIR), high surface area (BET), high thermal stability (TGA), and more amount of surface active cobalt species (XPS & ICP-AES). Fe_3O_4-CoTiLDH was further characterized by FEG-SEM, EDX, HRTEM, and VSM. Moreover, Fe_3O_4-CoTiLDH could be easily separated from the reaction system using external magnet with excellent recyclability for at least seven times without obvious deterioration of its catalytic activity.

OO-CYSA-02 : In silico screening of Covid-19 and Synthesis of (6-((1-(4-aminophenyl)-1H-1,2,3-triazol-4-yl)methoxy)substiyutedbenzofuran-2-yl)(aryl) Methanones using Green Synthetic Protocols towards Screening of their in vitro Anticancer, Antimicrobial Activities

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Benzofuran derivatives are an important class of heterocyclic compounds that are possessing vital biological activities such as anticancer, antiviral, antifungal antioxidant, antidepressant and antipsychotic. Similarly, 1,2,3-triazole and its derivatives have important biological activities for instance antimicrobial, analgesic, anti-allergic, anti-HIV, antimalarial and antituberculosis. In order to know the combined effect of both the benzofuran and 1,2,3-triazole moieties we have taken up the synthesis of title compounds. A series of novel 1,4-phenylenebisbenzofuran compounds were synthesized in conventional heating method and microwave irradiation method- an eco-friendly and a green synthetic approach. A series of well planned 4-aminophenyl-1H 1,2,3-traizole based benzofuran analogous were synthesized with high yields in a straight forward route via microwave irradiation method than conventional method. The entire synthesized compounds structures were confirmed based on IR, ^{1}H, ^{13}C NMR and HR mass spectral analysis. The presence of 1,2,3-triazole moiety, amino group and benzofuran base group may influence the biological applications. All the synthesized compounds subjected to evaluate their in vitro anticancer activity with MCF-7, PC-3 and HeLa cell lines by MTT assay, Further, in vitro antimicrobial activity of target compounds examined in Agar Disc Diffusion method by taking gram positive, gram negative and fungal strains and turned out with encouraged results compared with Ciprofloxacin and Fluconazole standards respectively. Furthermore, in slico studies carried out to find out H-bonding interactions, hydrophobic interaction with docking scores of prepared compounds. Off course, we have docked in silico covid-19 study with covid-19 main protease enzyme and got outstanding binding interactions.

OO-CYSA-03 : Hydromagnesite Sheets Crowned with Cobalt-Ferrite Magnetic Nanoparticles Facilitated Heterogeneous Approach for the Synthesis of Benzo[d]imidazo[2,1-b]thiazole Scaffolds

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The present work elicits an account of the one-pot robust multicomponent reaction (MCR) strategy catalyzed by novel hydromagnesite sheets embracing cobalt×ferrite ($CoFe_2O_4$×HMS) magnetic nanoparticles (MNPs) as environmentally benign nanocomposite to synthesize benzo[d]imidazo[2,1-b]thiazole derivatives. The high product yield (up to 94%) in minuscule reaction time, modest catalyst loading, estimable recyclability of catalyst and solvent without substantial loss of activity (up to five synthetic cycles), as inveterate by parameters of green chemistry, are the virtues of this protocol. The characterization of synthesized nanocomposite was accomplished through a number of spectroanalytical devices viz. powder X-ray diffraction (PXRD), field emission scanning electron microscopy (FE-SEM) with energy-dispersive X-ray spectroscopy (EDAX), high-resolution transmission electron microscopy (HR-TEM), Raman, FT-IR, TGA-DTA-DTG analyses, magnetic studies and nitrogen porosimetry analyses. The structures of the synthesized compounds were also endorsed by extensive spectroscopic studies (FT-IR, ^{1}H, and ^{13}C NMR, Mass) and elemental analyses. The reaction protocol is also scalable to the multi-gram scale, which is valuable to extend the methodology for the industrial process. The methodology affords several advantages to attain sustainable chemistry and opens up a new scope to further prospect the catalytic potential of ($CoFe_2O_4$×HMS) for the synthesis of biologically significant scaffolds.

OO-CYSA-04 : Structure-based Hierarchical Virtual Screening of Antiviral Libraries for the Discovery of New Molecular Entities as SARS-CoV-2 main Protease Inhibitors

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The novel coronavirus disease (COVID19) caused by a new strain of virus family SARS-CoV-2 in December 2019 has emerged as a deadly pandemic that affected millions of people worldwide leading to severe health and economic burden. As the world is suffering from the pandemic, key factors like lack of effective drugs, vaccines, inefficacy and cost of repurposed drugs motivated us to identify novel therapeutic strategies. The main protease enzyme (M^{pro}) of SARS-CoV-2 protein was identified as an attractive drug target which plays a key role in the viral replication and transcription. Here, we utilized structure-based virtual screening of antiviral libraries in Schrodinger suite to identify novel potential lead molecules against the crystal structure of protease protein (PDB ID:6LU7). The ligands were filtered in HTVS, SP, and XP modes against M^{pro} protein which resulted in 31 hit molecules. The top 6 ligand molecules (M1 –M6) were ranked as leads based on glide docking score, and glide emodel values as new molecular entities. M1, M3, and M6 ligands were showing good scoring functions and least binding energies from Prime MM/GBSA (-75.50, -70.31, -81.32 kcal/mol), and AutoDock (-8.21, -7.93, -7.64 kcal/mol) with high percent human oral absorption as 100%, 100%, and 93.2% obeying ADME parameters. These lead molecules fit into the main protease active site cavity by consistently interacting with key residues inhibiting the main protease of SARS-CoV-2 protein. A computational docking study was conducted using FDA-approved and repurposed drugs against M^{pro} to establish newly identified leads as potential SARS-CoV-2 main protease inhibitors.

OO-CYSA-05 : Development of Magnetic Copper Catalyst based on Biomass Derived Activated Carbon for the base-Free Chan-Lam Coupling and Oxidations

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Recently, biomass has attracted enormous interest for the preparation of different types of carbon-based materials as they possess tunable pore/surface properties, can be easily modified to generate active sites and have relatively low cost, which make them efficient to be used in the field of catalysis. Biomass derived activated carbon possess large specific surface area, highly porous structure and good thermal/chemical stability. Keeping the advantages associated with biomass derived activated carbon, we have synthesized inexpensive and environmentally benign magnetic catalysts [$Cu@KF\text{-}C/MFe_2O_4$, M= Co, Cu, Ni and Zn] using neem dead leaves (waste biomass) as a cheap and rich source of carbon material. In addition, KF modification was done to impart basic character to the catalyst that can perform C-N coupling under base-free conditions. Initially, BET analysis of the synthesized catalysts was carried out which indicated that Cu@KF-C/CoFe$_2$O$_4$ possess more surface area as well as pore volume and so accounted for the highest activity among the other synthesized catalysts. Further, XPS analysis was performed which inferred that Cu@KF-C/CoFe$_2$O$_4$ contains most of the copper in reduced form i.e Cu(0), which is the active species responsible for the better catalytic activity towards Chan-Lam coupling reactions as well as oxidation of alcohols and hydrocarbons. The physiochemical properties of the most active catalyst, Cu@KF-C/CoFe$_2$O$_4$ was examined by FT-IR, TGA, FEG-SEM, HR-TEM, EDX mapping, EDX, ICP-AES, XRD and VSM.

OO-CYSA-06 : Stereoselective Total Synthesis of Paecilomycin E

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A concise approach for the total synthesis of paecilomycin E is described involving Alder-Rickert reaction, Mitsunobu esterification and ring closing metathesis as the key steps. This approach has successfully demonstrated the Alder-Rickert protocol for the construction.

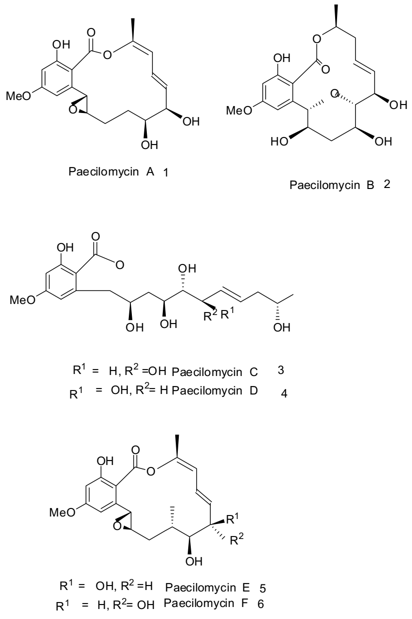

Figure 1: Structres of Paecilomycin A-F(1-6)

Figure 1: Structres of Paecilomycin A-F(1-6)

Restrocyclic acid lactones (RALs) are a group of fungal polyketide metabolites that are structurally consist of a C11 side chain. Majority of these naturalproducts have a 14-membered ring lactone as one of the core striuctural components. They are known to disply a wide rangeofbiologicalactivities such as estrogenic antifungal cytotoxic antimalarial, antiviral, antiparasitic and nematicidal behavior and also show inhibitory activities against ATPases and kinases.

OO-01 : Synthesis of Newdihydro Thieno-1, 8 Naphthyridine Derivatives and Evalution of their Anti-microbial Activity

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1,8-Naphthyridine derivatives are important class of heterocyclic compounds with attractive biological activity i.e. anti-cancer, ant-malarial, anti-uretic activities. Similarly newly derived dihydrothieno-1, 8-naphthyridine-phenyl urea and thiourea derivatives find important place among heterocyclic compounds as they are very prominent for their anti-microbial activity. The starting material, 2-aminonicotinonitrile in presence of dihydrothio phene3(2H)one gives 6,8-dihydrothieno[3,4-b][1,8]naphthyridin-5-amine, thus obtained was treated with Substituted Phenyl isocyanates and isothiocyanates in the presence of THF gives corresponding1-(6,8-dihydrothieno[3,4-b][1,8]naphthyridin-5-yl)-3-phenylurea and 1-(6,8-dihydrothieno[3,4-b][1,8]naphthyridin-5-yl)-3-phenylthiourea respectively in good yields.

All the new compounds were characterized by their spectral data and they were screened for their anti-microbial activity.

OO-02 : Natural Products - Their Importance

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Natural products are gaining importance in medicinal chemistry, as they exist as a part of traditional medicine in providing biologically active phyto constituents with lot of medicinal properties. The use of herbal medicines and extracts are increasing day by day across the globe and there is worldwide upsurge in the use of plant preparations for curing health disorders as codified in Ayurveda. Plants by nature synthesize unexpected novel structures by various biosynthetic pathways which provide valuable lead molecules in Drug discovery.

Flavonoids which form a group of plant pigments, isolated from plants show wide range of pharmacological activity on human beings including antihepatotoxic, anti inflammatory, anticancer, antioxidant activities.

OO-03 : Synthesis of Some Novel Isatin-Thiazole Conjugates and their Computational and Biological Studies

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The present work describes the synthesis of novel 3-[2-(5-phenyl-1,3-thiazol-2-yl)hydrazinyl]-1,3-dihydro-2H-indol-2-one derivatives 4(a-h) and precise characterization of synthesized hybrids using various spectroscopic techniques like FT-IR, NMR and HRMS. Through computational study, some global parameters and molecular electrostatic potential (MEP) were analyzed. The solvatochromic UV-Vis absorption study was performed using various solvents and the optical band gap of the synthesized compounds was determined by using Kubelka-Munk theory. The antimycobacterial activity of the synthesized compounds was evaluated against mycobacterium tuberculosis and the results suggested that, compounds 4d and 4e are effective inhibitors of mycobacterium tuberculi. The anti-inflammatory activity against MMP-2 and MMP-9 was determined using gelatin zymography, from the results it was evaluated that, the synthesized derivatives acts as good anti-inflammatory agents.

OO-04 : An Efficient p-TSA Catalyzed Synthesis of Some New Isoxazole Scaffolds and their Biological and Molecular Modeling Studies

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In the present investigation, we developed an easy and efficient protocol for the synthesis of a series of some novel isoxazole scaffolds (4a-j) via p-TSA catalyzed reaction of 1,3-dimethylbarbituric acid/ dimedone, substituted salicylaldehyde/2-hydroxy-nepthaldehyde and 3-phenyl-5-isoxazolone was administered in refluxed temperature in the presence of aqueous ethanol. All the obtained compounds were evaluated for their pharmacological and computational investigations, and structures were confirmed using analytical and spectroscopic techniques. The results of pharmacological investigations revealed that the compounds 4c, 4e and 4h possess excellent cytotoxicity efficacy, and compounds 4c, 4d, 4h and 4i have shown better anti-TB efficiency. The SAR study shows the importance of the electron-withdrawing group and additional phenyl nucleus enhancing the biological potency of the compounds. The results of the in silico molecular docking studies revealed that the compounds 4c and 4h effectively interacted with P38 MAP kinase and InhA-Enoyl-Acyl Carrier Protein Reductase proteins, respectively. DFT study suggested that the compounds are chemically and biologically more reactive due to less energy gap.

OO-05 : Synthesis and Cytotoxicity of Novel (E)-2-Phenylchroman-4-one-O-((1-substituted-1H-1,2,3-triazol-4-yl)methyl) Oxime Derivatives

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A series of new flavanone-triazole hybrids (4a-m) were synthesized from flavanone oximes (2a-c) via multistep synthetic strategy, involving Cu (I) catalysed azide, alkyne 1,3-dipolar cycloaddition by Click reaction. All the synthesized compounds were tested for their cytotoxicity against HCT-15, HeLa, NCI-H522 and HEK-293 (normal cell line) cell lines. Compounds 4a, 4b, 4d, 4e, 4j and 4m showed the significant cytotoxicity, wherein compound 4b showed potential cytotoxicity against NCI-H522 cell line and compounds 3a and 4a were offensive with HEK-293 in their toxicity profile.

OO-06 : Synthesis, Structural Characterization and Anti-Proliferative Activity of Pyrimidine-Curcumin Analogues

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A series of seven pyrimidine-curcumin analogues were synthesized and characterized by spectroscopic techniques. All structures showed the characteristic NMR peak of NH_2- group with a coupling constant J = 16 Hz for the trans confirmation. The synthesised analogues were screened for their anti-proliferative activities on two human cancer cell lines MCF-7 and MDA-MB-231 using MTT assay. The compounds displayed significant activity antiproliferative activity compared with the parent curcumin. Out of seven, the flouro derivative exhibited highest antiproliferative activity against MCF-7 and MDA-MB-231 cancer cells with IC_{50} values of 5.10 and 8.90 ìM respectively. Such compounds may be a good candidature as anticancer drugs in future.

OO-07 : An Eco-Efficient Approach for the Synthesis of 2-Amino-4-Phenyl-5, 6, 7, 8-Tetrahydronaphthalene-1,3-Dicarbonitriles via One-Pot Multicomponent Reaction using NaOH as a Catalyst

Edapu Harish Kumar[1], Ramakanth Pagadala[2] and Sathyanarayana Boodida[1,*]

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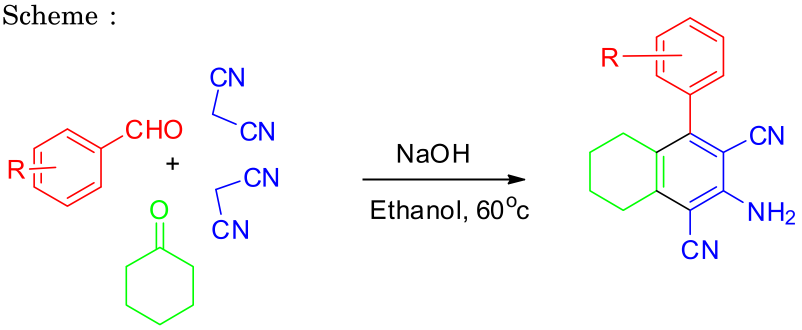
Multicomponent cascade reaction of aromatic aldehydes, malononitrile and cyclohexanone with catalytic amount of alkali in ethanol was carried to give 2-amino-4-phenyl-5, 6, 7, 8-tetrahydronaphthalene-1, 3-dicarbonitriles via Knoevenagel-Michael addition approach. The main features of the synthetic protocol are; moderate to good yields, mild reaction conditions, shorter reaction times, simple extraction of product and easily accessible catalyst. Its operational simplicity, less need for isolation techniques makes it an additional attractive route for the construction of these titled compounds. In view of the growing environmental concern in the field of chemistry, the proposed procedures for the synthesis of 2-amino-4-phenyl-5, 6, 7, 8-tetrahydronaphthalene-1, 3-dicarbonitriles are fit in the Green Chemistry criterion very well.

Scheme :



OO-08 : Eruca vesicaria Seed Oil : A Potential Source of Erucic Acid from Western Rajasthan

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Plant seeds are rich insource of oils that are important for nutrition, industry, and pharmaceuticals.The suitability of oil for a particular purpose, however, is determined by its characteristics and fatty acid composition. Eruca vesicaria (commonly known as taramira) is a short, tender perennial shrub belongs to Brassicaceae family found in the dry and arid regions of western Rajasthan (India). Eruca vesicariahas medicinal, ecological values in arid and semi-arid ecosystem. All parts of the plant including ripe fruit, leaves, root, stem and flowers may be used for the treatment of stress, anxiety, depression, insomnia and in rheumatic pains. In present work we studied fatty acid composition in seed oil of Eruca vesicariafrom arid region of western Rajasthan. It was observed that Eruca vesicariaseed oil contain 45.2% oil. The fatty acidcomposition of the oil as fatty acid methyl ester (FAME) was analyzed by gas chromatography coupled with mass spectrometer(GC-MS). The chemical composition ofEruca vesicariashows that the seedsare important source of oil (45–50%), protein (22–26%), carbohydrate (22.5%) and ash (6%). The major fatty acid present was Linoleic acid(6.39%), Linolenic acid (11.78%), Oleic acid (22.20%),Erucic acid (40.76%), Eicosenoic acid (6.37%), palmitic acid (9.72%), and stearic acid (1.59%).

OO-09 : Use of Some Metal Ferrites, MFe_2O_4 (M= Cu, Zn, Ni and Co) as a Catalyst in Aldol Reaction

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Aldol condensation of benzaldehydein presence of sodium hydroxide and acetone was catalysed by magnetic metal ferrites MFe_2o_4 (M = Cu, Zn, Ni, and Co). These metal ferrites were synthesized by hydrothermal method to improve product yield. The yield of product (dibenzalacetone) in presence ofCu, Zn, Ni and Co ferrites was found to be 90, 89, 80 and 65%, respectively. As-prepared metal ferrites were analysed by X-Ray Diffraction Spectroscopy (XRD), Energy dispersive X-Ray spectroscopy (EDX), and Scanning Electron Microscopy (SEM) to confirm morphology and particle size. The product was confirmed by m.p. and m.m.p.

OO-10 : Green Synthesis and Structure Elucidation of Some Benzothiazole Derivatives as Potential Antimicrobial Agents

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Benzothiazole is one of the most important heterocyclic compound, weak base, having varied biological activities and still of great scientific interest in application of drug discovery. In the present study, some substituted 2-(2-(1-phenylethylidine)hydrazinyl)benzothiazoles were synthesized with a green chemical route using water as a solvent. Structures of the synthesized compounds were elucidated on the basis of elemental analyses and spectral data. All the synthesized compounds were screened for their antimicrobial activity against E. coli, P. aeruginosa, S. aureus & S. pyogenus and antifungal activity against C. albicans, A. niger & A. clavatus. The result showed that these compounds exhibited moderate to significant activity.

OO-11 : Catalytic Effect of Phosphotungstic Acid-Functionalized Fe_3O_4 MNPs Blended with TiO_2 for Synthesizing Novel Spiro-Acridines and Evaluation of their Medicinal Potential on the Receptor Sites of the Main Protease of SARS-CoV-2

Shweta Potdar, Pratibha Sharma and Ashok Kumar*

The present work elicits an efficient and rapid three-component synthesis of a novel series of biologically significant spiro-acridine derivatives by integrating the pharmacologically dynamic hydantoin-phenytoin, substituted anilines, and dimedone as the prime synthetic equivalents. The process was enhanced by $Fe_3O_4@TiO_2$-PTA magnetic nanoparticles (MNPs), which acted as the heterogeneous catalytic system under ultrasonic irradiations. The reaction was accomplished in green solvent PEG-200 under aerophilic conditions to obtain products with excellent yields (90-96%). The core-shell structure and the characteristics of the prepared magnetic nano-catalysts were corroborated through powder X-ray Diffraction (PXRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDAX), FT-IR, and vibrating sample magnetometer (VSM) techniques. The average crystallite size of the magnetic nano-catalyst was found to be 24.36 nm having the saturation magnetization value of 21.146 emu g^{-1} indicating an easy recovery of the prepared magnetic nano-catalyst via the external magnetic field. Furthermore, the recyclability and the reusability of the magnetic catalyst and the solvent were also analyzed indicating an efficient approach up to five runs. Consequently, the structures of the synthesized compounds were ascertained based on elemental analyses and spectro-analytical data (^{1}H NMR, ^{13}C NMR, and mass spectrometry). High yields, smaller E-factor, considerable atom economy, easy recovery, and recyclability of the catalyst and solvent are the captivating features of the developed protocol. Moreover, in consideration of the ongoing global research on COVID-19, herein, we tried to identify the potential sites of the synthesized moiety that can suitably fit with the receptor sites of the main protease of SARS-CoV-2 (SARS-CoV-2 M^{pro}) through molecular docking studies.

OO-12 : Synthesis of Some New Novel Pyrazole and Pyrazoline Derivatives and their Computational Studies

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In the present investigation, we designed some new Pyrazole and pyrolzoline derivatives (3a-c) via Micheal addition. All the newly synthesized compounds were confirmed by ^{1}H NMR, IR and mass spectrometry. Also, the synthesized compounds subjected to DFT study were used calculate the chemical parameters such as chemical potential, electrophilicity and nucleophilicity and hardness. Moreover, synthesized compounds were screened for docking studies against the target enzyme SEC2 (PDB code: 1STE), from these results reveal that, compound 3b exhibited least binding energy -239.55 KJ/mol^{-1}. In future, these compounds can be used as antibiotics.

OO-13 : Bioassay Monitored Screening Leading to the Isolation of New Active Constituents from Medicinal Plants

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Research in drug discovery needs to develop robust and viable lead molecules or new chemical entities, which step forward from a screening hit to drug candidates. Medicinal plants have played significant role in the development of several clinically useful agents and continuously hold important status drug industries as development of new technologies have revolutionized the screening of plants constituents in discovering new drugs. The first commercial pure natural product introduced for therapeutic use is morphine marketed by Merck in 1826, and the first semi-synthetic pure drug aspirin, based on a natural product salicin isolated from Salix alba, was introduced by Bayer in 1899. This led to the isolation of early drugs such as cocaine, codeine, digitoxin, quinine and pilocarpine, of which some are still in use and several other recent plant derived compounds, which have undergone development and have been marketed as drugs

which include Paclitaxel from Taxus brevifolia for lung, ovarian and breast cancer, Artemisinin from traditional Chinese plant Artemisia annua to combat multidrug resistant malaria, Silymarin extracted from the seeds of Silybum marianum for the treatment of liver diseases. Keeping in view of the above facts and use of medicinal plants in discovery of new drugs or chemical entities and our continuous work and efforts to identify the new therapeutic agents, recently, in our laboratory, we have isolated and identified the many bioactive lead molecules from plants by using various chromatigraphic and spectral techniques. In this presentation, the detail techniques involved in the isolations, characterizations and biological screening evaluations of the isolated plant-derived lead molecules in our laboratories will be discussed.

OO-14 : Chitosan Supported Zinc Oxide Nanoparticles Catalyzed One-pot Synthesis of Azepine Analogues

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Multicomponent reactions [MCRs] have provided a strong dais to excess diversity as well as complexity in molecular and chemical bibliotheca in a short number of reaction steps. MCR is a very effective strategy in the sustainable and diversity-oriented synthesis of heterocyclic compounds. Also MCRs in accordance with the principals of green chemistry in terms of economy of steps and atom efficiency for development of improved organic synthesis pave the way towards sustainability approaches. In particular, synthesis of azepine derivates through MCRs has strongly attracted significant attention due to their various medicinal, biological and pharmaceutical activities. Present paper elicits the preparation of chitosan based nano composites containing the high content of ZnO nano particles as the support system to synthesize azepine derivative. Moreover, because of the ease of separation and no waste generation and the ability of reusing the catalyst, this work can be considered as a green and environmentally benign process. Also the clear work up procedure, high to excellent yields, relatively short reaction times and high atom economy are some added advantages associated with the protocol. All the synthesized compounds were characterized using various spectroanalytical techniques viz-FTIR, ^{1}H, ^{13}C NMR, Mass and elemental analysis. SEM, XRD, IR, TGA-DTA were used to established the structure and morphology of the synthesized catalyst.

OO-15 : Microwave Assisted Synthesis of N-Substituted Acridine-1,8-dione Derivatives: Evaluation of Antimicrobial Activity

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One-pot, four-component synthesis of the N-substituted acridine-1,8-dione derivatives in good yields reported. A simple and convenient one-pot method for synthesis of N-substituted acridine derivatives from condensation of 1,3-cyclohexanedione, substituted aryl amines and 1,2,3-triazole aldehydes using mixture of water/ethanol as a reaction medium is reported. The current protocol delivers numerous advantages such as good yields, short reaction duration, easy work-up and simplicity in procedure as it uses a green method and an eco-friendly catalyst. This method provides a quick access to the multi-functionalized N-substituted acridine-1,8-dione derivatives. The target compounds screened for their in vitro antimicrobial activity and most of the compounds found to exhibit good activity compared to standard drugs. The docking studies carried using Autodock 4.2 were proven that all the molecules exhibited good interactions with protein Glucosamine-6-phosphate synthase of Escherichia Coli and the Secreted aspartic proteinase from Candida albicans.

OO-16 : Molecular Docking Studies of Novel Imidazolones Against Fungal Proteinase and Sars Cov2 Main Protease

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Eleven active imidazolones were prepared using vilsmeier Haack reagent by cyclodehydration, condensation of azlactone derivatives with aromatic amines. Their structures were characterized by ^{1}H, ^{13}CNMR and mass spectroscopy. The compounds were screened against two fungal species candida albicans and fusarium ricini using griseofulvin as standard. Both invivo and insilico studies were carried out for novel imidazolones on candida albicans and insilico studies performed on SARs Cov2 main protease. Molecular docking studies on these compounds unravel the relative orientation, mode of interaction and nature of bonding with proteinase of Candida albicans and SARs Cov2 main protease.The compounds were docked against the enzymes with the help of AutoDock 4.2 software. The Autodock 4.2 results were visualized by using Biovia discovery Studio Visualizer and Proteins Plus Server.Evidence from docking pose and 2D interactions of compounds supported H-bonding, Vanderwaal's interactions and hydrophobic interactions with amino acid residues. Docking studies confirmed that all derivatives exhibit a good binding affnity with Autodock 4.2 software score in between "8.70 and "11.07 kCal/mol against the candida albicans proteinase and between -8.77 to -12.01 KCal/mol against SARs Cov2 main protease.

OO-17 : Carbohydrate Structural Elucidation by Mass Spectrometry

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We designed several new 1-hepta-O-benzoyl-â-D-maltosyl-3-phenyl thiocarbamides by the interaction of hepta-O-benzoyl-â-D-maltosyl isothiocyanate with various aryl amines. Analysis of newly synthesised derivatives have been investigated by mass spectrometry. The analysis method described in this paper demonstrate the structural characterisation of carbohydrate derivatives based on their molecular mass, as well as the mass of their respective fragment ions using mass spectrometry.

OO-18 : Conventional Synthesis and Study of Alkyl Substituted 1,3-Thiazole And its Nanoparticles with Special Reference to Plant Pathogens of Some Vegetable Crops

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The synthesis, spectral analysis and biological activities of 5-phenyl-2-hydroxy-chlorosubstituted-2-amino-1,3 thiazoles have been carried out. In this case 5-(2'-hydroxy-3',5'-dichlorophenyl)-4-(heptan-1-one)-2-phenyl amino-1,3-thiazole (K) has been screened. The compound K was synthesized from 1-(2'-hydroxy-3',5'-dichlorophenyl)-2-bromo-1,3-nonanedione (a_4) by the action of phenylthiourea. The nanoparticles of the compound K has been prepared by using ultrasonic technique. The titled compound and its nanoparticles were assayed for antipathogenic impact against some common crop pathogens viz -Aspergillus

OO-19 : Synthesis of 1-((2'-(2-(2-(Substituted Phenyl))-2-oxoethyl)-2H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)piperidine-4-carboxylic Acid Derivatives as Potent Biological Agents

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In the present work, we have discussed the synthesis of a series of 1-((2'-(2-(2-(substituted phenyl))-2-oxoethyl)-2H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)piperidine-4-carboxylic acid derivatives (7a-g) by the reaction of 1-((2'-(2H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)piperidine-4-carboxylic acid (5) with phenacyl bromides using acetonitrile and potassium carbonate at reflux condition. The key intermediate 5 have been synthesized by the reaction of 4-bromo biphenyl methyl triphenyl tetrazole with benzocaine(ethyl piperidine -4-carboxylate) in acetonitrile and K2CO3 under reflux temperature to get another intermediate 1-((2'-(2-trity-l2H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)piperidine-4-carboxylic acid which upon deprotection followed by alkali hydrolysis gave compound 5. The structures of all newly synthesized derivatives have been characterized using different spectroscopic techniques such as FT-IR, ^{1}HNMR, ^{13}C NMR and mass. The synthesized compounds (7a-g) were evaluated for their pharmacological and molecular docking studies.

OO-20 : Design, Synthesis, Characterizations and Antimycotic Activity of Some New Series of π Electron Deficient Polyfunctionalized Halogenated Pyrimidines

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Pyrimidines occupy a distinct and unique place in medicinal chemistry as this heterocyclic moiety has great biological and medicinal significance. A large array of pyrimidine drugs possess a variety of medicinal properties such as anticancer, antibacterial, antiprotozoal, antimicrobial, antiviral, antihypertensive, antihistaminic, anti-inflammatory, analgesic and CNS-active to metabolic adjuvants. The pyrimidine core is a structural constituent of critically important drugs like fluorouracil, etravirine, risperidone, iclaprim, avanafil, and rosuvastatin. Keeping in view the importance of pyrimidine moiety

drug discovery research, recently, we have synthesized the some new series of π electron deficient polyfunctionalized pyrimidines and evaluated their antimycotic activity in vitro against human pathogenic fungi. In this presentation, the detailed synthetic procedure, isolations, biological screening profiles and characterisations of the synthesized compounds by their spectral data (^{1}H NMR, ^{13}C NMR, EIMS, UV and IR) analysis will be discussed.

OO-21 : Regioselective Synthesis of Novel N-((1-alkyl-1H-1,2,3-triazol-4-yl)methyl)-2,2-dimethyl-2H-chromene-6-Carboxamides : Anti-Microbial Activity

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Regioselective click Cu(I) catalyzed [1,3] dipolar coupling of N-terminal alkyne tethered, 2,2-dimethyl-N-(prop-2-yn-1-yl-2H-chromene-6-carboxamide with a variety of organo azides gave exclusively 1,4 disubstituted triazole appended chromene derivatives, N-((1-alkyl-1H-1,2,3-triazol-4-yl)methyl)-2,2-dimethyl-2H-chromene-6-carboxamides in quantitative yield, which are characterized by IR,^{1}H-NMR, ^{13}C-NMR and MS. All the newly synthesized derivatives were screened for their antimicrobial activities, among them four compounds exhibited potent antibacterial and antifungal activity. The detailed results of synthesis and activity will be presented in discussion session

OO-22 : One-pot Multi-Component Synthesis of 2-((2-oxo-2-phenylethyl)thio-10-phenyl-4,10-dihydro-5H-indeno[2,1-d][1,2,4]triazolo[1,5-a]pyrimidine-5-one and their Characterization Study

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Design, synthesis of fused triazolo pyrimidine derivatives via a one-pot multi-component approach. The presence of bridgehead nitrogen atom these type of heterocyclic compounds is showing remarkable applications in the field of biological importance. The target compounds were synthesized by the reaction of 1,3-indane dione (1.0 mmol) on reaction with different types of aldehydes (1.0 mmol) initially the formation of chalcone and the insitu generation of chalcone in reaction vessel this on condensation reaction with 5-amino-4H-1,2,4-triazol-3-thiol in presence of acetic acid and few drops of piperidine to form a triazolo pyrimidines after completing of these reactants we added different phenacyl bromides to form a thio alkylated products with good percentage of the yields are obtained. All the final compounds were characterized by spectral techniques ^{1}H-NMR, ^{13}C-NMR, IR, MASS

OO-23 : Synthesis and Characterization of Oxazepine Derived from Symmetrical Azines and DFT Studies

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A new series of Novel oxazepine derivatives are synthesized from symmetrical azines w derived by the condensation of substituted aromatic aldehydes with Hydrazine hydrate in the presence of catalyst tetrabutylammoniumbromide. All the synthesized compounds are characterized by IR, ^{1}H, ^{13}C and HSQC NMR Spectral studies. Structure determination is optimized by Density Functional Theory (DFT) using B3LYP/6-311G++(d, p) method in the ground state.

OO-24 : Selective Synthesis of Novel Spiro Indenoquinoxaline-pyrrolidines by 1,3-dipolar Cycloaddition Reaction

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Multi-component 1,3-dipolar cycloaddition of azomethine ylides derived from cyclic ketones and a-amino acids with olefinic dipolarophiles for synthesis of divers spiro-pyrrolidines skeleton has received increasing interest. In continuation of our research program on the construction of structurally diverse spiro compounds by 1,3-dipolar cycloaddition reactions, here we described the synthesis of a series of novel structurally fascinating dispiroindenoquinoxaline hybrids with complete regio and diastereoselectivity via comprising three pharmocophoric cores i.e., indenoquinoxaline, pyrrolidine and thiazolidinone in single molecular framework by means of 1,3-dipolar cycloaddition reactions under microwave irradiations in high yields. In the present reaction azomethine ylide generated in situ, which subsequently react with dipolarophile alkyl-2-[(Z)-4-oxo-3-aryl/alkyl-2-(arylimino)thiazolidin-5-ylidene] acetate to construct thiazolidinone appended dispiro-indenoquinoxaline-pyrrolidines with unusual regio and endo-selective manner. The present study involves the generation of three new bonds and more than three stereogenic centers in a single operation under mild reaction conditions and short reaction time. The structure elucidation is based on NMR spectroscopic studies and regio-/stereochemistry has been concluded by single crystal X-ray diffraction analysis.

The details of present work and mechanism will be discussed during the conference.

OO-25 : Bovine Serum Albumin (BSA) Mediated Efficient One Pot Synthesis of 3,3'-(phenylmethanediyl)bis(4-hydroxy-6-methyl-2H-pyran-2-one) Derivatives and their Biological Studies

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Abstract. In this work, biocatalysis was achieved by the synthesis of 3,3'-(phenylmethanediyl)bis(4-hydroxy-6-methyl-2H-pyran-2-one) derivatives 3(a-h) using Bovine serum Albumin (BSA) as a catalyst. Substrate scope and various parameters involved on yield and time of the synthesis were investigated. The structure elucidation of the synthesised targets was assessed through different spectroscopic techniques like FT-IR, ^{1}H NMR, ^{13}C NMR and HR-MS analysis. Bio potency of the synthesised conjugates was examined towards anti-bacterial activity and most of the compounds showed effective results. Further, the anti-inflammatory activity of the synthesised compounds was evaluated against MMP-2 and MMP-9 using gelatin zymography technique. All the synthesised derivatives inhibited MMP-2 to good extent but displayed a moderate inhibition against MMP-9. Also the molecular docking studies were carried out to determine the interaction of synthesised bis-4-hydroxy-6-methyl-pyran-2-onederivatives with COX-2 receptor.

OO-26 : Greener Synthesis of Pyrido[2,3-d:6,5-d']dipyrimidines using Ag TiO$_2$ Nanocomposite as Heterogeneous Catalyst

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In recent years, the development of environmentally benign protocols has been extensively explored for the synthesis of bioactive heterocycles by eliminating the conventional catalysts. The use of heterogeneous catalyst specially nanocatalysts plays a crucial role in modern synthetic organic chemistry due to their salient advantages such as excellent catalytic activity, low toxicity, ease separation and reusability. Nitrogen-containing heterocycles are an important part of natural products and pharmaceutical agents and encompass distinct physical and biological activities. Amongst them, pyrimido-pyrimidines have remarkable position in synthetic and medicinal chemistry due to its diverse range of pharmacological activities.

In continuation of our endeavors towards the development of new green catalytic processes for sustainable synthesis of biologically active scaffolds, we report herein aqueous mediated and ultrasound-assisted three-component reaction of barbituric acid, various aromatic aldehydes and 6-amino-1,3-dimethyluracil/6-aminouracil to expedite the synthesis of a new series of 5-phenyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-2,4,6,8-tetraone under eco-compatible conditions in presence of green Ag-TiO_2 NCs as heterogeneous catalyst.

The details of present work and mechanism will be discussed during the conference.

OO-27 : Acetic Acid Catalysed Synthesis of Novel Imidazo[1,5-a] Quinoxalines and Spiro Imidazo[1,2-a] Quinoxalinones from Inactive 2-(1H-imidazol-1-yl) Aniline *via* Pictect-Spengler Reaction

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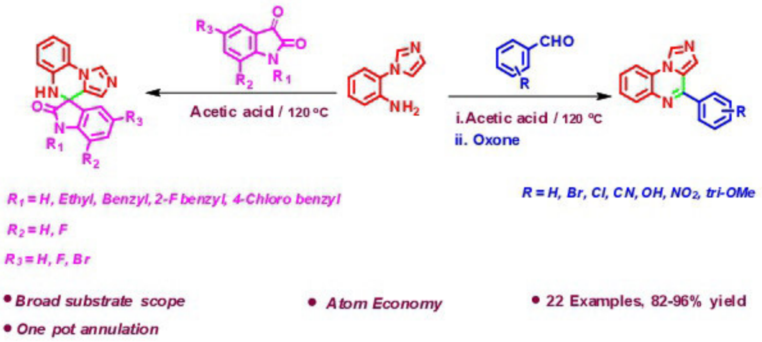
Nitrogen-containing compounds possess the high biological activity and are found to be present in both natural products and synthetic drugs. Quinoxalines are an important class of nitrogen-containing heterocycles that possess a broad spectrum of physiological and biological activities. Among them, imidazo[1,5-a] quinoxaline and spiroimidazo[1,2-a] quinoxalinone are fused-ring systems containing both imidazole and quinoxaline as well as indole in spiro quinoxalinone heterocyclic skeletons. This unique structural framework forms an integral part of several biologically active compounds and thus derivatives of these are well known for various types of biological activities like antibacterial, anticancer, anti-HIV agent, glucagon receptor antagonists, and angiotensin receptor activity and so on. So, the opportunity to prepare biologically important heterocyclic molecules in limited steps under mild reaction condition is an exciting goal for every modern organic chemist. To the best of my knowledge in the literature there was no straightforward method of synthesis of Imidazo[1,5-a] quinoxalines by using inactive 2-(1H-imidazol-1-yl) aniline and aldehydes. But the previous methods were involved ionic liquid supportted unconventional pictect-Spengler strategy, modified Pictect-Spengler strategy (To active starting substrate, introduced electron releasing groups at 2nd and 4th position of imidazole ring of starting substrate) and solid-phase strategy for the application of the pictet-spengler reaction and each method has its own limitation like low yields, expensive catalysts, harsh reaction conditions, and less substrate scope. Therefore, it is highly desirable to develop an efficient, nontoxic and convenient and straightforward approach for the synthesis of 4-substituted imidazoquinoxalines.

An efficient, straightforward, and green approch to access of the medicinally important Imidazo[1,5-a] quinoxalines and Spiroimidazo[1,2-a] quinoxalinones have been developed from inactive starting substrate (2-(1H-imidazol-1-yl) aniline) via Pictect-Spengler reaction using acetic acid as a catalyst. This protocol involves the general Pictect-Spengler strategy whereas the previous methods were involved ionic liquid supportted unconventional Pictect-Spengler strategy, modified Pictect-Spengler strategy (introducing electron releasing groups at 2nd and 4th position of imidazole ring of starting substrate) and solid-phase strategy for the application of the Pictet-Spengler reaction.. Further the substrate scope of the reaction has also been studied. The syntesis of spiro Imidazo[1,2-a] quinoxalinones were demonstrated first time by using 2-(1H-imidazol-1-yl) aniline and isatin or substituted isatins. so we can believe that the catalyst acetic acid was highly efficient, versatile, greener, inexpensive, stable and has great potential applications in the synthesis of various Imidazo[1,5-a] quinoxalines and spiro Imidazo[1,2-a] quinoxalinones

The detailed synthetic procedure, isolations, and characterisations of the synthesized compounds by their spectral data (1H NMR, 13C NMR, HRMS, and IR) analysis were discussed in this protocol.



OO-28 : Oxidation of Ethylbenezene Over New Heterogeneous Catalyst, {Co(II)[Cs- HACP- L]}

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The oxidation of ethylbenzene over {Co(II)[Cs- HACP- L]} was studying using 70% TBHP as an oxidative source. The reaction kinetics was affected by different parameters like TBHP ratio, reaction time, reaction temperature, reaction solvent and catalyst concentration. The heterogeneous catalyst, chitosan supported Co(II) Schiff base complex, abbreviated as {Co(II)[Cs- HACP- L]}, (where L = HACPANI) was synthesized and characterized using different analytical techniques; Fourier transform infrared spectroscopy, UV-VIS-NIR spectroscopy, scanning electron microscopy, energy dispersive X-ray analysis, X-ray powder diffraction etc. The main products of ethybenzene oxidation are acetophenone and benzoic acid, which were identified by GC-MS. The conversion of ethylbenzene (39.88%) and selectivity of products acetophenone (85.30%) and benzoic acid (14.70%) were obtained after 5 hours. The prepared catalyst was catalytically active and recyclable upto 7 cycles under optimized conditions.

PHYSICAL CHEMISTRY SECTION

Sectional President's Address

Pannuru Venkatesu

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Worldwide, there is growing awareness of the impact of hazardous chemical substances in the environment and economic view point. The judicious selection of chemicals and designing less toxic substances in chemical, purification processes and industries could offer safer and sustainable developments. Thus, control in generation of hazards and promotion of novel synthetic approaches must be followed. A wide area of research offering this incorporates the use of renewable feedstocks, catalysis and alternative solvents. Towards this, an environmentally benign solvent must be ascertained to ensure the biodegradability and enhanced applications in numerous fields like biotechnology and enzymology. Motivated by the demand for sustainable developments, researchers proposed ionic liquids (ILs) which fulfill the requirements of environmental sustainability. ILs render innumerable advantages over organic solvents in various fields like catalysis, electrochemistry, chemical synthesis and protein biochemistry. For a protein to be biologically active, the maintenance of its native structure becomes pre-requisite. Any deviation in native structure of protein results in misfolded or completely unfolded state of protein which in turn results in serious life threating ailments like type II diabetes, Alzheimer's disease and Huntington's disease. Most importantly, ILs as well as deep eutectic solvents (DESs) (a new generation of sustainable ILs) could be employed in enzyme biocatalysis as they enhance the solubility of products/ substrates without rendering them inactivation. The development of nontoxic ILs for biomolecules, the ability of ILs in dissolution, suppression and cryopreservation has potentially aided the developments in cryobiology, pharmaceutical industry as well in biomedical treatments.

PIL-01 : Ionic Liquids as Benign Solvent Systems for Sustainable Chemical Processes

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A novel class of molten salts referred to as ionic liquids possess the unique combination of particular properties, unlike molecular liquids, namely negligible vapor pressure (~ 10^{-11} to 10^{-10} bar at room temperature), wide thermal window (~ -50 °C to +250 °C), wide electrochemical window (~ ±3 Volt vs. NHE), non-flammability, high ionic conductivity and a highly solvating capacity for organic, inorganic and organometallic compounds. This unique combination of particular properties allows them to be exploited as "alternatives to organic solvents" and gives them increasing attention in academic and industrial research. The research areas on ionic liquids are growing very rapidly, and the potential applications are numerous, mainly because simple changes in the cation and anion combinations or the nature of the moieties attached to each ion allow the physical properties of ionic liquids such as hydrophobicity, viscosity, density, coordinating ability, ion selectivity, and chemical and electrochemical stability to be tailored for specific applications. The proposed talk will briefly introduce ionic liquids and understand the unique thermophysical properties of novel ionic liquids for metal ion extraction, CO_2 capture, desulphurization of fuels, and aqueous biphasic systems for the extraction of value-added products. Further, the effects of thermophysical properties of ionic liquids on these applications and current research trends on ionic liquids as solvents for the chemical industry will be discussed.

PIL-02 : Exfoliation and Decoration of Graphene with Nanoparticles for Photocatalysis in Aqueous Medium

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The advent of ionic liquids (ILs), the ionic compounds that are liquid at least below 100 °C, having unique physico-chemical properties, have exerted a great impact on research and development in different scientific avenues during last two decades.[1] The control over the properties of ILs, via altering the nature of cation, anion, length or nature of alkyl chain etc., have further widened the application arena of ILs. Many of the ILs have shown better surface active properties as compared to conventional ionic surfactants. Further, the ILs having a metal atom or metal ion in one of the constituent ions of IL are classified as Metal based ILs (MILs). Inspired by surface active nature of SAILs along with utilization of MILs for the preparation of variety of nanomaterials, our group conceived to synthesizes surface active MILs for liquid phase exfoliation of graphene and in-situ preparation of different nanomaterials in a sustainable manner for photocatalytic applications. The prepared nano-composites (ZnS@G; α-Fe2O3@G and Ag/AgBr@G) have shown enhanced photocatalytic efficiency towards degradation of toxic effluents in waste-water as compared to respective nanomaterials (ZnS, α-Fe_2O_3 and Ag/AgBr) under sun light or visible light. Not only this, we have successfully immobilized Cellulase on exfoliated G which showed 13-fold enhancement in catalytic efficiency as compared to that observed in buffer only.

PIL-03 : Perovskite Oxide as Advanced Electrode Materials for Charge Storage

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Unveiling the role of active sites is of large significance for the design and development of high performance energy storage materials. Defects in the form of vacancies and edges act as charge storage active sites and are not considered as imperfections. These defects have the ability to modulate electronic, surface and electrochemical properties. The active research on the supercapacitor these days involves the exploration of the fact that defects not always act as imperfections to the material and can be treated as energy storage sites. A number of questions that needs to be answered for the proper understanding of the field includes, which kind of lattice defects enhanced the performance of electrode material? How these defects can be generated in controlled, low-cost, scalable, and reproducible manner? How they can be identified and estimated in an appropriate way? How do they improve the activity of the material and what is the exact relation between structure and activity of the material? In recent years, oxygen vacancies rich perovskite oxide based super capacitor has seen an unprecedented popularity due to their structure/composition flexibility and anion intercalation charge storage mechanistic path. Still, a number of questions are left unanswered for the proper understanding of this field. Such as, what kind of structure modulation enhanced the stability of perovskite electrode? How the leaching of metal cations during electrochemical process can be prevented? What kind of doping positively influences the charge storage? How do oxygen vacancies contribute in the entire charge storage process? In this regard, we have tried to answer all these questions on the basis of extensive experimental and theoretical investigations that have been carried out by the researchers. Thus, we have made an attempt to comprehensively and critically review the factors favorable for design of high rate perovskite oxide based super capacitor electrode.

PIL-04 : Pharmaceutical Application of Ionic Liquids

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Antibiotic resistance is one of the biggest threats to global health, food security, and in development. Antibiotic resistance leads to longer hospital stays, higher medical costs and increased mortality. Hence, there is an emergence need to develop new class of antibiotics. Recent study showed the antibacterial efficiency of ionic liquids (ILs). Initially, ILs were proposed as an alternative solvent over conventional organic solvents; however, their unique physiochemical properties such as low vapour pressure and tune ability etc. has brought several new opportunities in variety of research fields such as bio-nanotechnology, biophysical [3], electrochemistry, and in biomedical. As a result, ILs have gained the interest of researchers towards their use for several purposes such as in drug development and in drug delivery system. Therefore, in present work a series of novel surface-active pyrrolidinium based ILs consisting of bis(trifluoro)sulfonylimide as an anion [Pyr Cx NTf3-] where,x=4,6,8,10,12 were synthesised and well characterised by ^{1}H NMR, ^{13}C NMR, FT-IR and mass spectroscopy. Different surface-active parameters were determined by surface tension and fluorescence spectroscopy. MTT was done to determine the cytotoxic effect of synthesised ILs. The synthesised ILs were screened for their antibacterial property against E. coli and S. aureus. Further, to increase the antibacterial property of MEL various combinations of MEL with ILs were prepared and their antibacterial activity was evaluated against E. coli and S. aureus. The results showed remarkable improvement in the antibacterial activity of MEL. Hemocompatibility showed good selectivity of non-covalent conjugate as a potential antibiotic agent. Moreover, the binding study was also performed to evaluate the binding efficiency and stability of MEL in presence of IL. Additionally, same study was performed with conventional drug, Levofloxacin to explore the efficacy of ILs in improving biological activity of drug.

PO-CYSA-01 : Correlation Analysis of Reactivity in the Oxidation of Substituted Benzaldehydes by Pyridinium Dichromate

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Oxidation of thirty six monosubstituted benzaldehydes by pyridinium dichromate (PDC) in dimethylsulphoxide (DMSO), leads to the formation of corresponding benzoic acids. The reaction is of first order with respect to PDC. A Michaelis-Menten type kinetics was observed with respect to the reactants. The reaction is promoted by hydrogen ions; the hydrogen ion dependence has the form kobs= a + b [H+]. The oxidation of [2H] benzaldehyde (PhCDO) exhibited a substantial primary kinetic isotope effect. The reaction was studied in nineteen different organic solvents and the effect of solvent was analysed using Taft's and Swain's multi-parametric equations. The rates of the oxidation of para and meta substituted benzaldehydes showed excellent correlation in terms of Charton's triparametric LDR equation, whereas the oxidation of ortho-substituted benzaldehydes were correlated well with tetraperametric LDRS equation. The oxidation of para-substituted benzaldehydes is more susceptible to the delocalized effect than is the oxidation of ortho- and meta- substituted compounds, which display a greater dependence on the field effect. The positive value of ? suggests the presence of an electron-deficient reaction centre in the rate-determining step. The reaction is subjected to steric acceleration by the ortho-substituents. A suitable mechanism has been proposed.

PO-CYSA-02 : High Energy Density of Supercapacitor with BioActivated Carbon and Solid Electrolyte Containing Ionic Liquid and Anion-Trapping Boron Moieties

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Fabrication of high energy density supercapacitors (SCs) with long cycle life using sustainable materials for next-generation applications is of supreme significance. The ongoing challenge is to raise the energy density of SCs comparable to that of batteries while maintaining the high power density and cyclability. In addition, achieving superior performance with low-cost and renewable bio-mass derived compounds

is very vital to address the growing environmental concerns. In order to address these issues, we proposed the use of bio-activated carbon and focussed on developing boron-containing high conductive ionic liquid (IL) based gel polymer as electrolytes. Herein, high surface area, hierarchical porous carbon materials were derived from a biowaste from commonly available non-edible fruit. It showed outstanding specific capacitance of 210 F g^{-1} at a current density of 2 A g^{-1} in an aqueous electrolyte. In order to improve the performance, boron-containing gel polymer electrolyte (B-GPE) with a semi-interpenetrating polymer network (IPN) structure was successfully prepared. In this electrolyte, polyvinylidene fluoride (PVDF) acts as polymer host, the novel borate ester monomer (BEM) as the cross-linker, and LiTFSI and imidazolium-based IL as the plasticizer and electrolytic salt, respectively. Due to the incorporation of anion-trapping boron sites, the ionic conductivity of the prepared GPE at 25 °C was enhanced by more than 5mS $cm^{-1,}$ and it also shows constructive mechanical strength, excellent thermal stability, and extremely low flammability. Imidazolium IL based solid electrolytes support in achieving high energy density due to its high potential window. Further flexible solid state symmetric SC devices are to be fabricated with the same active carbon electrodes employing B-GPE. These results will be aroused our interest to optimize the system further to develop high-performance, green energy storage devices using eco-friendly materials for future generation electric vehicles and other advanced energy storage systems.

PO-CYSA-03 : Thermophysical Properties of Binary liquid mixtures at different Temperatures and ATR-FT- IR Spectral Studies

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The thermo physical properties of density (p), speed of sound (u) data of binary liquid mixtures of Phenetole (ethoxy benzene) with aniline , N-methylaniline and NN,dimethylanilinehave been estimated at 303.15K 308.15K, and 313.15K temperatures at atmospheric pressure. From the data of measured densities, the excess molar volumes (V^E) and excess isentropic compressibilities (κ_s^E) have been calculated at all the estimated temperatures. The V^E and κ_s^E values were fitted to Redlich-Kister equation. Further the measured sound speed data were compared with Schaffs Collision factor theory (CFT) and Jacobson's Free Length theory (FLT) to check their predictive capability. The resultant properties were explained interms of molecular interactions owing to physicochemical effects between the unlike components of binary liquid mixtures. Further AT FT-IR data was also collected to confirm the existence of intermolecular Hydrogen bonding between phenetole and amines components.

PO-CYSA-04 : Expanding the Potential Role of Deep Eutectic Solvents toward Facilitating the Structural and Thermal Stability of α Chymotrypsin

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Since the introduction of deep eutectic solvents(DESs), numerous reports have surfaced describing its tunable properties and environmentally benign nature. Due to such favorable properties of DESs, they have found a wide variety of applications. Moreover, in order to harness the potential of proteins in numerous industries, there is an emergent need to find a suitable cosolvent that is biocompatible with protein and is also environmentally safe. In this context, this work presents a systematic evaluation of effect of two deep eutectic solvents (DESs), namely, choline chloride-urea (ChCl-urea) and choline chloride-glycerol (ChCl-gly) on the structural and thermal stability along with activity of enzyme á- chymotrypsin (CT) using circular dichroism (CD), UV"visible, steady state, and thermal fluorescence spectroscopy. It was observed that the presence of DESs does lead to enhancement in the thermal stability of CT along with the preservation of activity. The enzymatic activity was well maintained in both the DESs, and the deleterious effect of urea was overcome by ChCl-urea on the enzyme. Thus, the negative outcome of urea was overpowered by the combination of ChCl and urea. Overall, both the DESs can be described as potential biocompatible, sustainable, and promising cosolvents for CT with enhanced structural and thermal stability along with preservation of its activity.

PO-CYSA-05 : Green Synthesis of Pomegranate Leaf Extract Cobalt Ferrite Nanoparticles and their Anticancer Activity against Breast Cancer (MCF-7) Cell Lines

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Cobalt ferrite nanoparticles were prepared by green synthesis method using pomegranate leaf extract. XRD analysis confirmed the cubic structure of $CoFe_2O_4$ nanoparticles with an average crystallite size of 23.55 nm using Scherer formula. SEM images revealed that the synthesized nanoparticles are in spherical shape. EDAX spectrum showed the elemental composition of as synthesized nanoparticles. Vibrating Sample Magnetometer analyses revealed that the synthesized nanoparticles have ferrimagnetic behaviour.The anticancer activity was assessed at the in vitro level by MTT assay against breast cancer (MCF-7) cell lines

PO-CYSA-06 : Development of Electro Analytical Methods and Oxidation Mechanism for the Determination of Nonsteroidal Anti-inflammatory Agent, Phenylbutazone Inpharmaceutical and Biological Fluids

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The electrochemical oxidation of Phenylbutazonewas investigated for the first time on carbon paste electrode using cyclic, linear sweep and square wave voltammetry. The results indicated that the carbon paste electrode showed excellent electro-catalytic activity towards the oxidation of phenylbutazone in phosphate buffer solution of physiological pH 7, than the bare glassy and graphite pencil electrodes. To optimize the experimental conditions for the determination of phenylbutazone, the dependence of the peak current on pH, concentration, and scan rate were evaluated. The anodic peak was characterized and process was diffusion controlled. For the estimation of phenylbutazone, a square wave voltammetric method with high accuracy and precision was developed with a limit of detection (LOD) of 5.2 nM and a limit of quantification (LOQ) of 17 nM, in the concentration range 0.8 to 10 µM. The method was employed for the determination of PBZ in biological and pharmaceutical samples. This approach can be used in clinical diagnosis, quality assurance and drug screening.

PO-CYSA-07 : Influence of Magnetic Nanoparticles on the Conformational Stability of Hen-Egg White Lysozyme

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From the last decade, nanotechnology has been explored to fabricate, characterize and specially tailor the functional properties of nanoparticles for therapeutics and biomedical applications. Based on

the unique physical, chemical, thermal, and mechanical properties magnetic nanoparticles (Fe_3O_4) have ability to interact with biomolecules such as proteins to tune their most versatile and useful transition ability to good extent and offer a high potential for several biomedical applications. The present work focuses on studying the conformational stability and molecular level interactions of lysozyme (Lys) in the presence of two novel synthesized nanoparticles, namely, Fe_3O_4 and Fe_3O_4 coated with choline hydroxide using UV-visible, steady state fluorescence spectroscopy, activity of lysozyme, circular dichroism (CD) and dynamic light scattering (DLS).However, the fluorescence study reveals that there is a concentration dependent quenching of the fluorescence intensity after addition of nanoparticles. Different interactions with proteins at the molecular scale may be the reason for this unexpected behavior. Therefore, the present work provides an insight towards designing the next-generation protein friendly nanomaterials.

PO-01 : Tetra Hydro Furan Solvent Effect on Kinetics and Mechanism of Hydrolysis of Biologically Active Esters

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The chemical reaction in nature and in living beings proceeds with particular rate constant, energy change with well defined mechanism to a chemical reaction whether formation, oxidation or hydrolysis, the reaction needs proper medium, definite temperature, manifested either by thermal or by photochemical process for generating final product. The nicotinamide, nicotinic esters and nicolinyl hydrazide etc are useful pharmacologically active molecules and used, since long as pro drugs. The mechanistic approach and study of hydrolysis of these products will through their mode of activities in quite interesting and important from the view of kinetic study. Transition state theory inspires a thermodynamic approach of reaction rates in which the rate constant is expressed in terms of thermodynamic parameters, the simplest account of reaction rates is provided in terms of collision theory. The reaction in solution are classified into two types namely diffusion controlled and activation controlled. When a chemical reaction proceeds energies are being redistributed among bonds old bonds are being cleaved and new bonds are being formed. The extent of hydrolysis of biological esters like ethyl nicotinate in aqueous THF solvent in various ratio(0, 20, 40, 60, and 80%) at fixed temperature(200, 300 and 400 C). then its rate constant and mechanism is affected. Different analysis process are measured by conductometric, pH and titrometric method. Addition of metal oxide (nanoparticles) as a catalyst inhance the extent of hydrolysis.

PO-02 : Oxidative Transformation of Amino Acids using Transition Metal Oxidants

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Kinetics and oxidation of POLAR and non polar amino acids by Diethylammonium chlorochromate (DEACC) in dimethylsulphoxide (DMSO) is leading to produce its consecutive sulphoxide.To better understand the reaction, this work investigated the reaction kinetics and transformation pathways of selected amino acids towards DEACC. The rate was dependent on the first power of the concentration of the Polar amino acids and DEACC.The reaction was studied at constant ionic straight and over the temperature range 310-320K.The reaction consists of three steps - induction period, complexation and oxidation. Addition of an acid enhances the reaction rate; the effect of acidity is expressed by the relation $k_{obs} = a + b\,[H^+]$. The effect of solvent medium was studied in nineteen different organic solvents and temperature effect has also been studied. The solvent effect is evaluated by the models of Kamlet and Swain multi parametric equations. Importance of the cation solvating powers is predominantly seen in the effects of solvent medium. On the basis of results and discussion a suitable mechanism is proposed.

PO-03 : Correlation Analysis of Reactivity in The Oxidation of Some Vicinal and Non-Vicinal Diols by Tripropylammonium Chlorochromate : A Kinetic and Mechanistic Approach

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The kinetics of oxidation of four vicinal, four non vicinal diols by tripropylammonium chlorochromate (TPACC) have been studied in dimethylsulphoxide (DMSO). The main product of oxidation is the corresponding hydroxycarbonyl compound. The reaction is first order each in MFC. Michaelies-Menten type of kinetics is observed with respect to the diols. The reaction is catalysed by hydrogen ions. The

hydrogen ion dependence is taking the form: $k_{obs} = a + b[H^+]$. The oxidation of [1,1,2,2 $^2H_4$] ethanediol exhibits a substantial primary kinetic isotope effect ($k_H/k_D = 5.73$ at 298 K). The reaction has been studied in nineteen different organic solvents and the solvent effect has been analysed using Taft's and Swain's multiparametric equations. The temperature dependence of the kinetic isotope effect indicates the presence of a symmetrical transition state in the rate determining step. A suitable mechanism has been proposed.

PO-04 : Inhibition Effect Study of the Newly Synthesized Pyrazoline Derivative on Mild Steel in Hydrochloric Acid Medium by Experimental and Theoretical Approach

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The novel pyrazoline derivative 5-[5-(4-bromophenyl)1-1(pyridine-2-yl)-4-5-dihydro-14-pyrazol-3-yl]-2-methoxy pyridine (BPPM) was synthesised and the spectral analysis has been carried out using ^{1}HNMR, ^{13}CNMR and FT-IR spectra. The evaluation of the inhibition effect of BPPM on the corrosion of mild steel in 0.5M HCl solution has been carried out by Tafel polarization and electrochemical impedance spectroscopy techniques with the variation of its concentration from 10ppm to 40ppm at the temperature range from 303K to 323K. The theoretical analysis of the inhibition effect was performed with quantum chemical calculations using density functional theory (DFT) which proved the ability of protonated form of BPPM to interact with the vacant d-orbital of iron to arrest the rate of corrosion. The scanning electron microscopy with EDX studies and UV-Visible spectroscopy technique confirmed the formation of metal-BPPM complex. The experimental and theoretical data proved BPPM as a potent corrosion inhibitor at considerably low concentration exceeding not more than 40 ppm.

PO-05 : Green Synthesis of Bismuth Selenide Nanoparticles using Ascorbic Acid

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Synthesis of Bismuth Selenide (Bi_2Se_3) at nanoscale has received

quite some attention during the past decades owing to its semiconductor (with a gap of 0.3 eV) and thermoelectric properties. It has been the subject of ongoing scientific research by several groups because topologically protected surface states have been observed in Bismuth Selenide.

In the present study,a greener synthetic method has been developed using economically cheap desktop chemicals such as ascorbic acid (vitamin C), $BiCl_3$, ethylene diamine tetra acetic disodium salt (EDTA) and Selenium dioxide (SeO_2). In a typical synthesis process 10mmol of SeO_2, 6.66mmol $BiCl_3$,and 0.666g EDTAethylenediammine tetra acetic disodium salt were mixed with 135 ml distilled water in a 250mL R.B flask. After thorough mixing 1.166g of NaOH, 1.166g ascorbic acid were added to the contents of R.B flask. The contents of the flask were heated in an oil bath to a temperature of 150 ^{0}C with constant stirring for 48 hrs with a speed of 100 rpm. The precipitated dark grey powder was filtered, washed with distilled water and ethanol several times and air dried samples were obtained. These samples were further calcinated for about 6hrs at 100^{o}C. Samples thus obtained were characterized by X-ray powder diffraction measurements and scanning electron microscopy (SEM), which revealed the formation of nanoparticles (34nm before calcination and 12nm after calcination).

PO-06 : Terminalia Chebula Fruit Aqueous Extract

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Nowadays, the biological synthesis of nanoparticles attains researchers' interest in removing hazardous pollutants from water. Due to eco-friendliness, cost effective, non-hazardous and avoids the usage of catalyst and stabilizing agents. Herein, biosynthesized NiO nanoparticles were prepared at the ambient conditions by using aqueous Terminaliachebula fruit extract. Terminaliachebula fruit extract contains many phytochemicals like polyphenolic compounds, terpenoids, carbohydrates and flavonoids, which can be responsible for the nucleation of NM in biological synthesis. The resulted biosynthesized NiO nanoparticles were characterized via UV, FTIR, Zeta potential, XRD, EDX, SEM and TEM. The UV and XRD analysis confirmed the formation and cubic crystalline nature of biosynthesized NiO nanoparticles, receptively. FTIR, EDX and zeta potential confirmed the functional groups, elemental composition and surface charge. Additionally, they explain that phytochemicals were responsible for the reduction and stabilization of biosynthesized NiO nanoparticles.

The average size of biosynthesized NiO was found to be 14.08 nm and spherical in shape with TEM. In addition, antioxidant and catalytic activities performance of the NiO nanoparticles were also investigated.

PO-07 : Oxidation Kinetics and Mechanistic Studies of Organic Acids by Tripropylammonium Chlorochromate

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Kinetics and mechanism of oxidation of formic and oxalic acids by diethyammonium chlorochromate (TPACC) have been studied in dimethylsulphoxide. The main product of oxidation is carbon dioxide. The reaction is first order with respect to TPACC. Michaelis Menten type of kinetics were observed with respect to the reductants. The reaction is acid catalysed and the acid dependence has the form: kobs = a + b[H+]. The oxidation of deuterio formic acid exhibits a substantial primary kinetic isotope effect (kH/kD = 5. 79 at 298 K). The reaction has been studied in nineteen different organic solvents and the solvent effect has been analysed using Taft's and Swain's multiparametric equations. The temperature dependence of the kinetic isotope effect indicates the presence of a symmetrical cyclic transition state in the rate determining step. Suitable mechanisms have been proposed.

PO-08 : Reaction Kinetics between Paracetamol and N-Bromosuccinimide in Presence of Mercuric Acetate

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The Reaction kinetics of oxidation between Paracetamol and N-bromosuccinimide in the presence of mercuric acetate in the acid medium has been performed. The overall reaction is second order viz. First order with respect to each reactant and rate of reaction is retarded by hydrogen ion concentration. A plausible reaction mechanism has been suggested. The thermodynamic parameters such as energy and entropy of activation have been calculated by employing Eyring equation.Correlation Analysis Of Reactivity In The Oxidation Of Some Vicinal And Non-Vicinal Diols By Tripropylammonium Chlorochromate: A Kinetic And Mechanistic Approach

PO-09 : Effective Bioglycerol Conversion to Solketal over Sulphated Al-MCM 41 Catalysts

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Conversion of glycerol, a by-product in the biodiesel productionto valuable chemicals can make it a sustainable process and at the same time glycerol can be exploited as a renewable chemical feedstock as well. Solketal is one such valuable product fromacetalization of glycerol that is used as a fuel additive to reduce carbon emissions and enhance octane number. Further, solketal has several other applications in solvents, inks, paints and pharmaceuticals. Acetalization of glycerol involves carbocation production by the activation of ketone carbonyl group through a protonation step or polarization by the Lewis or Brønsted acid sites.The present work is a report of highly efficient sulphated Al-MCM 41 catalyst for the selective synthesis of Solketal by acetalization of glycerol at room temperature.Al-MCM41 was prepared by templating method followed by sulphonation with H_2SO_4 (1N) to obtain sulphated Al-MCM 41. The catalyst was characterized by low angle XRD, BET-SA and Pore size measurements, SEM-EDAX and py-adsorbed FT-IR studies. The XRD patterns clearly show the mesoporous structure of MCM 41 from the low angle peak and BET-SA obtained was ~ 600 m^2g^{-1} with a typical adsorption isotherm of type-IV, a characteristic feature of mesoporous materials. The py-adsorbed FT-IR patterns of the Al-MCM 41and sulphated Al-MCM 41 clearly indicate the generation of enhanced Bronsted acidity on the surface of the catalyst which explains the higher activity of the sulphated catalyst over the non-sulphated one. The catalyst activity was compared with simple Al MCM41 and also sulphated zirconia and results have shown sulphated Al MCM 41 to be superior to the other two catalysts tested. This clearly indicates the role of mesoporous structure that gives a stable and enhanced surface.

PO-10 : Reaction Kinetics between Paracetamol and N-Bromosuccinimide in Presence of Mercuric Acetate

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The Reaction kinetics of oxidation between Paracetamol and N-bromosuccinimide in the presence of mercuric acetate in the acid medium has been performed. The overall reaction is second order viz. First order with respect to each reactant and rate of reaction is retarded

by hydrogen ion concentration. A plausible reaction mechanism has been suggested. The thermodynamic parameters such as energy and entropy of activation have been calculated by employing Eyring equation.

PO-11 : Synthesis of Fatty Acids Stabilized Gold Nanoparticles : Effect of Experimental Conditions on Particle Size

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In this abstract, Synthesis of gold nanoparticles stabilized by myristic, palmitic and stearic acids is discussed . Three reducing agents formaldehyde, triethanolamine and dimethylformamide which are moderate strong to mild are used. The synthesized nanoparticles are dispersible in non-polar solvents such as benzene and toluene. The existence of adsorbed fatty acids is shown by IR spectra. The toluene solution of these nanoparticles exhibited a surface Plasmon resonance in the range 405-426 nm. The results show the gold nanoparticles have an enhanced stability on increasing chain length of the fatty acid.

The size of the nanoparticles is greatly influenced by the experimental conditions such as temperature and concentration. The nanoparticles are characterized by FTIR, XRD, UV–Vis, and TEM techniques.

INDIAN COUNCIL OF CHEMISTS

Indian Council of Chemists (ICC), was founded at Agra on 19th September, 1981 with an initial membership of more than 100 fellows. However, over the past 41 years it has grown in strength and popularity. At present there are more than 1850 Life Fellows and about 8200 annual floating fellows. The membership includes Scientists, Professors, Researchers, Teachers and Scholars from various IITs, CSIR Laboratories, Universities, Colleges, prestigious academic institutions and scientific organizations spread all over the country. The first Annual Conference of ICC was held at **Agra** and subsequent conferences were held and hosted by various universities / institutions throughout the country such as; Kashmir University, **Srinagar,** Karnataka University, **Dharwad,** Gorakhpur University, **Gorakhpur,** Central Fuel Research Institute, **Dhanbad,** Madurai Kamraj University, **Madurai,** Jiwaji University, **Gwalior,** Sri Venkateshwara University, **Tirupati,** Gulbarga University, **Gulbarga,** Goa University, **Goa,** Bihar University, **Muzaffarpur,** Kakatia University, **Warangal,** Jammu University, **Jammu,** The Institute of Science, **Mumbai,** Dr. BR Ambedkar University, **Aurangabad,** Mangalore University, **Mangalore,** Madras University, **Chennai,** North Maharashtra University, **Jalgoan,** Kuvempu University, **Shimoga,** Mysore University, **Mysore,** Rani Durgavati University, **Jabalpur,** Indian Institute of Technology, **Roorkee,** KC College, **Mumbai,** Birla Institute of Technology, **Ranchi**, Birla College, **Kalyan**, Dr. H.S. Gour University, **Sagar,** Gurukul Kangari University, **Haridwar,** H.N.G. University, **Patan,** Panjab University, **Chandigarh,** Osmania University, **Hyderabad,** Saurashtra University, **Rajkot,** Karnatak University, **Dharwad,** Indian School of Mines, **Dhanbad**, Uka Tarsadia University Bardoli, **Surat** and **Haribhai V. Desai College, Pune** in association with **College of Engineering, Pune,** School of Chemistry, Andhra University, **Visakhapatnam,** National Institute of Technology Karnataka (NITK) Surathkal, Mangalore, **Karnataka,** Jaipur National University, **Jaipur,** Veer Narmad South Gujarat University, **Surat** & **6 International Conferences** at **Bangkok, Kuala Lumpur, Dubai, Tashkent, Bali** and **Paris** were highly successful and well attended.

OBJECTIVES

(i) To advance and promote the cause of chemical research & education in the country.
(ii) To strive for strengthening co-operation on the national level and promoting contacts amongst scientist of the country.
(iii) To publish such proceedings, journals, transactions and other material as may be considered desirable.
(iv) To organize symposium, discussions, special lectures, exhibitions and other related activities for a better understanding of chemical research and its applications for the economic, social and industrial progress of the country.
(v) To under take any or all other acts, matters and things as are conducive to, or incidental to, or necessary for, the above objectives.
(vi) To work in association with International Societies of Chemistry and to co-operate with other organizations having similar objectives

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