International Conference

on

Recent Trends in Chemistry of Materials 2021

(ICRTCM 2021) – Virtual Mode

Date: 20th September to 24th September, 2021

Organized by

Department of Chemistry, ICFAI Science School

ICFAI University Tripura

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ICFAI University Tripura

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Mr. Sujit Sutradhar
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Message

It is gratifying to note that distinguished academicians and scientists from across the country and abroad are invited to deliver their lectures in International Conference on Recent Trends in Chemistry of Materials 2021 (ICRTCM 2021) during 20th -24th September 2021 organized by the Department of Chemistry in virtual mode.

I am confident that this International Conference would be the conglomeration of the galaxy of internationally and nationally renowned academicians and scientists and research scholars and this conference will provide a direction in the future research activities in the field of Chemistry.

It is appreciated that the Organizing Committee has decided to publish a Book of Abstract. This will serve as a chronicle for the event.

I take this opportunity to welcome all the delegates and participants in the international conference and wish a grand success for ICRTCM 2021.

Prof. Dr. Biplab Halder
Pro - Vice Chancellor
ICFAI University Tripura

Message

I am indeed happy to learn that the Department of Chemistry of ICFAI University Tripura is organizing an International Conference on Recent Trends in Chemistry of Materials 2021 (ICRTCM 2021) during 20th -24th September 2021 in virtual mode.

I am further delighted to note that academicians and scientists from all over the country and abroad are going to present their lectures during this Conference. Focused on new and innovative chemical technologies, this event will continue to be the ideal platform to share scientific knowledge and expertise in the area of chemical applications. The scope of this conference is to encompass the latest research in the field of Inorganic, Organic, Physical, Theoretical, and Material Chemistry. I am certain that this Conference will be a grand success and will have a major impact on the scientific community.

All my good wishes to you all.

Dr. A. Ranganath
Registrar
ICFAI University Tripura

Message

The inherently empirical nature of Chemistry provides a great challenge to the chemists in bringing out the deterministic aspect of the science. I am glad that the Department of Chemistry, ICFAI University Tripura is hosting an International Conference on Recent Trends in Chemistry of Materials 2021 (ICRTCM 2021) from 20th - 24th September 2021 in virtual mode. This Conference will open many horizons to the researchers and the scientific community of our country. Notably, the eminent speakers from our country and abroad are going to participate to communicate sound knowledge and expertise in trending research fields through keynote lectures. This is a tremendous opportunity for all of us to listen to these great scientists and enhance our knowledge.

I appreciate the hard work of the organizing committee members for hosting the conference in virtual mode.

I wish all the good luck to the organizers of the Department of Chemistry, ICFAI University Tripura.

Prof. Dr. Priyangshu Rana Borthakur
Dean, FST
ICFAI University Tripura

Message

The Department of Chemistry, ICFAI University Tripura, feels honoured to organize this International Conference on Recent Trends in Chemistry of Materials-2021 (ICRTCM 2021) from 20th to 24th September 2021. The mission of this conference is to provide a platform for constructive ideas on recent trends and innovative approaches with efficient use of materials in the field of Chemistry and to draw together the scientists of academic and industrial institutes among the global nation on a greater understanding and collaborative approach for a marvellous design to make a modern world. Chemistry of Materials is a multifaceted topic dealing with the discovery and design of new materials. Research in Chemistry of Materials is vibrant and a breakthrough in material science would bring significant impact on future technology.

The ICRTCM-2021 aims to provide an opportunity for academicians, scientists, researchers, as well as students to come together and engage in a fruitful exchange of views and ideas across a broad range of disciplines in the fields of Chemical and Material sciences through a comprehensive and eventful virtual gathering. The scope of this conference is to encompass the latest research in the field of Inorganic, Organic, Physical, Theoretical, and Material Chemistry. This will provide opportunities for new researchers to explore new directions in their research through interaction with the leaders in the field. It also aims to communicate sound knowledge and expertise in selected research fields through keynote lectures deliver by eminent speakers from India and abroad. The program of action includes nine technical sessions covering the thrust areas by the invited talks and contributed lectures delivered by the experts who have expertise in the field of materials chemistry globally.

With a galaxy of speakers from across the globe, this forum aims to give an excellent opportunity for academicians, scientists and participants all over the country and abroad to come together and share their knowledge and to interact on the latest development in the interdisciplinary areas of chemical sciences.

I would like to thank the Organizing Committee members, distinguished invited speakers, presenters, participants, all my colleagues and friends who have directly or indirectly contributed towards the planning of this Conference in making it an enlightening, enriching and memorable experience for all of you.

Snath

Dr. Swarnali Nath Choudhury

Associate Prof. & HOD, Chemistry

BRIEF SCHEDULE

	10 am – 11 am	11 am – 12 pm	12 pm – 1 pm	1 pm – 2 pm	2 pm – 3 pm	3 pm – 4 pm	4 pm – 5 pm	5 pm – 6 pm
20.09.2021	**Inaugural Session**	**Plenary Lecture** **Prof. Dr. Sourav Pal** Director, Indian Institute of Science Education and Research Kolkata, India	--	LUNCH BREAK	**Invited Lecture** **Dr. Amal Kumar Mandal** Senior Scientist, CSIR-CSMCRI Bhavnagar, India	**Plenary Lecture** **Prof. Dr. Richard Catlow** University College London, Royal Institution	**Invited Lecture** **Dr. Mousumi Das** Associate Professor, IISER Kolkata, India	--
21.09.2021	**Invited Lecture** **Prof. Dr. Parameswar K. Iyer** Professor, Department of Chemistry & Centre for Nanotechnology, IIT Guwahati, India	**Invited Lecture** **Prof. Dr. Amitava Das** Professor, Dean of Research & Development, IISER Kolkata, India.	**Technical Session I**		**Invited Lecture** **Prof. Dr. Rajadurai Chandrasekar** Professor, School of Chemistry, University of Hyderabad, India.	**Invited Lecture** **Prof. Dr. Thomas Wirth** Professor of Organic chemistry at Cardiff University	**Technical Session II**	
22.09.2021	**Invited Lecture** **Dr. Tapas Kuila,** Senior Scientist, Surface Engineering and Tribology, CSIR-CMERI, India.	**Invited Lecture** **Prof. Dr. Debashis Ray** Professor & Head, Department of Chemistry, IIT Kharagpur, India.	**Technical Session III**		**Technical Session IV**	**Invited Lecture** **Dr. Sangita Sen** Assistant Professor, IISER Kolkata, India.	**Invited Lecture** **Dr. Pradip Kr. Tarafdar** Assistant Professor, IISER Kolkata, India	--
23.09.2021	**Invited Lecture** **Dr. Raj Kumar Arya** Associate Professor, NIT Jalandhar, India.	**Invited Lecture** **Dr. Krishnandu Makhal** Assistant Professor, School of Physical Sciences, JNU, India.	**Technical Session V**		**Technical Session VI**	**Invited Lecture** **Dr. Alakananda Hajra** Associate Professor, Department of Chemistry, VisvaBharati University, India.	**Technical Session VII**	
24.09.2021	**Technical Session VIII**	**Invited Lecture** **Prof. Dr. Chandan Mukherjee** Professor, Department of Chemistry, IIT Guwahati, India.	**Technical Session IX**		**Invited Lecture** **Dr. Jan K. Zareba** Assistant Professor, Faculty of Chemistry at Wrocław University of Science and Technology, Poland.	**Invited Lecture** **Prof. Dr. Michael D. Ward** Professor and Head, Department of Chemistry, University of Warwick, Coventry CV4 7AL, UK	**Valedictory Session**	

TABLE OF CONTENTS

TABLE OF CONTENTS

TABLE OF CONTENTS

TABLE OF CONTENTS

TABLE OF CONTENTS

ICRTCM 2021

Plenary Speakers

Inaugural Plenary Lecture-1

Prof. Dr. Sourav Pal,
FNA, FASC, FNASc, FRSC
Director, IISER Kolkata,
Former Director, CSIR -NCL
Pune
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Title: Computational Chemistry: de novo design of molecules and materials

Plenary Lecture-2

Prof. Dr. Richard Catlow,
FRS, FRSC
University College London,
Royal Institution, UK,
Foreign Secretary and Vice
President of the Royal Society
email: catlowr@cardiff.ac.uk

Title: STRUCTURE, DYNAMICS and REACTIVITY in CATALYTIC and ENERGY SYSTEMS

Functional Supramolecular Materials for Bio-and Opto-electric Application

Dr. Amal Kumar Mandal
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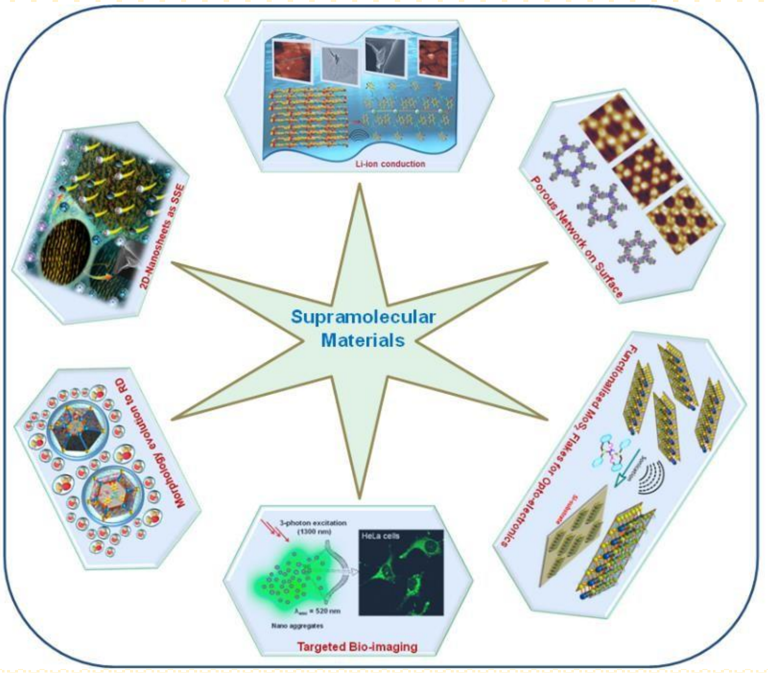
ABSTRACT:

The quest for new materials for tailor-made applications and understanding the complexity of living matter has led to a tremendous research activity exploring the possibilities of various kinds of functional building blocks to design nanostructured material. Supramolecular materials, where each monomeric unit is self-assembled together to form the desired structure, are arguably hot topics these days. While they have been around as natural materials for thousands of years, chemists are only now learning how to make them, modify and adapt their functionalities, and quantify and understand their uniquely diverse yet highly specialized properties. Their usefulness and market potential have attracted so much attention that almost every scientist will find a subject related to supramolecular materials that are interesting to them.



In this contemporary effort, my research ambition is to combine *chemistry and self-assembly* at the nanoscale, to create nanostructured materials for bio- and optoelectronic applications. Around chemistry and self- assembly at the nanoscale, I have developed two independent research lines that I will present. To illustrate this, I will start from a tunable three-photon active molecular probe to morphology tuned organic nanoparticles used for the three-photon excited targeted bio-imaging application.

After this, facet selective self-assembly of a small organic molecule into unique rhombic dodecahedral morphology. Following this, supramolecular organic nanosheets as solid-state electrolytes for efficient lithium-ion conduction. For optoelectric application, I will present how the self-assembly at the liquid-solid interface offers attractive features to fabricate the precise nano-porous structure on the surface. Apart from this, engineering optical property of two-dimensional thin flakes of *2H*-MoS2 semiconductors with the aid of molecules and organized molecular networks on their surfaces.

STRUCTURE, DYNAMICS and REACTIVITY in CATALYTIC and ENERGY SYSTEMS

Prof. Dr. Richard Catlow
University College London, UK; School of Chemistry, Cardiff University; UK Catalysis Hub, Research Complex at Harwell, UK
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ABSTRACT:

The concerted use of synchrotron, neutron and modelling techniques has proved to be a powerful approach in probing catalytic structures and processes at the molecular level. We will illustrate the approach by recent applications to a range of systems including:

- Hydrocarbon dynamics and reactivity in microporous catalysts, where we will describe how the concerted use of modelling with neutron spectroscopy can yield unique information on molecular transport and reactivity in hydrocarbon synthesis and auto-exhaust catalysts.

- Structural and electronic properties of nano-particulate catalysts, including photocatalysts, where the focus will be on the combination of modelling with synchrotron techniques in developing detailed structural models of supported nano-particles.

- Carbon dioxide, ammonia and methane activation on oxide, and nitride catalysts where the focus will be on developing models for the activation mechanisms.

- The electronic Structure of Photoactive oxides

We will discuss how this powerful combination of techniques might be applied more widely in catalytic and Energy Materials science.

Theoretical and computational investigations on low-lying excited states of cabron-based molecular systems

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ABSTRACT:

The low-dimensional many-electron quantum systems are the centre of research interest in the multidisciplinary areas of Physics and Chemistry. The carbon- based molecules and materials are less expensive and environment-friendly. The optoelectronic properties of these molecular systems are governed by relative energy ordering of their low-lying singlet and triplet excited states. This talk will discuss the available many-body methods to solve the correlated model Hamiltonian that describes these carbon-based molecular systems including exact diagonalization as well as Density Matrix Renormalization Group (DMRG) techniques. The calculations of low-lying excited states of some real molecules will be discussed in the context of their applicability in optoelectronics[1-4].

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2. S. Naskar, **M Das** "The use of low-lying excited states of zethrene and its homologs in singlet fission within Pariser-Parr-Pople model Hamiltonian: A Density Matrix Renormalization Group study", *Chem. Phys.* , **533**, 110717(2020).

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Multifunctional Organic and Hybrid Materials for Sensors, Optoelectronics and Healthcare Applications

Prof. Dr. Parameswar Krishnan Iyer*
Professor
[1]*Department of Chemistry*, [2]*Centre for Nanotechnology, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India.*
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ABSTRACT:

New functional luminescent dyes, including conjugated polymers and oligomers based on the principle of aggregation-induced emission (AIE) have been designed and developed.[1-7] They have been utilized for chemosensors,[1,2] biosensors,[3] bioimaging,[3-6] optoelectronic devices[5-13] and latent finger printing applications. By introducing specific functional groups aggregation caused quenching (ACQ) molecules were converted to bright AIE/AIEE dyes which were utilized as excellent platforms in solution as well solid phase for the detection of important analytes of relevance to environment, cancer therapeutics, anti-amyloid activity as well as wash-free bioimaging applications. These organic dyes and functional materials displayed strong self-assembling nature in water, in crystalline and amorphous forms on desired surfaces, in physiological environment allowing them to be applied as sensors, healthcare probes and optoelectronic devices.[1-13] This lecture will present the design principles that were utilized to develop several advanced materials and their remarkable applications by introducing functional group engineering.

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Designer Molecule and Assemblies for Organelle-specific Drug Delivery

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ABSTRACT:

Stimuli-responsive release of a drug molecule or an appropriate fluorescent marker with spatial and temporal precision at the targeted site of an organism remains a challenge. An appropriate design could help in maximizing therapeutic efficacy; minimize undesired side effects and real-time monitoring of the site-specific drug release. The present lecture aims to discuss examples of usages of polymeric nanocarriers with the option of having a tunable composition, favorable biocompatibility and visualization of the site-specific drug release. These could help in improving the drug efficacy or theranostics. Some of our recent efforts on these issues are to be discussed in the presentation.

A Roadmap to All-Organic Photonic Integrated Circuits from Nano/Micro Organic Solids

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ABSTRACT:

Recently, nano/micro organic solids have emerged as promising materials for producing miniaturized organic photonic components, such as optical waveguides (active/passive), lasers, resonators (including chiral ones), filters, and modulators suitable for constructing organic photonic integrated circuits (OPICs).[1-2] Miniature crystal (rigid/flexible) optical waveguides[1-3,5-11,14] are useful for controlling and manipulating light propagation down to micro scale. In optical resonators,[4,10,12,13] their mirror-like geometry allows them to trap the photons tightly by repeated total internal reflection at the air-matter interface and produce multimodal optical emissions. Low-optical-loss (high Q) resonators are good optical gain media, therefore potential elements for microlasers. The guided light-intensity and- speed can be modulated using light-driven refractive index changes in photochromic optical waveguides.[10(iii)] Selective reabsorbance of broad-band optical emission in microcrystal waveguides lessens the bandwidth of the propagating light signal producing a long-pass filter effect.[15]

Atomic force microscopy (AFM) is an effective technique to mechanically micro manipulate miniature organic photonic components towards OPICs - an approach known as Mechanophotonics.[1,2,15-17] I will introduce examples of miniature organic photonic (optically linear and nonlinear[12,14]) components in my talk. I will also discuss the construction of OPICs with active, passive, and energy-transfer attributes using mechanophotonics. The fabricated OPICs switch, split, direct, and filter optical signals useful for signal enhancement, sensing, information processing and switchable photonic device applications.

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Advances in Iodine Chemistry

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ABSTRACT:

Many known iodine(III) reagents for organic synthesis have structures of type $ArIL_2$ or Ar_2IL with Ar being an aryl moiety and L a heteroatom-containing ligand. Surprisingly, iodine(III) compounds with three heteroatom ligands on the iodine of type IL_3 have been rarely investigated owing to their relative instability.

This work investigates the reactivity and structural features of iodine triacetate $I(OAc)_3$ and iodine tris(trifluoroacetate) $I(OCOCF_3)_3$. We discovered that non-iodinated arenes are easily and selectively converted into [bis(acyloxy)iodo]arenes$ArI(OCOR)_2$ in a single step under mild conditions using iodine triacetates as reagents.[1]

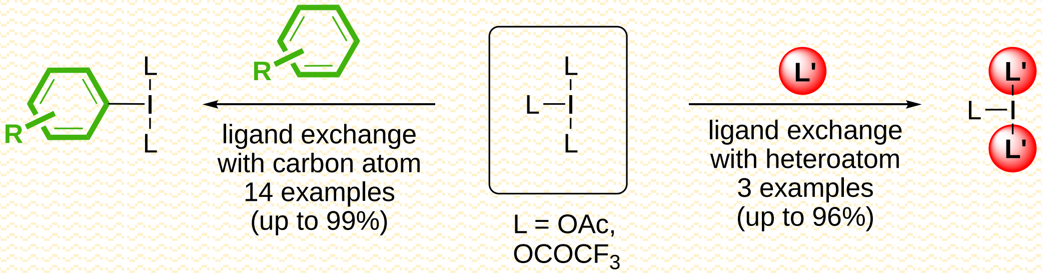

Fig. 1 Use of iodine triacetates in synthesis

Difficult oxidation steps can also overcome with electrochemical synthesis. We will also report recent results in the electrochemical generation of iodine(III) reagents and their use in synthesis,[2-5]especially in fluorinations.[6]

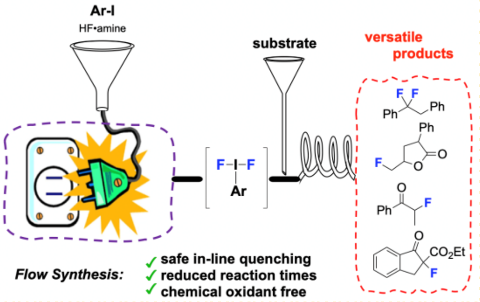

Fig. 2 Electrochemical fluorinations using hypervalent iodine reagents

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Chemically Derived Graphene for Clean Energy Applications

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ABSTRACT:

The rapid depletion of fossil fuels has forced researchers to find alternative energy sources for the survival of human civilization on this planet. In addition, the irreversible burning of fossil fuel produces harmful gases which results in global warming. Therefore, there is an urgent need for a cheap, lightweight, and environmentally-friendly new energy storage device that can partially or completely alleviate these problems. These findings encourage researchers to develop various types of advanced energy storage devices, such as supercapacitors, batteries, and fuel cells. The energy storage performance of such devices depends on the characteristics of the electrode materials. Compared with graphene grown by other physical technologies, chemically derived graphene has shown great potential as an efficient energy storage and conversion material due to its ease of synthesis, low cost, and the presence of chemically active sites. Graphene oxide (GO) is an intermediate product of a chemical method that uses natural graphite as a raw material to prepare graphene. The oxygen functional groups present in GO can be functionalized with various surface modifiers, metal oxides, sulfides, etc. Various types of organic surface modifying agents such as sulfonated poly-ether-ether-ketone (s-PEEK), 6-amino-4-hydroxy-2-naphthalenesulfonic acid (ANS), sulfanilic acid azocromotrop etc. were used for the improvement of capacitive properties of functionalized graphene through pseudocapacitive contribution. Different types of metal oxides such as $MnCO_3$, MnO_2, Co_3S_9, Ni_3S_2@Co_3S_4/Mn_3O_4-RGO, Ni-Co binary hydroxide etc were as the positive electrode materials for supercapacitor device fabrication. Graphene-based materials can also be used in lithium-ion batteries, zinc-ion batteries, photovoltaic cells, etc. Recently, it has also been found that graphene-based materials are very effective as electrocatalysts for hydrogen evolution reactions. Therefore, chemically derived graphene is considered to be an effective energy material to reduce the carbon footprint by replacing fossil fuels.

Synthesis and Structure of Multimetallic Coordination Aggregates: Design and Choice of Ligands Showing Variable Reactivity Patterns

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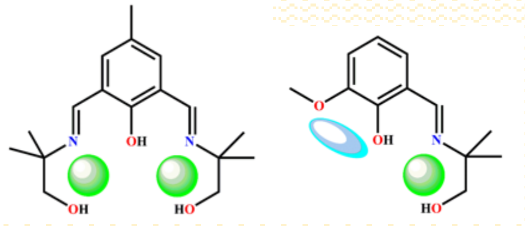
ABSTRACT:

From coordination chemistry of *3d* ions in biology to functionally active industrially important catalysts, knowledge and understanding of formation of multinuclear constellations of 3d and 4f ions is of current interest. For this purpose, the fabrication and easy synthetic availability of different ligand systems having two adjacent metal ion trapping sites is crucial, because the initially formed bimetallic fragments are allowed show varying course of self-multiplication. During this process the terminal donors from the ligand backbone along with ancillary couplers are exploited to take control over multiple metal ions. For different *3d* ions newer synthetic strategies towards the reacting ligand anions have been attempted and developed. Attempts are also made to categorize some of the most successful methods for *3d*-*3d* and *3d*-*4f* aggregates. The characteristics of the synthetic outcome and their molecular structures in terms of nuclearity, form, shape, architecture, etc. are unpredictable depending on the specific structural features of the used Schiff bases, reaction conditions and other factors. The majority of the aggregates to be presented in this talk are of special interest not only for their fascinating structures but also because they sometimes display interesting magnetic phenomena, such as ferromagnetic exchange interactions, large ground state spin values and single-molecule magnetism behaviour. Choice of two types of ligands can show coordination selectivity.



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A Study of Molecular Response to Strong Non-Uniform Magnetic Fields

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ABSTRACT:

In this talk we discuss the properties of the electronic states optimized in the presence of non- uniform magnetic fields strong enough to compete with the Coulombic forces in the molecule. We study the relative contribution of the spin and orbital effects to the variational energy, the probability of lighting up the ordinarily spin-disallowed dark bands and the computation of induced magnetic anapole moments. Conventionally the isotropic response of an atom or molecule to a uniform magnetic field as encoded in its magnetizability forms the criterion for classification as ’diamagnetic’ or ’paramagnetic’. We propose a more general criterion encompassing non-uniform fields.

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Membrane Transport Inspired Chemistry

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ABSTRACT:

The entry of enveloped viruses requires the fusion of viral and hosts cell membranes. An effective fusion inhibitor aiming at impeding such membrane fusion may emerge as a broad-spectrum antiviral agent against a wide range of viral infections. Mycobacterium survives inside the phagosome by inhibiting phagosome-lysosome fusion with the help of a coat protein coronin 1. Structural analysis of coronin 1 and other WD40-repeat protein suggest that the trp-asp (WD) sequence is placed at distorted β-meander motif (more exposed) in coronin 1. The unique structural feature of coronin 1 was explored to identify a simple lipo-peptide sequence (myr-WD, myr-WDWD), which effectively inhibits membrane fusion by modulating the interfacial order, water penetration, and surface potential. The mycobacterium inspired lipo-dipeptide was successfully tested to combat type 1 influenza virus (H1N1) and murine coronavirus infections as a 'potential broad-spectrum' antiviral agent.

Drying in thin film polymeric coatings: current and future scope of research

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ABSTRACT:

Several thin films polymeric coatings are used such in transparent films, batteries, solar cell, separation membrane, reflective coating, optical coatings, blood collection tubes, antimicrobial coatings, etc. The purposes of these thin films are to modify surface, to reduce mass and amount of light absorbing material and to decrease the weight and bulkiness of the materials. Thin film polymer coatings use less material for manufacturing, are flexible and non-breakable, no infrastructure is needed to support cells etc. The presentation gives brief description on glassy polymeric coatings, antimicrobial coatings and water-based coatings. The presentation majorly focuses drying of thin polymeric coatings. The aim of drying is to remove solvent from a wet coating to desired levels without inducing any defects such as saponification, fading, wrinkling, blistering, cracking and blush.

Earlier natural drying was used to preserve food but it depends on sun and weather conditions so the natural drying is replaced by mechanical drying. Drying of thin polymeric coating is governed by diffusion. Several different models of diffusion are explained in presentation given by Alsoy and Doda; Zielinski and Henry; Prince and Romdhane; etc. Non-fickian diffusion model in glassy binary polymer coatings is also explained in Polystyrene – p-Xylene System and poly(methyl methacrylate) – Ethylbenzene System.

The past research in thin polymeric coatings is very limited and need to be elaborated. Focus can be given in drying & diffusion in cross linking polymeric coatings. Water-based coatings, surfactant-enhanced coatings and glassy coatings can be studied in an elaborative manner. None of the available diffusion models are uniformly applicable in all cases for entire drying. Models are to be generalized and modified which can be executed efficiently. A broader approach can be given in the field of applications includes drug encapsulation and release from coatings and to develop biocompatible and long-acting antimicrobial polymer coatings against broad range of pathogens.

Magneto-electric effects in homogeneous media

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ABSTRACT:

The subject of electromagnetism has often been called electrodynamics to emphasize the dominance of the electric field in dynamic light–matter interactions that take place under nonrelativistic conditions. In this talk I shall show the experimental results that the often neglected optical magnetic field can nevertheless play an important role in a class of optical nonlinearities driven by both the electric and magnetic components of light at modest (non-relativistic) intensities. At first, I shall mainly focus on the optical interactions involving both electric and magnetic fields in two-photon scattering which stimulate molecular librations/rotations via torque-enhanced magnetic transitions. Torque is shown to account for unpolarized rotational components in the magnetic scattering spectrum under conditions that produce only polarized vibrational features in electric dipole scattering. Secondly, I shall specifically discuss the observation of magneto-electric rectification in a centrosymmetric media which is previously unexplored. This nonlinearity at the molecular level has important potential for energy conversion, ultrafast switching, nano-photonics and nonlinear optics. These experiments were carried out in nonmagnetic dielectric media in condensed phase & in thin films possessing spatial inversion symmetry that prohibited second-order, all-electric nonlinearities but allowed magneto-electric rectification.

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Photo, Synthesis, and Chemistry

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ABSTRACT:

The development of new methodologies in an energy-efficient pathway is also important from the aspect of twelve principles of green chemistry. In this regard, visible light photocatalysis is a hot topic from the last two decades.[1] Due to the employment of visible light as renewable energy, this has become a promising strategy in organic synthesis under environment-friendly conditions. However, the inability of the majority of organic molecules to absorb visible light is the main challenge to perform an organic reaction under the irradiation of visible light. In this context, photocatalysts play a crucible role as they have the capability to absorb the visible light.[2] Different transition metal salts and organic dyes have emerged as excellent photocatalysts by the continuous efforts of the chemists on the visible light promoted transformations. Various photocatalyst-free methodologies have been also developed employing the substrates which are capable of absorbing the visible light.[3] Additionally, the photocatalyst-free strategy has been also developed employing the (a) photoexcitation of the intermediate or (b) photoexcitation of electron donor-acceptor (EDA) complex between the substrates or substrate-intermediate. As a result of this continuous evolution of visible light photocatalysis, this has become an important tool for the synthetic chemist for the synthesis of bioactive natural products and pharmaceuticals.[4] We will discuss in details in this lecture.[5]

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Geometrical Confinement of Aquated Gd(III) Complex via Non-covalent Electrostatic Interaction within the Inner-Layer of Porous Silica Nanoparticles Results a Highly Efficient T1 Contrast Agent for Magnetic Resonance Imaging

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ABSTRACT:

Contrast agent enhanced magnetic resonance imaging has emerged as an indispensable imaging modality for the early-stage diagnosis of many diseases. Magnetic resonance imaging (MRI) is an NMR-based noninvasive bioimaging modality that provides anatomical tissue images with high spatial resolution despite using any ionizing radiation. However, the low intrinsic sensitivity of the technique is the main disadvantage. In this context, contrast agent enhanced magnetic resonance imaging has been under continuous investigation for the conspicuous images of lesions and early-stage detection of tumors.

To develop T_1 contrast agent with high relaxivity value, herein, porous silica nanoparticles internalized with about 20 numbers of aquated, cationic Gd(III) complexes (**1**) and of hexadentate ligand H_2hbda has been synthesized. The Gd(III) complex exhibited a longitudinal relaxivity value per mM Gd(III) ions, r_1 = 9.05 $mM^{-1}s^{-1}$ (pH 7.4, 37 °C, 1.41 T), which amplified to 86.41 $mM^{-1}s^{-1}$ upon the geometrical confinement (complex **1**@SiO_2NPs) *via* the rigidity enhancement through the electrostatic interaction between the silica surface and the cationic complex **1** molecules. The relaxivity could further be amplified by the interaction of complex **1**@SiO_2NPs with serum albumin protein. The kinetic inertness, cellular uptake property and *in vitro* imaging efficiency will be discussed.

Switch me on, switch me off: novel SHG switching schemes and beyond

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ABSTRACT:

Second harmonic generation (SHG), also referred to as "frequency doubling" is a parametric nonlinear optical (NLO) process in which two photons interact with a NLO material to create new photon with doubled frequency. SHG is a second-order NLO process, thus it occurs only in noncentrosymmetric matter. Coordination polymers (CPs) are rich playground for SHG studies, since the interplay of organic and inorganic components not only shapes in manifold ways the NLO response,[1] but also provides for their diverse phase transition behavior. Indeed, thus far the focus of interest was primarily on CPs displaying reversible structural phase transitions between noncentrosymmetric and centrosymmetric crystal phases, which successfully served as materials for temperature-induced SHG-*on* - SHG-*off* switching.

This presentation is divided into two parts. The first part is devoted to methodological aspects of SHG switching experiments. We are going to explain two the most common types of SHG switching measurement setups (oscilloscope and spectrograph-based) and will overview the most common critical factors that convolute analysis of obtained temperature-dependent NLO responses. Here, in particular, we will pay attention to the influence concomitant NLO phenomena such as two-photon excited luminescence or third harmonic generation.

The second part of the talk will discuss SHG switching schemes that go beyond classic SHG-*on* - SHG-*off* scenario. We will have a look on example of SHG switching in hybrid organic-inorganic perovskite lead methylhydrazinium chloride, $MHyPbCl_3$, whose SHG response is present in its two crystal phases.[2] Even more intriguingly, low temperature $Pb2_1$ phase features lower SHG activity than high-temperature $Pb2_1m$ phase, which gave rise to an uncommon kind of SHG switching in which a second-harmonic response is switched between a room-temperature, SHG-*low* state and a high-temperature, SHG-*high* state.

We have also recently demonstrated that novel dicyanamide CP comprising benzyltrimethylammonium cations ($BeTriMe^+$) of formula $BeTriMe[Mn(dca)_3(H_2O)]$ which features effectively irreversible temperature-induced change of SHG response.[3] This compound served as a case study to introduce the class of *remote NLO markers*, referred also to as *NLO threshold temperature sensors*. Distinguishing feature of *NLO threshold temperature sensors* is that they can inform on the thermal shocks that affected probed object in the past, contrary to classical (reversible) SHG switches. Specifically, they can be used to deduce whether a certain threshold temperature was achieved by the object or not. This kind of markers can be therefore particularly useful as safety control labels of goods that are sensitive to elevated temperature, such as chemicals but also food.

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Orthogonal binding of different guest types to interior and exterior of coordination cages - consequences and applications

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ABSTRACT:

An octanuclear cubic M8L12 coordination cage that is soluble in water can bind strongly small, neutral organic guests in the central cavity, principally driven by the hydrophobic effect. In addition, the cage can bind anionic guests at polar recognition sites around the exterior surface, binding up to six anions, one on each face of the cubic host. Many examples of the strengths of both types of guest binding have been determined, and the two are approximately orthogonal, with binding of each type of guest (cavity-bound or surface-bound) being variable independently of the other type of guest. The ability of the host cage framework to bring together neutral organic molecules in the cavity, surrounded by a shell of anionic guests around the cage surface, has remarkable consequences for applications in catalysis, sensing, and supramolecular photochemistry.

The exposed amino acids on protein skeleton control protein absorption on surface engineered silver nanoparticles

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ABSTRACT:

Absorption of protein on the surface of silver nanoparticles (Ag NPs) could be controlled by modulating the surface using cyclodextrin (CD). The CD nanocavities were tactically arranged over the Ag NPs with the help of surfactants. Two different model proteins, one with an exposed tryptophan residue and the other with the amino acid (tryptophan) captivated inside the folded structure, showed different motifs of surface absorption based on host guest interaction.

Keywords:
silver nanoparticles, cyclodextrin, surface modification, protein absorption

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Ru(II)-Catalyzed Divergent Synthesis of 2-Methylindoles and Indolines through a C–H Allylation/Cyclization Cascade

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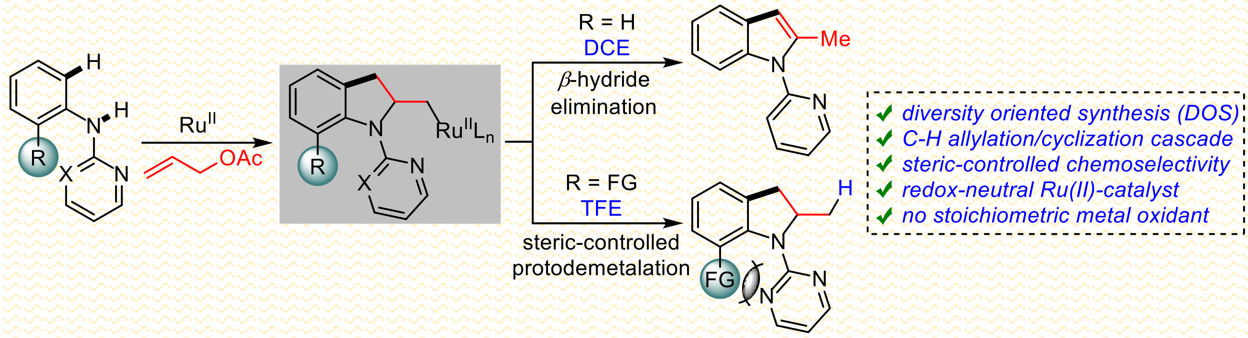
ABSTRACT:

Indole and indoline core structures are ubiquitously found in medicinal scaffolds, natural products, agrochemicals, and functionalized materials. Because of its high importance, over a century the synthesis and functionalization of indoles has been a major area of research to synthetic organic chemists. Although an extensive study has been performed by several research groups for the synthesis of indoles through traditional cross coupling and amination approach for the development of mild and scalable methods, in recent years transition metal catalyzed cascade C-H activation methods have been attracted to synthetic organic chemist to develop functionalized indole and indoline moiety to improve the atom economy and more importantly the step-economy in organic syntheses.

In this vein, a Ruthenium-catalyzed synthesis of 2-methylindole was accomplished via C-H allylation, oxidative cyclization cascade. Also a novel strategy to suppress β-hydride elimination from the σ-alkyl-Ru intermediate by steric hindrance from a remote position is explored. Hence diversity oriented synthesis (DOS) of 2-methylindoline from the corresponding *ortho*-substituted anilines was achieved via protodemetalation in lieu of β-hydride elimination. This mild intermolecular annulation cascade proceeds smoothly by redox-neutral ruthenium catalyst without stoichiometric metal oxidants such as silver(I) or copper(II) salts providing excellent functional group tolerance.



- ✓ diversity oriented synthesis (DOS)
- ✓ C-H allylation/cyclization cascade
- ✓ steric-controlled chemoselectivity
- ✓ redox-neutral Ru(II)-catalyst
- ✓ no stoichiometric metal oxidant

Keywords:
cascade reaction, step-economy, divergent synthesis, metal oxidant free.

Reference:

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Experimental and Computational investigation on employment of Dansyl derivatized fluorescent probe in detection of remnant water in hygroscopic deuterated solvents

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ABSTRACT:

A Dansyl based fluorescent probe has been designed, synthesized and well-characterized by NMR, IR, Mass spectrometry, SEM, SCXRD. The fluorescent compound is capable of sensing trace amounts of water contaminant in hygroscopic deuterated solvents by providing colour change under UV irradiation. A distinct bathochromic shift in the emission spectra of the probe has been observed along with visual colour change (Green to Yellow) under UV lamp. These are the key evidence of the presence of water in the deuterated solvents. The limit of detection (LOD) and limit of quantification (LOQ) for probe DFFP have been estimated. For MeCN LOD and LOQ are found to be 0.0440% (v/v) and 0.1469% (v/v) and in case of DMSO 0.0354 % (v/v) and 0.1182 % (v/v) respectively. To prove the potentiality of the probe while detecting the remnant water, along with experimental studies exhaustive theoretical evaluation was done. DFT (Energy optimization and other calculations) helped in better understanding the sensing mechanism and the mode of interactions among probe-water-solvent. Total electron density has been mapped over Electrostatic Potential Surface and calculation of ESP charges helped in locating more electron-dense regions in the ground state. The involvement of TD-DFT studies helped in finding the possible electronic transitions and corresponding absorption bands. Moreover, the probe is capable of sensing ethanolic water vapour in the gaseous phase. Due to high fluorescence and being nontoxic to cells, the probe could be used as a potential cell imaging dye. It has been employed in human cancer cell lines (A549), and fluorescent confocal microscopic images were obtained.

Nanocellulose reinforced biopolymer nanocomposites materials for sustainable food packaging applications

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ABSTRACT:

Nano-materials have largely attracted interest of many researchers due to their enhanced properties compared to bulk materials. Nanocomposites represent a new alternative of conventional composites for improving polymer properties e.g. mechanical strength, thermal stability, reduced water absorption, gas barrier properties, etc . The rapid progress of nanofillers was a breakthrough, and since, nowadays Nanocellulose incorporated bionanocomposites (BNCs) is gaining utmost interest in the area of barrier films for food packaging as reinforcing filler to make biodegradable BNCs with different biopolymer. The development of these nanocomposites is a new strategy to improve physicochemical properties of polymers, including thus the proper and detail experimental studies are crucial, especially in the early stages of the development of nanomaterials, in commencing before the potential human health risks of this nano material which calls for investigation correctly, which could potentially incur substantial future social, health and economic repercussions. NCs have proven to be nontoxic in nature and possess the ability to enhance the biocompatibility of its nanocomposite products. Biodegradable biopolymer based nanocomposites with cellulose nanocrystals (CNCs) were carried out following solution mixing technique. The crystalline nature of CNCs has been scrutinized by X-ray diffraction study. The FESEM of CNCs revealed a network of CNCs morphology. The Fourier transform infrared spectroscopy results of cellulose nano-fibrils confirmed the removal of lignin and hemicellulose from raw jute (Corchorus olitorius L.) fibres. The storage modulus and tensile properties of BNCs films also studied by ultimate tensile machine (UTM). BNCs film are expected to be highly promising in the area of food packaging applications.

Keywords:
Nanofiller, Cellulose nanocrystals, Bionanocomposites (BNCs), Food packaging.

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Design, synthesis, and molecular docking studies of some novel N'-(1,3-benzothiazol-2-yl)-arylamide derivatives

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ABSTRACT:

In the present work we carried out hydroxybenzotriazole (HOBT) and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDCl) mediated synthesis of new N'-(1,3-benzothiazol-2-yl)-arylamides C1-18 in high yields under relatively milder reaction conditions using dimethyl formamide as solvent. Synthesized compounds were characterized by FT-IR, 1H-NMR, 13C-NMR and HRMS spectral data. In the extra-precision docking compounds C1-18 exhibited interactions mainly with the N-terminal and central domains of S. aureus GyrB catalytic pocket. Binding free energy (ΔGbind) of compounds C1-18 for both pdb.3U2K and pdb.4URN complexes were computed by MM-GBSA approach. Free energy components indicated Coulomb energy term as favorable for binding, while van der Waals and electrostatic solvation energy terms strongly disfavored the binding. Cytotoxicity study of selected compounds performed using on VERO cells. ADMET properties of synthesized compounds C1-18 are also computed.

Key words:
N'-(1,3-benzothiazol-2-yl)-arylamides, HOBt/EDCl, MM-GBSA approach, Cytotoxicity study.

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Penta-Fluoro-Pyridine Assisted One Pot Synthesis of Esters from Carboxylic Acids

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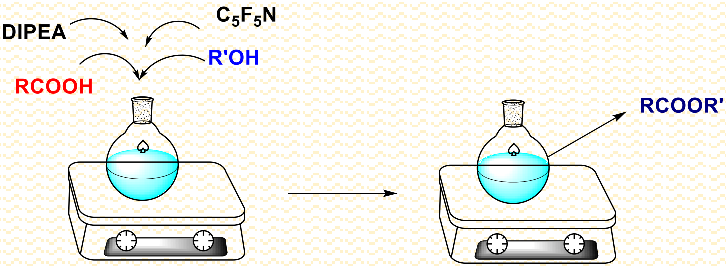
ABSTRACT:

Herewith I report a new single-pot sequential strategy in which carboxylic acid with the help of C_5F_5N are converted to corresponding acyl fluorides which subsequently transformed into respective esters on exposure with alcoholic molecules. The process reveals that C_5F_5N initially activates carboxylic acid to the corresponding acyl fluoride which later gives ester on reaction with alcoholic functionalities. This one pot strategy produces ester in good to nice yields.



Keywords:
Penta-Fluoro-Pyridine, Acyl Fluorides

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A stilbazolium dye-based chromogenic and red-fluorescent probe for recognition of 2,4,6-trinitrophenol in water

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ABSTRACT:

Abstract: The nitroaromatic compounds (NACs) show absorption maxima below 400 nm and their determination using absorption and colour change requires probes with absorption beyond this region. Herein, we report a stilbazolium-based probe DMAS-DP, which undergoes aggregation in HEPES buffer with an absorption maximum at 475 nm (red colour) and these aggregates demonstrate a highly selective and sensitive change in their colour from red to light yellow with 2,4,6-trinitrophenol (TNP). The LOD for the determination of TNP is 100 pM, the lowest in the literature by using visible spectroscopy. Moreover, the aggregates of DMAS-DP emit fluorescence in the red region with a maximum at 615 nm (red under 365 nm light), which is quenched selectively by TNP. 2,4,6-Trinitrotoluene (TNT) and other NACs show insignificant changes in the visible spectrum of the aggregates of DMAS-DP, even when present in excess. Density functional theory (DFT)-based structure optimization studies reveal that the DMAS-DP attains the Z-conformation and its dimethylamino moieties form strong interaction with the protons of TNP and are responsible for the reduced force constant (color). This constitutes the first probe where a stilbazolium dye has been used for constructing a TNP-selective chromogenic and red-fluorescent probe.

Keywords:
Stilbazolium, Chromogenic, NIR-fluorescent, Nitroaromatics, 2,4,6-trinitrophenol, red-fluorescence

References:

New J. Chem., 2020, 44, 10870 -10877

An ESIPT based versatile fluorescent probe for bioimaging strong acidic conditions in Live-cells and *E. coli*

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ABSTRACT:

Probe **BTNN** undergoes a drastic upsurge (~146-fold, Φ = 69%) in fluorescence intensity (bright green, λ_{em} (530 nm) while moving from pH 7 to pH 2. MG-63 cells and *E. coli* bacteria internalize **BTNN** without toxicity and their fluorescence intensity is directly correlated to pH in the cells / bacteria (Figure 1A). This response to pH is instantaneous, reversible and stable over a week. The protonation of diethylamino nitrogen followed by efficient normal and ESIPT processes from protonated **BTNN** are responsible for remarkable increase in fluorescence intensity and quantum yield under acidic conditions. For **BTNNH**, the experimentally observed emission maxima at 530 nm is in the middle of calculated values of emission peaks from S_1 (normal) and S_4 (ESIPT) state *i.e* at 517 nm and 561 nm and considerably point to the participation of both normal and ESIPT excited states in emission of **BTNNH** (Figure 1B).

Furthermore, polystyrene-**BTNN** thin films can be used for efficient detection of HCl vapour (2 ppm). This is first example where 2-(2-hydroxyphenyl)benzothiazole derivative can image strong acidic conditions.

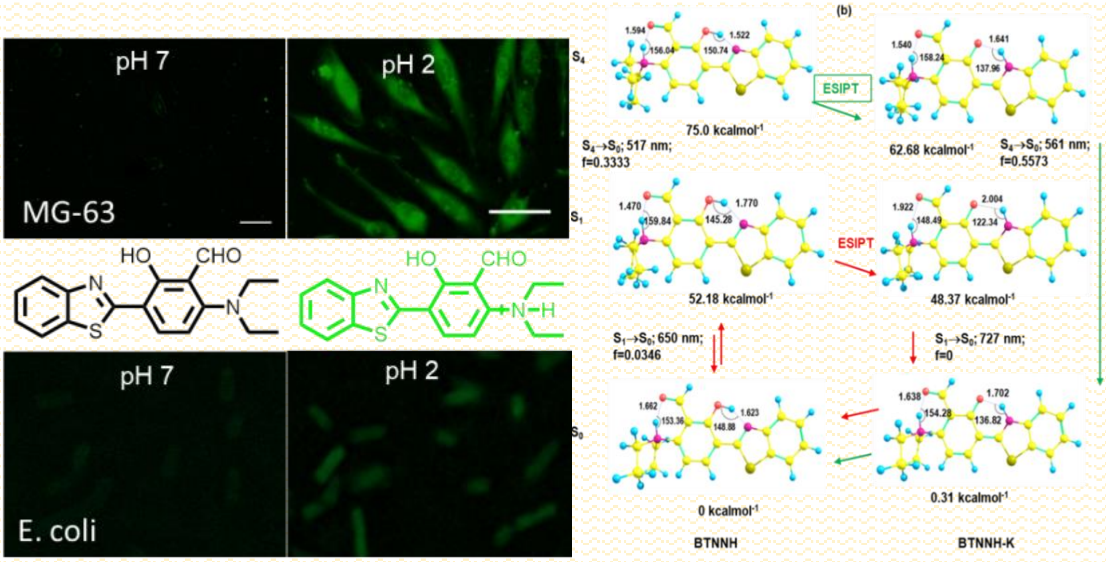

Figure 1. (A) the effect of pH on the fluorescence of live MG 63 cells and *E. Coli*; (B) The mechanism involved in fluorescence of BTNN under acidic conditions

Keywords:
2-(2-hydroxyphenyl)benzothiazole, fluorescence enhancement, pH, MG-63 cells, *E. coli*, HCl vapour

A Molecular Ruthenium(III) Complex Supported by Anionic, Redox-Non-Innocent Ligand: Redox Metal-Ligand Cooperativity for an Efficient Water Oxidation Catalysis

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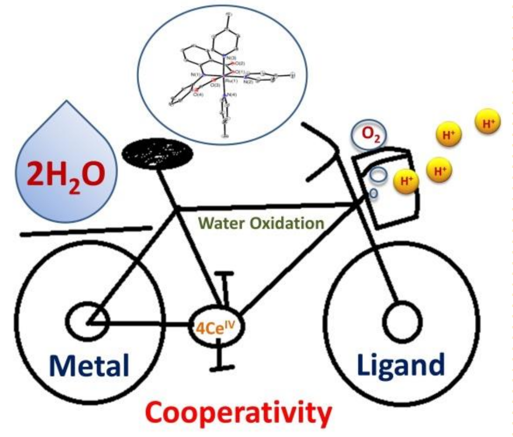
ABSTRACT:

The world's energy crisis directs us to develop sustainable energy conversion processes. In this context, the splitting of H_2O to O_2 and H_2 is one of the best alternatives. The critical step in such solar-to-fuel scheme is the four-electron oxidation of H_2O to O_2. In this work, we report the catalytic water oxidation activity of a mononuclear ruthenium(III) complex $[Ru(L)(pic)_3]$ (H_3L = 2,2'-iminodibenzoic acid, pic = 4-methylpyridine), using Ce(IV) as an oxidant in pH 1. The detail mechanistic investigations of water oxidation have been carried out by the use of spectroscopy, electrochemistry, kinetic analysis and computational studies. Electrochemical study suggests that water oxidation proceeds via formal high-valent Ru^{VII} species. The capability of accessing such a high-valent state is derived from the redox-non-innocent behavior of the anionic-tridentate ligand framework which helps in accumulation of oxidative equivalents in cooperation with metal center. This metal-ligand cooperation is important to facilitate the multi-electron oxidation of water. Mechanistic investigation reveals that O-O bond formation takes place via heterometallic radical coupling pathway between the oxygen atom of ruthenium-oxo species and the oxygen atom of hydroxocerium(IV) ion.



Keywords:
Non-innocent Ligand, Ruthenium Complex, Water Oxidation, Catalysis.

Reference:

Kundu, A.; Dey, S. K.; Dey, S.; Anoop, A.; Mandal, S. *Inorg. Chem.* **2020**, *59*, 1461−1470.

A highly selective novel chemodosimeter in estimation of noxious cyanide in common water hyacinth (*Eichhornia crassipes*): An environmental refinement

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ABSTRACT:

In recent decades selective and simple sensing of cyanide ion is one of the most demanding research interests, due to its lethal and toxic properties and rapid reactivity.[1] Strong interaction of cyanide ion with heme Fe of cytochrome c oxidase imprinted this anion as a super poison, resulting in interference in the electron transport process, hence causing hypoxia in mammals and imposes severe damage in the central nervous system.[2] According to the guideline of WHO, the permissible level of cyanide is 1.9 μM in drinking water.[3] An elevated level can affect several functions of human health and also cause death. Despite these fatal effects CN^- has been irresistibly used in industrial production, such as electroplating, metallurgy, tanning, and the synthesis of fibers, nylon, and resin industry and the waste of these industries plays a crucial role in environmental pollution.[4] Thus it is desirable to introduce a simple portable tool to monitor the involvement of this toxic contaminant CN^- into the biological and environmental systems.

For this a naphthaldehyde-pyridoxal conjugated chemodosimeter (**NPLC**) was developed and employed for the sensitive and selective detection and estimation of cyanide in common water hyacinth (*Eichhornia crassipes*), a free floating macrophyte used in phytoremediation process since ancient time. The involvement of the probe in chemodosimetric fashion towards cyanide was elucidated by experimental and computational studies.[5]

Keywords:
Chemodosimeter, Cyanide sensing, Turn-On response, Estimation in Water Hyacinth

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Preparation and characterization of heteronuclear complexes of N,N’-l,2-phenylenebis(salicylaldiminato)copper(II) Schiff base and thallium salts

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ABSTRACT:

Several Schiff base metal complexes have been studied because of their industrial and biological applications. Schiff bases are extensively used for the preparation of homo and hetero-binuclear complexes. For the past thirty years, transition metal complexes of Schiff bases have been used as ‘metal complexes as ligands’ for the study and investigation of Nitrogen and Oxygen-bridged complexes. The investigation on oxygen bridged complexes has been extended by preparing the ligand N,N’-l,2-Phenylenebis(salicylaldiminato)copper(II) i.e. CuPhS. This paper describes synthesis and characterization of heteronuclear complexes of thallium(I) chelates of nitrophenols such as 2-nitrophenol, 2,4-dinitrophenol, and 2,4,6-trinitrophenol with CuPhS.

It has been observed that $\upsilon_{\text{C-Ostr.}}$(phenolic) occurs at higher energy side in comparison to alcoholic/enolic $\upsilon_{\text{C-Ostr}}$. In aromatic Schiff bases, nitrophenols and salicylaldehyde, the $\upsilon_{\text{C-Ostr.}}$(phenolic) should occur around 1530 cm^{-1} but in case of alcoholic/enolic (C–O), the band should occur around 1150-1250 cm^{-1}. The $\upsilon_{\text{C-Ostr.}}$(phenolic) is exhibited by the metal complex ligand CuPhS at 1522-1538 cm^{-1}. On complexation, the $\upsilon_{\text{C-Ostr.}}$(phenolic) band in the heteronuclear complexes of CuPhS with thallium(I) chelates of organic acid shifted towards higher energy side by ~55-56 cm^{-1} and also split into two bands. The observed shifting and splitting of $\upsilon_{\text{C-Ostr.}}$(phenolic) bands on complexation may be due to the presence of C–O bond in thallium(I) chelates of organic acids. The shifting of $\upsilon_{\text{C-Ostr.}}$(phenolic) towards the higher energy side on complexation indicates coordination through phenolic oxygen. The shift of frequency toward the higher energy side is expected due to ring current developed from electron delocalisation in chelating ring. The major shifting of $\upsilon_{\text{C-Ostr}}$ frequency by ~55-56 cm^{-1} in adducts indicates the presence of phenoxo-bridge. It is also suggested that in these adducts, the phenolic C–O bond have partial double bond character.

The heteronuclear thallium metal adducts show bands in the far-IR region between 445-536 cm^{-1} and 542-627 cm^{-1} which are tentatively assigned to $M–N_{str}$ and $M–O_{str}$ modes respectively. The $\upsilon_{\text{M-Ostr}}$ appear at higher stretching frequency than the $\upsilon_{\text{M-Nstr}}$. These bands are absent in the ligand (Schiff base obtained on reacting o-phenylenediamine and salicylaldehyde) but present in the neutral transition metal chelate CuPhS at 505-591 cm^{-1}. The above data confirms the coordination of oxygen-atom of phenolic group and N-atom of $–NO/–NO_2$ group to Tl(I) metals in all the heteronuclear complexes. Spectral analysis and magnetic data shows that the thallium metal coordinate through the two phenolic oxygen atoms. The magnetic moment value of heteronuclear complexes, it has been suggested that CuPhS and most of its adducts have square planar geometry with coordination number 4.

Key words:
Schiff base, CuPhS

First total synthesis of the proposed structure of pandangolide 1

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ABSTRACT:

The first total synthesis of proposed structure of pandangolide 1 is reported. The construction of the 12-membered core was achieved via both MNBA-mediated intramolecular Shiina lactonization and RCM protocol. The structure of target molecule was confirmed unambiguously by the single crystal X-ray analysis, though the optical rotation and NMR data of synthesized pandangolide 1 were found to be inconsistent with the proposed structure. (Figure 1).

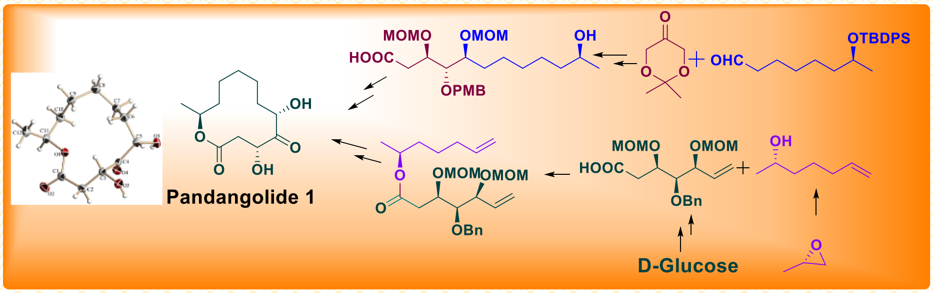

Figure 1. First total synthesis of the proposed structure of pandangolide 1

Keywords:
Macrolide • Aldol reaction • Macrolactonization • Hydroboration-oxidation • Ring-closing metathesis

References:

Krishanu show and Pradeep Kumar; Eur. *J. Org. Chem* (Doi: DOI: 10.1002/ejoc.201800675)

New analytical method development for the estimation of some common alcohol denaturants and its validation

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ABSTRACT:

Analytical method development and validation are the continuous and inter-dependent task associated with the research and development, quality control and quality assurance departments. The objective of analytical method development and validation procedure is to demonstrate that it is suitable for its intended purpose. Denatured alcohol is ethanol made unfit for human consumption by the addition of one or more chemicals (denaturants) to it. In specially denatured alcohol (SDA), the denaturants are selected in such a way that the product is fit for use in some fields like cosmetics, pharmaceutical, chemical manufacturing etc. completely denatured alcohol (CDA) is alcohol that has been thoroughly denatured that the product is utterly unfit for beverage use and the denaturants used are very nearly inseparable from the alcohol. Usually in India, methyl alcohol is used as a common denaturant for use in this industry. But for some specific purposes like that for use of alcohol in cosmetics, pharmaceutical etc. other denaturants are also used. Hence, qualitative as well as quantitative analysis for these additives is very important. Many chemicals like brucine, formaldehyde etc. have been newly introduced as denaturants especially in that case of power alcohol. Some of these additives have no validated wet chemical methods available for quantitative as well as qualitative analysis. This procedure is directed to the four most common type of analytical procedures are identification test, quantitative test, limit test and quantitative test of the active moiety in samples. Development in scientific and concrete analytical methods has been resulted from the advancements of analytical instruments. Validation parameters are explained in term of accuracy, precision, linearity, specificity, limit of detection (LOD), limit of quantification(LOQ), ruggedness, robustness and system suitability.

Keywords:
Analytical method development, Method validation, Alcohol denaturants, Strategy, validation parameters.

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Synthesis, Structure, and Characterization of Multinuclear Ni−Ln Complexes: Role of Ligand Backbone in Topology and Magnetic Properties

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ABSTRACT:

Phenol group bearing Schiff bases are useful in providing multinuclear *3d-4f* complexes showing interesting magnetic property. The variable coordination behavior of 2-{[(2-hydroxy-3-methoxybenzyl)imino]methyl}-6-methoxyphenol (H_2L1) having O_4N donor atoms and its hydrolyzed congener was investigated towards $NiCl_2{\cdot}6H_2O$ and Ln^{III} nitrate salts, provide a family of coordination aggregates containing a $[Ni_5Ln_3]$ octanuclear core structure. Room temperature reactions in $MeOH–CHCl_3$ medium and in the presence of NEt_3 yield isostructural $[Ni_5Ln_3(L1)_4(\mu\text{-}OH)_2(\mu_3\text{-}OH)_6(o\text{-val})_2(H_2O)_6]NO_3{\cdot}7H_2O$ (Ln = Dy^{III} (**1**), Tb^{III} (**2**), and Ho^{III} (**3**); *o*-val = *o*-vanillin) heterometallic complexes. Direct current magnetic susceptibility measurements showed an upsurge at low temperature for complex **1** and **2**, indicative of ferromagnetic interactions. AC magnetic susceptibility measurements were not able to show any slow relaxation property to the magnetization. CASSCF calculations for complex **1** indicates all three Dy^{III} centers have anisotropic axes but the relative orientation of the magnetic axes reduces the probability of this molecule to behave like a SMM which further established by the POLY_ANISO calculations. To modify the molecular topology by utilizing all the ligand donor atoms we have synthesized the new Schiff base ligand H_2L2, (2-{[(2-hydroxy-3-methoxybenzyl)imino]methyl}phenol) providing O_3N donors. A series of hexanuclear complexes having formula $[Ln_2Ni_4(L2)_4(\mu_{1,3}\text{-}CH_3CO_2)_2(\mu_3\text{-}OH)_4(MeOH)_2]{\cdot}xCH_3OH{\cdot}yH_2O$ (where Ln = Dy^{III} (**4**), x = 4, y = 0; Tb^{III} (**5**), x = 0, y = 4 and Ho^{III} (**6**), x = 4, y = 0) was obtained from the sequential use of Ln^{III} nitrate salts and $Ni(CH_3CO_2)_2{\cdot}4H_2O$. DC magnetic susceptibility studies hint to the possibility of ferromagnetic interactions occurring in all the aggregates, whereas AC susceptibility measurements find the complex **4** to show out-of-phase component at zero applied DC field, characteristic of single molecule magnet (SMM) behavior. Micro-SQUID studies reveal open hysteresis loops for **4**, corroborating its SMM character. Detailed CASSCF and DFT calculations were also performed supporting the experimental findings in complex **4**.

Keywords:
Schiff Base, Multinuclear Complexes, *3d-4f*, Ferromagnetism, SMM.

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Effect of Nanoclay on Organic-Inorganic Hybrid Nanomaterials Based on TPEs

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ABSTRACT:

In recent years much attention has been focused on polymer nanocomposites due to their promising potential for versatile applications in automotive industry, packaging, aerospace etc. Amongst all the potential nanocomposite precursors, those based on clay and layered silicates have been more widely investigated. This study aims at investigating the effects of pristine and modified laponite clay on a model LDPE/EVA TPE blend system. Two different types of nanoclay particles are melt-blended with this system at 1.5 wt% loading. The clay particles are modified by ion exchange method to improve the interaction of clay particles with the polymer matrix. The blends are compression moulded and their mechanical, dynamic mechanical & thermal properties, and morphology are evaluated. The properties of the blends are found to be strong function of the extent of modification. A significant improvement in the mechanical properties is observed in all the nanoclay-based films. Morphological studies and dynamic properties clearly indicate that the differential properties of these blend systems primarily stem from the extent of dispersion and alternation of crystalline morphology, which in turn is a strong function of preferential incorporation in the LDPE or EVA matrix and the agglomeration tendency of the nanofillers.

Keywords:
Blends, TPE, clay, dispersion, morphology, nanocomposites

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Design, Synthesis and Characterization of Achiral Unsymmetrical Four-ring Based Hockey-stick Shaped Liquid Crystals: Structure-Property Relationship

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ABSTRACT :

Hockey-stick-shaped liquid crystals are interesting due to their unusual physico-chemical properties. Nematic phase observed in these materials have shown interesting properties like ferroelectric-like switching, ease of alignment in coated cell, large flexoelectricity, etc. Polar moiety viz. F, Cl, NO_2 etc., in the molecular architecture of hockey-stick-shaped molecules originate permanent dipole moment that affects the phase structure and physical properties [1-2]. Herein, we have designed and synthesised a new series of four-ring-based hockey-stick-shaped molecules having polar Cl group at one end and variable aliphatic chains at another end of the molecular long axis [2]. The four phenyl rings are attached via one ester and two imine linking groups. All the compounds exhibited enantiotropic mesomorphism. The lower homologs (**1–5** to **1–8**) exclusively showed nematic phases and higher homologs exhibited nematic and/or smectic A phase. Compound **1–5** showed a stable nematic phase with highest phase range of about 110 °C. Small and wide-angle X-ray scattering (SAXS/WAXS) experiments have been performed that elaborated the internal arrangement of molecules in layers. Density functional (DFT) study confirmed that the molecules had a resultant dipole moment (~6 Debye) which in turn cancelled out when the molecules, in the bulk phase, arranged preferably antiparallelly as a dimer.

Keywords:
liquid crystals, hockey-stick shaped, structure-property relationship, SAXS/WAXS

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COBALT CATALYZED MECHANISTIC INVESTIGATION ON THE INTERMOLECULAR [3+2] CYCLOADDITION REACTION & SELECTIVITY OF PRODUCTS OF THE ALLENES AND CYCLOPROPANOL DERIVATIVES, A DFT STUDY

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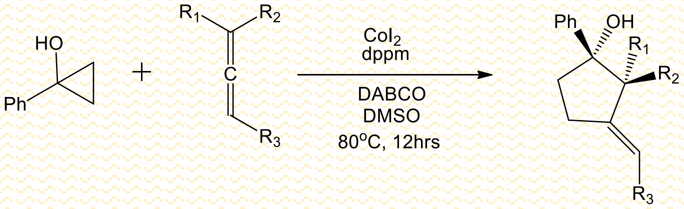
ABSTRACT:

Substituted cyclopentanols are important precursors of several synthetic and natural products. As a result strategic synthesis of cyclopentane scaffold is an attractive problem in synthetic organic chemistry. [3+2] cycloaddition reaction is probably the most direct and conceptually the simplest way for the generation of the pentacyclic ring system. While exploring in such direction Yoshikai et. al. observed regio and diastereoselective aspect of a cobalt catalysed [3+2] type of cycloaddition reactions of cyclopropanols and allene derivatives (Scheme-1).



Scheme-1

Our study reveals that a stepwise pathway involving cleavage of cyclopropanol derivatives and carban-carbon single bond formation leading to a pentacyclic cyclopentane products with exocyclic double bonds. The cleavage of cyclopropanol ring with following cyclisation process occurs with lower activation barrier. The steric interaction by the variation of substituents decides the reaction to progress selectively in a specific direction leading to a specific diastereoselective product in high yield. The relative order of the favourability of the transition structures remain unaltered with the variation of substituents (electron releasing or withdrawing), it may be concluded that the electronic nature of the substituent on the phenyl ring does not affect the diastereoselectivity of the overall reaction. The origin of diastereoselectivity of the reaction is the steric effect between the substituent present on the cyclopropane derivatives and allene derivatives. No effects were observed for the presence of substituent in the ligand of cobalt. Such a favourable configuration results the diastereomeric structure of the cyclopentane derivatives with the orientation of the substituents as observed in experimentally reported products.

Keywords:
Intermolecular [3+2] cycloaddition, metal catalysis, cyclopropanol, allene, DFT, reaction mechanism.

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Fluorescence ‘off–on–off’ signaling with zinc ensemble to investigate prevalence of ATP in liver cancer cells

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ABSTRACT:

Adenosine 5'-triphosphate (ATP), the primary energy source of all living organisms, is responsible for intracellular energy transfer that in turn controls several cellular functions. In normal mammalian cells, ATP is generally obtained both from glycolysis and mitochondrial oxidative phosphorylation (OXPHOS). However, in cancer cells, ATP is produced only through upregulated glycolysis even when oxygen is abundant[1]. The internalized ATP was found to substantially increase the intracellular ATP concentration and promote the cancer cell growth, proliferation, and resistance to anticancer drugs[2]. Several cancer drug resistance mechanisms have so far been recognized, and among these, numerous mechanisms are known to be ATP dependent[3]. Thus the continuous monitoring of ATP levels in cancer cells possesses great importance for disease diagnosis and prognosis. In this work, we have developed a new fluorescent chemosensing ensemble consisting of a 2-hydroxy naphthaldehyde–picolylamine conjugate (**NPAC**) with Zn^{2+} for the efficient and selective recognition and estimation of ATP via a turn ‘‘off–on–off’’ mechanism. UV-vis, fluorescence measurements, NMR titrations, TDDFT calculations have been performed in order to understand the sensing mechanism and electronic properties of receptor–donor complex. The cell permeable ensemble **NPAC–**$\mathbf{Zn^{2+}}$ exhibits highly sensitive and selective response towards ATP over other biologically important organic phosphates at pH 7.0. Furthermore, the sensing mechanism has successfully been implied in human liver cancer cells to detect and quantify ATP through fluorescence imaging studies. This study could be employed in biomedicine and diagnostics research by further exploring the cellular dynamics of ATP and its functions in biological systems.

Keywords:
Adenosine 5'-triphosphate (ATP), Fluorescence ‘‘off–on–off’’, Chemosensing ensemble, human liver cancer cell

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Assessment of the nutritive value of *Prunus domestica*

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ABSTRACT:

Medicinal plants have been used traditionally by the native inhabitants since the ancient time for the treatment of many diseases. *Prunus domestica* also a medicinal plant used to cure many diseases such as leucorrhoea, irregular menstruation and debility following miscarriage. In addition to this it also exerts many biological activities such as antioxidant, antidiabetic, hepatoprotective, cytotoxic and many other activities. Its origin is thought to be near the Caspian Sea and it is found in Kashmir, Swat division of Pakistan and Uttarakhand region of India as well. *Prunus domestica* is commonly known as plum. In Hindi it is called as Aloo Bukhara. *Prunus domestica* is the member of the family *Rosaceae* and genus *Prunus*. This family is the 19th largest family of the plant which consists of more than 2000 plant species. About 36 plant species of the genus *Prunus* have been reported in India, of which 18 species are used for the cultivation purpose. Keeping the eye on its medicinal aspects, in the current study we have evaluated the nutritive value of this plant.

Keywords:
Medicinal plants, *Prunus domestica,* Uttarakhand, nutritive value

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Application of Photo Catalytic Nanomaterials for Durability of Built Environment

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ABSTRACT:

Environmental issues and climate change have highlighted another major problem with concrete. Concrete's ingredients like cement, sand, rocks & water are all nature sourced. But with sand & stone mining ban and with water becoming progressively costly, what should be the new alternatives? Till recently, major developments in cement-concrete performance were achieved with the use of micro-fine waste particles viz. fly ash, slag and silica fumes. Not a long ago discovered exotic nano-scale materials, asserts of alleviating the problem of natural materials scarcity and reducing all types of wastes including green-house gas (GHG) emissions. Nano titanium synthesized from waste materials has excellent self-cleaning properties and is the most widely used nanomaterial in commercia-environmental applications. The photocatalytic mechanism of this self-healing material also has a disinfection mechanism which includes *decomposition* of the cell wall and disinfection of novel viruses such as *SARS-CoV* and *COVID-19*. Nano-TiO_2 or Nano-Titania a product of nanotechnology has already been applied in many buildings as in the construction of Jubilee Church, Umberto Tunnel and Ara Pacis archaeological museum -Rome, Hotel-de-Police, Bordeaux-France. Recently the self-healing properties of nano-TiO_2 have been launched in India, marketed and distributed by *Zuari Cement* (part of the Heidelberg Cement Group) which are available under brand names *TX Aria-Architectural Line* and *TX Aria-Environmental Line*.

Our work reports the effect of adding hydrophobic 40 nm dia. nano-sized Titania (NT) particles by functionalized them to hydrophilic via. surface modification or wrapping by new generation pH neutral polymeric admixtures & added them to cement: sand ratio of 1:3 with a water-cement ratio of 0.4. Mechanical strength results of the cementitious composites were taken at all terms up to 365 Days(D). The optimized quantity of NT as found in cement composites are then added to a M-40 Grade concrete composites for compressive strength testing at both shorter & longer terms following Indian standard protocols. Simulating sea water behaviors in laboratory conditions– results of sulphate and chloride attacks on standard concrete at medium and longer terms is discussed. Results reveals that the application of NT in cementitious systems has an improved effect when compared with non-NT cementitious systems and also the former is more durable. Photocatalytic NT is also time durable and the micro-structural investigations disclose that crystallographic nature of NT, which is the main reason for their favorable mechanical impacts.

Keywords:
Cement; Composites; Concrete; Environment; Strength; Titania

Oxime Radicals – A Potential Intermediate in Synthetic Organic Chemistry

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ABSTRACT:

Applied from the catalysis of selective Oxidation processes and mechanical studies to the manufacturing of polymers, energy storage, magnetic material design and spectroscopic studies of biological objects, N-Oxyl radicals, molecules with the N–O• fragment, are a rich family. As a helpful intermedium for organic synthesis compared to other N-oxyl radicales, oxime radicals (or iminoxyl radicals), although the precursors of oxides are widely disseminated and readily available organic molecules, have long been undervalued. In addition, oxime radicals are unusual in structure. The N—O• fragment is connected to an organic movement with a double bond, but the R_2N–O• Fragment with two C–N bonds is included in all other classes of N-oxyl radicals. Although oxime radicals have been known since 1964, they were not recognised until the previous decade when various select reactions were identified from oxidative cyclic, functional and iminoxyl radical couplings. Most works focus on intramolecular oxime radicals reactions. These reactions are characterised as cycling with C-H bond splitting and cycling with double C = C bond splitting.

Keywords:
iminoxyl radicals; isoxazolines; oxidative cyclization; oxime radicals; oximes

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pH-responsive adsorption of cationic/anionic dyes from their aqueous solutions by Katira gum-*cl*-*poly*(acrylic acid-*co*-N-vinyl imidazole) hydrogel

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ABSTRACT:

pH responsive hydrogel of katira gum (KG) with a copolymer mixture of acrylic acid (AA) and N-vinyl imidazole (NVI) (termed as KG-*cl-poly*(AA-co-NVI) were synthesized by free radical co-polymerization technique using KPS as initiator and N, N'-methylene-bis-acrylamide (MBA) as a cross-linking agent. FTIR, XRD, and SEM were used to characterise the pH-sensitive hydrogel. Hydrogel showed two maximums at pH = 4.5 and pH = 9 in swelling studies with water. The cationic [methylene blue (MB), methyl violet (MV)] and anionic [Tartrazine (TA), Carmoisine-A (CR-A)] dyes were removed from their aqueous solutions using the hydrogel as an adsorbent. The anionic dyes were adsorbed at pH = 2 for TA and pH = 3 for CR-A, while the cationic dyes were adsorbed at pH = 7. Pseudo second order kinetics and the Langmuir isotherm model were used to explain the adsorption. For the MB, MV, CR-A, and TA, the highest adsorption capacity was found to be 331.5, 286.01, 273.5, and 201.53 mg/g, respectively. Several thermodynamic parameters, including Gibbs free energy change (ΔG^0), enthalpy change (ΔH^0), and entropy change (ΔS^0), were also studied. The dyes were removed by the hydrogel in the following order: MB > MV> CR-A> TA. It was found that hydrogel absorbed the cationic dyes more effectively than the anionic dyes.

Keyword:
pH responsive, adsorption, katira gum

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ANALYSIS OF EXTRACTION-SULFATION EFFICIENCIES, STRUCTURAL FEATURES AND ANTIVIRAL ACTIVITIES OF SULFATED POLYSACCHARIDES FROM DIFFERENT NATURAL PRODUCTS

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ABSTRACT:

Natural resources represent a rich and valuable platform for the development of new biologically active experimental compounds and drug candidates [1–4]. The identification of new molecular entities for drug development remains a need in many therapeutic areas. The compounds with a high degree of diversity and appealing pharmacological properties is a limiting step in drug development. This study reports the production of highly bioactive sulfated polysaccharides, originally present in a nonsulfated form, and demonstrates their antiviral activity (human cytomegalovirus) at a low degree of cytotoxicity. Experiments strongly propose that the main mode of antiviral action is the inhibition of virus entry. Oleum-DMF reagent is utilized to generate a range of sulfated polysaccharides from various natural sources, possessing different sugar compositions, degrees of sulfation and molecular masses. This reagent is not only used to solubilize polysaccharides but also converts their hydroxyl functional group into sulfates. The most active sulfated polysaccharide is proved to be a branched glucan with sulfates. Summarizing, the important factors responsible for the antiviral activity are: (i) degree of sulfation, (ii) molecular mass and (iii) structural features. Thus, our goal is to improve the utilization of natural source-derived compounds, mainly biologically active polysaccharides with varied chemical profiles.

Keywords:
Natural Resources, Chemical modification of Polysaccharides, Structural features, Antiviral activities

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Recent advances in the synthesis of 3d-4f heterometallic complexes using compartmental ligand approach and their applications as molecular magnetic materials

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ABSTRACT:

In recent decades 3d–4f heterometallic discrete complexes have growing special attraction in the field of molecular magnetic materials with potential applications in the information storage device, quantum computer, spintronics, and magnetocaloric materials.The significant magnetic anisotropy of Ln(III) ions like Tb(III),Dy(III), Ho(III), and Er(III) ions allowed the synthesized complexes as captivating candidates to construct molecular nanomagnets. Compartmental ligands like phenol-based Schiff bases are useful candidates in the construction of 3d-4f heterometallic multinuclear complexes as there are different pockets are available for different types of metals according to the hard and soft acids and bases (HSAB) principle. 4f ions like Tb(III), Dy(III), Ho(III),and Er(III) prefer hard pockets and preferentially interact with the oxygen-rich parts of ligands, while 3d ions like Cu(II), Ni(II), Fe(II) and Mn(III)prefer soft donor atom-like nitrogen atoms for binding. Although the study of 3d-4f heterometallic complexes is a well-established field as many databases related to the structural topology and nanomagnet materials are available in the literature, still, we believe that a lot of effort remains to be carried out on the development and understanding of the complicated magnetic exchange interactions between the 3d and 4f spin carriers and subsequent theoretical computational simulation of the observed magnetic behaviours.Here we review the synthetic approaches, structural topology,and magnetic properties of 3d–4f heterometallicdiscrete complexes.

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Inductive Coupled Plasma Optical Emission Spectrometry (ICPOES) in ensuring Food Quality and Safety

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ABSTRACT:

Increasing global industrialization has made a tremendous pressure on the food safety expert to ensure the quality and safety of food products for human consumption. Green revolution has improved the agriculture production but has made us dependent on various agrochemicals including pesticides. As a result, soil and water quality deteriorates and most of the food especially the roots vegetables have the high probability of such carcinogenic components. International regulatory guidelines have also been reframed with the more stringent permissible limit to safeguard the human being.

Analytical instrumentation has a vitol role for precise identification and quantification of these toxic contaminants. Inductive Coupled Plasma Optical Emission Spectrometry (ICPOES) is one of the advanced analytical techniques in this direction to ensure and limit the heavy metal contaminants in the food chain. Present paper covers the case studies related to heavy metals and their limits as per Indian standards along with the brief overview of ICPOES for detection and estimation of minerals and heavy metals as per the regulatory guidelines for food safety and quality.

Key words:
Inductive Coupled Plasma Optical Emission Spectrometry (ICPOES), Food, Heavy metals.

MOLECULAR ORBITAL COMPOSITIONS, STRUCTURAL AND SPECTROSCOPIC PROPERTIES AND REACTIVITY OF A SERIES OF RHODIUM COMPLEXES -A DFT STUDY

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ABSTRACT:

The present study has aimed to perform density functional theory (DFT) and time-dependent density functional theory (TDDFT) studies to explain the structural and spectral properties along with reactivity, of two different series of rhodium diaryltriazenide complexes. In all the calculations Gaussian 16 [B3LYP/SDD-6-31G(d,p)] package with the help of GaussView visualization program, has been used. A group of five 1,3- diaryltriazenes have been utilized, differing in the inductive effect of the *para*-substituents (R) on the aryl fragment (R = OCH_3, CH_3, H, Cl, NO_2) in order to understand their effects, if any, on the properties and reactivity of the complexes. The energy and compositions of the frontier molecular orbitals of the complexes have been evaluated using DFT. The global indices parameters *viz*., chemical potential (μ), chemical hardness (η) and electrophilicity indices (ω) have been calculated to gain insight into the reactivity of the complexes. The electronic spectral and cyclic voltammetric properties of the complexes have been explained with the help of frontier molecular orbital compositions. The calculations show the lowest energy absorption of the complexes (near 400 nm) may be assigned to an electronic transition from the filled rhodium orbital (HOMO) to the vacant π*–orbital (LUMO) localized on the triazene fragment of a coordinated diaryltriazene ligand. In a similar way, the cyclic voltammetric responses have been assigned to a Rh(III)-Rh(IV) oxidation and the reductive response being designated as the reduction of the triazene fragment of the coordinated ligand.

Keywords:
DFT studies, optimized structures, global reactivity indices, frontier molecular orbital compositions.

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Effective Cd^{2+} ion Adsorption by Amylopectin–g-poly (methylacrylate-co-sodium acrylate)

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ABSTRACT:

AP-g-poly (methylacrylate-co-sodium acrylate) was prepared by partial alkaline hydrolysis of the synthesised graft copolymer amylopectin-g-polymethacrylate. The study of characterization of the AP-g-poly (methylacrylate-co-sodium acrylate) was carried out by measuring saponification equivalent (SE), FTIR, ^{1}H NMR and ^{13}C NMR spectroscopy and thermal analysis (TG / DTG). Amylopectin–g-poly (methylacrylate-co-sodium acrylate) was used for Cd^{2+} ion adsorption study. The adsorption data were well fitted by the pseudo-second-order and Langmuir Isotherm Model. Several adsorption parameters like change of enthalpy, change of free energy and change of entropy were calculated. The spontaneous nature of the adsorption process was confirmed by negative value of free energy change.

Keywords:
Graft copolymer, Biodegradation, Cd (II) ion removal, Amylopectin, Methylacrylate

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Hydrogeochemical comparison between two aquifer and their possibility for safe drinking water supply: A case study in an arsenic affected area of West Bengal

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ABSTRACT:

Natural elevated level of arsenic (As) in groundwater poses a serious threat to millions of inhabitants of Bengal Delta Plain (BDP). Access to safe arsenic water (which is used as drinking and farming water) is thus of prime importance and must be implemented. It is known for instance that deep wells (> 150 m) are generally safer and contains lower concentration of As, thus providing safer water to the community. The problem is that these deep tube wells installation requires advanced drilling technology with very high installation costs. The concentration of arsenic (as well as the chemical signature of the water) varies with depth, with deep aquifers having less arsenic than the shallow ones. However, in the latter case, the arsenic content is dependent on the sediment. Present study investigates a hydrogeochemical comparison between Brown sand aqifer (BSA) and Grey sand aquifer (GSA) within shallow depth (< 70 m) in an As affected area of West Bengal followed by the potentiality of BSA as safe drinking water source. Higher concentration of NH_4^+, PO_4^{3-}, Fe and As along with lower Eh in groundwater of GSA indicates the reductive dissolution of Fe oxyhydroxides coupled to the microbially catalyzed mineralization of organic matter releases As in groundwater of this aquifer. BSA accomodates much lower As concentration (< 10 ppb) than GSA and it can be used for sustainable drinking water supply source.

Key words:
Arsenic, Bengal Delta Plain (BDP), Aquifer, Brown sand aqifer (BSA), Grey sand aquifer (GSA)

Assessment of polyphenols and free radical scavenging activities of wild edible fruit of North-West Himalaya, Uttarakhand

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ABSTRACT:

The Indian Himalayan Region owns approximately 675 wild edible plant species, out of which 340 were exclusively reported in Uttarakhand. of these, wild edible fruits are of great interest due to their nutritional values, vitamins, and mineral contents. They have served as dietary staples and medicines for thousands of years, particularly in the tribal and rural areas of Uttarakhand. Limited studies on wild edible fruits of Uttarakhand have shown the presence of abundant polyphenol contents and antioxidant activities. There are a lot of wild edible fruits which are still under exploration regardless of their nutritional values. The promotion and consumption of indigenous fruits could help to mitigate food insecurity and alleviate malnutrition in developing countries. The antioxidant capacity of *Ficus subincisa* Buch-Hm Ex.Sm. Fruits were investigated during the present study. Solvents have an important role in the chemical or pharmaceutical industry. Toxic solvents may cause inimical effects on human safety and health. Therefore, green solvents are encouraged to be utilized because they are environmentally friendly and easily acquired during crop processing results of the antioxidant analysis showed that all the green solvent extractives were studied had significantly different quantities of antioxidants. Hence the *F.subincisa* fruits could serve as effective free radical scavengers which may be an opportunity for pharmaceutical plant-based products. However, further exploration is necessary for effective use in both modern and traditional systems of medicines.

Keywords:
Wild edible fruits of Himalaya, Free radical scavenging activities, *Ficus subincisa* fruit, Green solvents, Phenolics, Flavonoid.

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Apoptosis inducing 1,3,4-oxadiazole conjugates of Capsaicin: Their in vitro anti-proliferative and in silico studies

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ABSTRACT:

Series of 1,3,4-oxadiazole conjugates of capsaicin were synthesized by exploiting one point modification at the hydroxy position of vanillyl group of capsaicin. All synthesized compounds were evaluated for their anti-proliferative activity against NCI-60 human cancer cell lines at 10 μM. *In vitro* assay revealed that compound **20a** exhibited good cytotoxic activity against HCT-116, NCI-H460 and SKOV3 human cancer cell lines with IC_{50} 8.55 μM, 5.41 μM, and 6.4 μM respectively compared to parent natural product, capsaicin. Further on, it significantly inhibited the colony formation in NCI-H460 in dose dependent manner and enhanced ROS effect. It also induced cell arrest at S phase and caused apoptosis by suppressing Pro parp marker. Compound **20a** exhibited anti-migratory property and suppressed the expression of VEGF marker in dose dependent manner. Furthermore, compound **20a** also suppressed the effect p-Erk, p-p38 and P-CNA maker. *In silico* studies supported the interaction of this class of compounds with VEGFR2 protein.

Keywords:
Capsaicin, Cancer, Anti-proliferative, 1,3,4-oxadiazole, VEGFR.

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Efficient removal of chlorpyrifos and dimethoate pesticides from water medium using dextrin-graft-*poly*(2-acrylamido-2-methyl propane sulfonic acid-co-acrylic acid) copolymer by adsorption

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ABSTRACT:

A graft copolymer is synthesized by grafting of mixture of acrylic acid (AA) and 2-acrylamido-2-methyl propane sulfonic acid (AMPS) monomers onto the dextrin backbone by free radical copolymerization technique. Several characterization techniques like ^{1}H NMR, FT-IR and SEM analysis are used to characterize the graft copolymer. The polymer is used as an efficient adsorbent for the removal of toxic pesticides namely chlorpyrifos (CP) and dimethoate (DM) from their aqueous solutions. Different operating variables, kinetic, isotherm and thermodynamic parameters are investigated for the two pesticides. The pesticide adsorption process over polymer surface is directed by pseudo-second-order kinetic model. Langmuir and Dubinin-Radushkevich isotherms both correlate well with the equilibrium data. Maximum adsorption capacity (q_m) of the polymer is found to be 172.41 mg g^{-1} for DM and 108.69 mg g^{-1} for CP.

Keywords:
Pesticide; Graft copolymer; Adsorption; Dextrin.

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Gymnema sylvestre as potential antiglycation agent against the complication in advanced glycation of BSA

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ABSTRACT:

The non-enzymatic protein glycation is a condensation reaction between amino and carbonyl groups of proteins and reducing sugars irreversibly and spontaneously under hyperglycaemic condition. The process involves multistep organic reactions involving the formation of Schiff base, which is subsequently stabilized by Amadori rearrangement [1]. This complex series of reactions leading to the formation of many reactive carbonyl species (RCS) intermediates such as glyoxal, methyl glyoxal [2–3] and advanced glycation end-products (AGEs) [4], which are a heterogeneous group of high-molecular weight aggregates stabilized by non-reducible cross-linking with characteristic fluorescence [5]. Among those, protein cross-link is believed to be potential cause of complications in diabetes including retinopathy, neuropathy, nephropathy, cardiovascular and neurodegenerative diseases like Alzheimer. AGEs can be obtained both endogenously and exogenously in the body. Natural defence system in the body is the primary firearm to prevent glycation. Synthetic inhibitors also prevent glycation through several possible mechanisms such as by interfering with the attachment of sugars with proteins, by inhibiting the late stage of glycation or by averting Amadori product formation. Furthermore, their ability to scavenge free radicals and to break cross-links might be other mechanisms responsible for their potential inhibition of glycation. Naturally occurring phytochemicals have been found to be relatively non-toxic as compared to synthetic compounds, and are inexpensive and available in an ingestible form.

A large number of plants and natural biomolecules have been shown to have antidiabetic effects. Alternatively, phytochemicals play pivotal role in preventing many diseases and are great importance owing to their diverse structures and functions. One of such phytochemical is gymnemic acid (GA), a triterpenoid saponins possessing β-amyrin skeleton from *Gymnema sylvestre R. Br*. GA is known for antidiabetic agent by blocking the receptors responsible for the absorption of glucose in intestine and thereby lowering blood glucose level significantly. The selection of GA as antiglycation agent is rational since the process of diabetic and glycation are assimilated to each other after a certain period. In addition to antidiabetic effect, the triterpenoid saponins possessing β-amyrin skeleton has shown microbial resistance e.g. influenza A virus in mice. Prompted by these evidences, we emphasis in this article about the role of GA as inhibitor of AGEs and draw a correlation on how a saponin natural product from antidiabetic medicinal plant origin can be effective as antiglycating agent for preventing the secondary complication of DM. We observed that Gymnemic acid well following the inhibition of non-enzymatic glycation of Bovine Serum Albumin (BSA) *in vitro*. The extensive spectroscopic studies using UV-Visible, fluorescence spectroscopy indicate that saponin type compounds can be targeted for AGEs inhibition.

Keywords: Non-enzymatic, Glycation, AGEs, diabetes complication, natural inhibitors, gymnemic acid.

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Exploring Photocatalytic Degradation of Methyl Violet (MV) & beta vulgaris dyes with Gallic Acid Surface Passivated CdS QD's

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ABSTRACT:

This study was focused on the application of Methyl Violet (MV) & beta vulgaris dyes with the Gallic Acid(GA) passivated colloidal CdS quantum dots (QDs) as sources for the photocatalytic degradation of organic dyes in liquid phase. Photo induced interaction of passivated colloidal CdS quantum dots with Methyl Violet (MV) & beta vulgaris dyes have been studied. Distinctive photo induced interaction were observed between Methyl Violet (MV) & beta vulgaris dyes that reflects charge transfer interaction of both the dyes with CdS QDs as reflected by UV-VIS absorption studies. The dye adsorption on the CdS surface causes an increase in optical density as well as a quenching of dye molecule emission intensity. The apparent association constant (K_{app}) between dye and CdS QDs was calculated using spectroscopic data. The electron transfer from the excited state dye to the colloidal CdS conduction band is responsible for dye quenching.

Keywords:
Gallic Acid(GA), Cadmium sulphide, Surface functionalization, Photocatalysis, beta vulgaris dye, Methyl Violet

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Applications of highly novel nanocellulose-based biopolymer nanocomposites in novel drug delivery

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ABSTRACT:

Green chemistry based eco-friendly, eco-efficient, available and sustainability nano-materials and their composites are presently the main drive for the development of the next generation of materials, products, and processes. This presentation explores some of the studies on nanocellulose (NC) based transdermal drug delivery system as a novel drug delivery system and also NC based ophthalmic drug delivery systems having highly sustained bio-availability of ophthalmic drugs in our laboratory. The skin can be readily used as an accessible surface for transdermal drug delivery. An average adult body covers ~ $2m^2$ and benefits from 1/3 of the blood circulating throughout the body. The synthesis of nanocellulose based drug release materials using diverse routes has been a point of attraction for researchers with the aim of applying these materials in biopharmaceuticals. The skin has attracted considerable interest as a novel site for drug application for local and systemic effect. Within the last 2 decades, challenges in drug delivery have been partially met through modification of the transdermal and ophthalmic formulations using viscosity enhancing polymers or hydrogels or nano-fillers aimed at increasing the drug's retention time, along with the least side effects. In this regard, nanocellulose has proven beyond doubt as a novel nanomaterial that enhances the overall performance of its biopolymer nanocomposites especially the sustained delivery of drugs and other particles. Though, there are some challenges that need to be addressed such as the application from the research bench top using animals into patients' specific applications, product quality consistency, structural control, and cost-effectiveness.

Keywords:
Drug, Nanocellulose (NC), Ophthalmic drug delivery, Release kinetics, Transdermal drug delivery

A dinuclear and a trinuclear Ni(II) complex formation on slight variation of experimental conditions: Magnetic Studies

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ABSTRACT:

A tridentate reduced Schiff base ligand HL (HL = 2-[(2-dimethylamino-ethylamino)-methyl]-phenol) has been used to synthesize a diphenoxido bridged dinuclear Ni(II) complex $[Ni_2L_2(NO_2)_2]$ (**1**) and a μ_2 and μ_3-phenoxido, μ_3-hydroxido, and μ_2-nitrito (1κ*O*:2κ*N*) bridged trinuclear Ni(II) complex $[Ni_3L_3(OH)(NO_2)]\cdot ClO_4$ (**2**). Both complexes were characterized by X-ray structure determination and variable-temperature magnetic susceptibility measurements. In both complexes the nickel atoms are six-co-ordinate with a distorted octahedral environment. The interesting feature of the trimeric complex **2** is that the three mononuclear units are assembled around a μ_3-hydroxido ion in such a way that the three phenoxido groups and one nitrito group form a cyclic bridge that markedly modify the magnetic properties. Complex **1** presents a moderate antiferromagnetic Ni-Ni coupling (J = -39 cm^{-1}) through the phenoxido bridges with a wide Ni-O-Ni bond angle of 101.77(6)° whereas the lower Ni-O-Ni bond angles, in the range 86.66(6)-96.07(7)°, lead to a moderate ferromagnetic coupling (J = + 18.2 cm^{-1}) in the trimeric complex **2** with a weak antiferromagnetic contribution (J' = -0.51 cm^{-1}).

Keywords:
Nickel(II), Reduced Schiff base, Nitrite, Crystal structure, Magnetic properties

Potentiality of Chitinase Enzyme in Medicinal Field and their Contribution in Applied Research

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ABSTRACT:

Chitinases have a significant use in human health care, as recommended in augmenting the activity of anti-fungal drugs in therapy for fungal diseases, using in antifungal creams and lotions. Chitin derivatives are non-toxic, non-allergic, and biocompatible and biodegradable therefore has huge potential in the preparation of a number of medical articles such as artificial skin, contact lenses, and surgical stiches. Chitooligosaccharides also have novel pharmaceutical potential to be used in the human medicines because of its wound healing property, anti-hypertensive and anti-tumor activity shown by chitohexaose and chitoheptaose. A chitin monomer, NAG acts as anti-inflammatory agent. The involment of AMCase is found to increase the Th-2 inflammation and play a key role in the pathogenesis of asthma and allergic inflammation was novel and unexpected because of the fact that mammals do not produce any chitinase structure, nor do they used chitin as an energy source. It is found that the patients with the respiratory disease have the great quantity of YKL-40 (chitinase-like protein) in respiratory organ tissues. Chitinase-3-like-1 enzyme (CH13L1) is a therapeutic target that mediates the effect of Aging in COVID-19. The angiotensin-converting enzyme 2 (ACE2) that act as the host cell receptor for SARS-CoV-2, CH13L1 protects the lung against injury.

Keywords:
Chitooligosaccharides, AMCase, YKL-40, COVID-19, anti-tumor.

Solvation behaviour of streptomycin sulphate in aqueous L-aspartic acid solutions at temperatures from 293.15-313.15 K

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ABSTRACT:

Comprehensive study of thermodynamic mixing properties of binary and ternary mixtures has intense importance in theoretical and applied areas of exploration that helps in mapping methods in chemical, petrochemical and pharmaceutical industries[1,2]. For the illumination of action of drugs, metabolic processes in the body, the properties like density, ultrasonic speed, viscosity, etc. are mostly studied[3,4]. These physical properties for varying concentrations of streptomycin sulphate in water and in (0.01, 0.02, 0.03) mol kg^{-1} aqueous solutions of L-aspartic acid have been calculated at five discrete temperatures (T =293.15-313.15) K and ambient pressure (101.03) kPa. The ρ and u data have been used to determine apparent molar volumes, V_{ϕ}, limiting apparent molar volumes, V^{0}_{ϕ}, apparent molar isentropic compression, $K_{\phi,s}$, limiting apparent molar isentropic compression, $K^{0}_{\phi,s}$, and their transfer values. The η data has been analyzed viscosity B-coefficients, and viscosity B-coefficients of transfer, $\Delta_{tr} B$. Further, the derived data has been designated in terms of solute-solute and solute-solvent interactions and structure making / breaking characteristics of streptomycin sulphate in aqueous solutions of L-aspartic acid.

Keywords:
Density, apparent molar volumes, streptomycin sulphate, L-aspartic acid.

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Volatile Constituents of Essential oil of *Amra Haridra* from North India

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ABSTRACT:

The essential oil of the rhizomes of *Amra Haridra* (*Curcuma amada* Roxb.) from North India was obtained by hydrodistillation Clevenger apparatus method and investigated by GC-FID and GC-MS. More than 40 components have been identified with camphor (9.01%), 2-(2,5-dimethoxyphenyl)cyclohex-2-enone (7.93%), isoborneol (6.86%), germicrone (6.61%), curzerene (6.6%) and β-elemene (5.87%) as the main constituents.

Keywords:
Amra Haridra, Zingiberaceae, essential oil composition, GC/MS, camphor.

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Drug-amino acid interactions: A physicochemical approach

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ABSTRACT:

Physicochemical studies on amino acids with drugs help in understanding the conformational stability and folding/unfolding characteristics of the protein. The binding of drug with protein is an essential process in ascertaining the activity and mechanism of action of the drug across biological membrane. The complex conformational and configurational factors, make direct studies on protein interactions very difficult [1,2]. Hence, for a better understanding of the complex biological processes or metabolic pathways occurring inside the body, numerous model compounds of low molecular weight such as peptides, amino acids and their derivatives are studied [3]. Drugs play a crucial biological role in living organisms [4]. These are imperative chemical compounds that are used for the recognition, prediction and alleviation of diseases. Studies of thermophysical properties such as densities, viscosities, speeds of sound etc. help to understand drug action in aqueous solution as they exert their activity by interaction with biological membrane [5,6]. These investigations also attract the attention of researchers owing to the unique features and the important role that drugs play to understand the pattern of molecular aggregation and complexation. Dependence of thermophysical properties of drug-amino acids systems on temperature in aqueous media provides valuable information in pharmaceutical industries. Physicochemical properties are helpful in understanding drug-protein interactions.

Keywords:
Drugs, amino acids, physicochemical properties

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Interplay of Hückel and Möbius Aromaticity in Metal-Metal Quintuple Bonded Complexes of Cr, Mo, and W with Amidinate Ligand: Ab initio DFT and Multireference Analysis

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ABSTRACT:

The aromaticity of metal-metal quintuple bonded complexes of the type M_2L_2 (M=Cr, Mo, and W; L=amidinate) are studied employing gauge including magnetically induced ring current (GIMIC) analysis and electron density of delocalized bonds (EDDB). It is found that the complexes possess two types of aromaticity: i) Hückel aromaticity through delocalization of ligand π electrons with metal-metal δ-bond-forming 6 conjugated electrons (4π and 2δ) ring; ii) Craig-Möbius aromaticity through delocalization of π electrons of both the ligands with metal d-orbitals in Craig type orientation forming 10π electrons ring with a double twist. Extended transition state natural orbital chemical valence (ETS-NOCV) and canonical molecular orbital natural chemical shielding (CMO-NCS) analysis confirm the Craig-Möbius type arrangement of the orbitals. Furthermore, the unprecedented Hückel and Möbius type aromaticity is confirmed from the plot of the current pathways using 3D line integral convolution (3D-LIC) plots. The metal-metal bond order also increases down the group as justified from the complete active space self-consistent field (CASSCF) analysis. Due to an increase in the π and δ electron conjugation, both the Hückel and Möbius aromaticity increase down the group.

Synthesis, characterization, DNA binding ability, in vitro cytotoxicity, electrochemical properties and theoretical studies of copper(II) carboxylate complexes

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ABSTRACT:

Four copper(II) carboxylate complexes, namely [Cu_2(μ-3,5-dinitrobenzoate-O,O')$_4$(4-(dimethylamino)benzaldehyde)$_2$] (**1**), [Cu_2(μ-benzoate-O,O')$_4$(benzoic acid)$_2$] (**2**), [Cu_2(μ-benzoate-O,O')$_4$(H_2O)$_2$] [Cu(benzoate-O, O')$_2$(imz)$_2$].2H_2O (**3**) and [Cu(benzoate-O,O')$_2$(2-Me-imz)$_2$] (**4**) (imz = imidazole, 2-Me-imz = 2-methyl-imidazole), were synthesized and comprehensively characterized by elemental analysis, spectroscopic methods, single crystal X-ray diffraction, cyclic voltammetry (CV), topological analysis as well as theoretical studies. Single crystal X-ray diffraction revealed that products **1** and **2** are dinuclear paddle-wheel complexes, compound **3** is a co-crystal containing mononuclear and dinuclear blocks, while compound **4** is a mononuclear complex. Hirshfeld surface analysis of the compounds rationalized different types of hydrogen bonds, which also lead to the generation of H-bonded networks in **3** and **4**. Their topological analysis disclosed a uninodal 4-connected 2D layer with sql topology in **3** and a uninodal 2-connected 1D chain with 2C1 topology in **4**. The interaction of **1–4** with calf thymus DNA was investigated by UV–visible and fluorescence spectroscopy, revealing a moderately strong non-intercalative mode of interaction. In vitro cytotoxicity study of the complexes on HepG2 (human liver hepatocellular carcinoma) cell lines revealed a significant inhibition activity. Electrochemical study of the complexes in CH_3CN (**1–3**) and DMSO (**4**) solution showed a one electron transfer corresponding to Cu(III)Cu(II)/Cu (II)Cu(II) and Cu(II)Cu(II)/Cu(I)Cu(II) redox couples. The ΔE and Ipa/Ipc values suggest that the redox couples are quasireversible. The DFT study was performed to further rationalize the crystal structures and nuclearity of the obtained copper(II) complexes.

Keywords:
Copper carboxylates, Crystal structures, DNA binding, Cytotoxicity, Cyclic voltammetry, DFT calculations.

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Protein denaturation inhibitory activity of the seed of *Prunus domestica* L.

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ABSTRACT:

Plants are being used as the main therapeutic agents since the ancient time by the native inhabitants. There are many systems of the medication like Ayurveda, Siddha, Unani and Homeopathy etc. which purely based on the plants and plant-based medicines. Natural products are the main source of the nutrients like phenolic vitamins, tocopherols, pigments and minerals for the human health. The plant *Prunus domestica* L. (plum) is one of the medicinal plants used to cure many diseases like leukorrhea, alzheimer disease irregular menstruation, debility following miscarriage and many other diseases. This plant is the member of the family *Rosaceae* and genus *Prunus*. This family is one of the largest family of the plants having more than 2000 plants. This plant also shows many biological activities like antioxidant, antidiabetic, antibacterial, antifungal, hepatoprotective activity etc. Our work is mainly done on the seed of this specific plant. Usually, people eat then fleshy part of the plum and seed is discarded away. The present work is done to evaluate the protein denaturation inhibition activity of the seed.

Keywords:

Prunus domestica L., *Rosaceae*, phenolic, biological activities, seed

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Insights into the thermophysical properties of L-ascorbic acid and thiamine hydrochloride in aqueous 1-ethyl-3-methyl imidazolium hydrogen sulphate media at various temperatures (293.15-318.15)K

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ABSTRACT:

Studies on thermophysical properties of vitamins in aqueous ionic liquids play a significant role in different biochemical processes as well as in the designing of several industrial processes.[1,2] An investigation of molecular interactions through the procured thermophysical properties is very important because it provides an insight into the forces that are operating in the liquid mixtures.[3,4] The physical properties like density, speed of sound and viscosity provide a crucial information regarding the various sorts of interactions existing amid the solutions.[5,6] These physical properties were interpreted for L-ascorbic acid and thiamine hydrochloride in water and in (0.05, 0.10, and 0.15) mol kg^{-1} aqueous 1-ethyl-3-methyl imidazolium hydrogen sulphate media at six discrete temperatures. Through the use of this data, different thermophysical parameters were investigated. These parameters include apparent molar volume (V_ϕ), apparent molar isentropic compressibility ($K_{\phi,s}$), partial molar volume ($V^o{}_\phi$), partial molar isentropic compressibility ($K^o{}_{\phi,s}$), partial molar expansivity ($E^o{}_\phi$), volumetric and acoustic interaction coefficients (V_{AB}, V_{ABB}, K_{AB}, K_{ABB}), Hepler's constant, viscosity coefficients (A and B) etc. In addition, the structure breaking capability of both the vitamins have been assessed via positive sign of $\left(\frac{dB}{dT}\right)$ values and negative sign of $\left(\frac{\partial E^o{}_\phi}{\partial T}\right)_P$ values. Also, through Cosphere overlap model, different assorted interactions prevailing in the systems have been analysed.

Keywords:
Thermophysical properties, 1-ethyl-3-methyl imidazolium hydrogen sulphate, L-ascorbic acid, thiamine hydrochloride, viscosity coefficients

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Computational studies of microwave assisted solvent-free tandem cross-metathesis/intramolecular isomerisation-cyclisationto pyrroles

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ABSTRACT:

Pyrrole and its multi-substituted derivatives in natural origin and biologically active molecules confirms biological importance of this ubiquitous heterocyclic core like Neolamellarin A(HIF-1, antitumor) and Vonoprazan (neuroprotective activity, potassium-competitive acid blocker) The microwave-assisted solvent-free reaction has been developed for the rapid synthesis of *N*-substituted pyrrole using cross-metathesis between *N*-allylamines and *α, β*-unsaturated carbonyl compounds. The effect of microwave irradiation is demonstrated through a series of comparative cross-metathesis reactions. In the present eco-friendly approach, the combination of solvent-free conditions and microwave irradiations leads to a substantial reduction in reaction times with improved yields. The computational analysis revealed that the microwave irradiation conditions the interconversion of ruthenacyclobutane is approximately 10 folds more facile than the conventional heating. Thus, we have found that microwave irradiation assisted green synthesis of *N*-acyl pyrrole under one pot condition offers environment benignness, easy handling fast reaction, higher regioselective yields and evaded the need of column chromatography.

Keyword:
Metathesis, *N*-Pyrrole, microwave, solvent free.

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