Abstract Volume

INTERNATIONAL SYMPOSIUM ON CURRENT TRENDS IN CHEMISTRY

Organised by
Department of Chemistry
Diamond Harbour Women's University
(SPONSORED BY HIGHER EDUCATION DEPARTMENT, GOVT. OF W.B.)

10th January, 2020
Venue:
Diamond Harbour Women's University
Sarisha, WB, India

In assocation with

INDIAN CHEMICAL SOCIETY

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Prof. Anuradha Mukhopadhyay
Vice Chancellor

DIAMOND HARBOUR WOMEN'S UNIVERSITY
Diamond Harbour Road, Sarisha
South 24 Parganas, West Bengal - 743368

Message

Date: 27th December, 2019

It is a pleasure to learn that the Department of Chemistry, Diamond Harbour Women's University is organising an International Seminar in collaboration with the Indian Chemical Society on 10th January, 2020.

It is expected that this International Seminar on such a broad topic as **"Current Trends in Chemistry"**, jointly organised with fresh young minds from the Department of Chemistry, Diamond Harbour Women's University and the valuable counsel of the Indian Chemical Society will prove to be an enriching experience for all participants and students.

I hope that this seminar will be successful in providing a platform for interaction not only between fellow participants and delegates but also with experts in the field.

I congratulate all members of the organising committee and my colleagues in the Department of Chemistry for organising this seminar.

I wish the seminar a grand success.

Anuradha Mukhopadhyay
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Established by Diamond Harbour Women's University Act 2012 (West Bengal Act XXXVII of 2012)

Indian Chemical Society
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Web : http://www.indianchemicalsociety.com

Date: December 29, 2019

Message from the President, Indian Chemical Society

It is matter of great pleasure that the Department of Chemistry, Diamond Harbour Women's University, Sarisha, South 24 Parganas, West Bengal and the Indian Chemical Society have ventured to organize an International Seminar on January 10, 2020. It is my proud privilege to bring to the notice of all concerned that the Indian Chemical Society, since its foundation in 1924, has been continuously striving for generation and dissemination of knowledge of Chemical Science and Technology throughout the entire world. Being inspired by a nationalist spirit - J. N. Mukherjee, J. C. Ghosh, S. S. Bhatnagar, N. R. Dhar and other distinguished contemporaries took an undaunted endeavor to establish the Indian Chemical Society with Acharya Prafulla Chandra Ray as its founder president. At a later stage, the Society received the scholastic services of Priyadaranjan Ray, B. C. Guha, P. B. Sarkar, B. N. Ghosh, Jagdish Shankar, T. R. Seshardri, R. C. Mehrotra, Sukh Dev, T. R. Govindachari, Sushil K Mukherjee and some other stalwarts in the field of chemical science in our country.

A linguist, having proficiency in major languages of the world and a voracious reader of literature, Prafulla Chandra was the founder of Indian School of Modern Chemistry and a pioneer of chemical industries in India. By leading a simple life of ascetic self-denial, by his patriotism, philanthropy and entrepreneurship and also with his erudition and wisdom Prafulla Chandra had set up a transcendental idealism to be cherished by his countrymen from generation to generation.

I presume that some basic issues of global interest would find place in the deliberations and I hope that new ideas will emanate and new directions of future research will be indicated in the international seminar.

The organising committee of this international seminar deserves applause and appreciation for undertaking the commendable task of organising such an important event.

I wish the seminar a grand success.

Dulal C Mukherjee
Professor (Retd.) of Chemistry, University of Calcutta
& President, **Indian Chemical Society**

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Prof. Chittaranjan Sinha, Honorary Secretary
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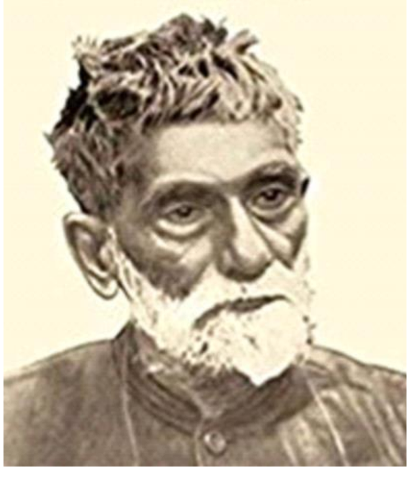
Message from The Honorary Secretary

The Chemical Education and Research along with Chemistry based Industry in the country is initiated by Acharya Prafulla Chandra Ray. He is the scientific spirit of India – a fusion of sacrificial love for country and chemistry and the condensed humanity. His tireless efforts to use Chemistry to establish first pharmaceutical industry in the country, Bengal Chemical and Pharmaceutical Works. Ltd on spending his own earnings is nonetheless a unique example in the British Ruled India. He was an inspiring teacher not only to Chemistry students but also to all. A man of real scientific tempers, a nationalistic spirit, philanthropic and was a great stimulation to entrepreneurship. With his leadership as Founder President, his students started the initiation of Indian Chemical Society on May 09, 1924 with Professor J. N. Mukharjee as the Honorary Secretary and Prof. J. C. Ghosh, Prof. S. S. Bhatnagar and others as its members. With funding of Acharya Ray a part of floor on Palit Building in newly established University College of Science, University of Calcutta was constructed in Rajabazar and is serving as the Office of Indian Chemical Society. He donated a lump sum of Rs. 1,80,000/- to the University of Calcutta for its development and to many other organizations. Anti-British drive against Rawlatt Act his spirit “Science can afford to wait SWARAJ cannot.” catalyses the freedom movement. In 2011, the International Year of Chemistry and 150th Birth Anniversary of Acharya Ray the Royal Society of Chemistry decided to honour his memory by establishing in Presidency College an *International Chemical Landmark Plaque* first-ever in outside Europe. The inscription reads as follows: '*To commemorate the life and achievements of Acharya P. C. Ray, father of Indian Chemistry, philanthropist and entrepreneur who founded modern chemistry teaching and research in India*'.



The Indian Chemical Society organizes Seminar, Symposia, Annual Convention of National and International level along with school level competition to promote chemistry from school to research institute. To encourage quality research in the country the Society has instituted nineteen Endowment Awards for the researchers in chemistry and also number of Convention Awards for young chemists along with Life-Time Achievement Awards. Besides, the Society has arranged Lectureship program for newly formed PG Colleges and Universities to teach chemistry based on their course curricula. In the global perspective society is communicating the world of chemistry through the monthly publication, the **Journal of the Indian Chemical Society** (JICS) since its inception and is also trying to act as nodal agency to popularise Chemistry among the student community by publishing "Education in Chemical Science and Technology". The journal publishes current research in Chemistry and related fields in regular issue and also in Special issues.

It is our great satisfaction that Department of Chemistry, Diamond Harbour Women's University, Sarisha, South 24-Parganas, a newly established only Women University in the state organizes an "International Seminar" on 10th January, 2020 in collaboration with the Indian Chemical Society. The Society conveys heartfelt thanks and gratitude to the members of the Department and Vice-Chancellor along with other Officials for giving us the opportunity to meet the young generation of the country. Your selfless striving and uncompromising emotion towards growth of nationalistic spirit through the service to the Chemistry can improve the Society's health and activity. Our sincere thanks are due to the Young Chemists and participating international and national chemists for their deliberation and other activities.

I do hope that all you will help to improve the all-round growth of the Society to full fill the 'dream' of founder President Sir P. C. Rây.

Best wishes to all for a successful conference!

Chittaranjan Sinha

(Chittaranjan Sinha)

Honorary Secretary, Indian Chemical Society

Kolkata

6th December, 2019

ISCTC-2020@DHWU

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ISCTC-2020@DHWU

One day

International Symposium on Current Trends in Chemistry

(Sponsored by Higher Education Department, Government of West Bengal)

Organized By

Department of Chemistry;

Diamond Harbour Women's University

In Association with

Indian Chemical Society

January 10th, 2020

Programme Schedule

Registration: **09.00 to 10.00 AM**

Inaugural Session: **9.30-10.15 AM**

- Inaugural Song: **By Students**
- Welcome address and Inaugural Speech: **Professor Anuradha Mukhopadhyay**, The Hon'ble Vice Chancellor, Diamond Harbour Women's University
- Felicitation to all delegates present in dais.
- Speech from Guest of Honor: **Prof. Jacques Maddaluno**, Director, INC, CNRS
- Speech from Secretary from Indian Chemical Society by **Prof. C. Sinha**
- Vote of Thanks: **Dr. Md. Sayeedur Rahman**, The Registrar, DHWU

High Tea/Breakfast: 10.15-10.45 am
(Parallel Poster Session) *

Plenary session (10.45 am to 12.15 pm.)
Chair Person: Prof. Asok Kumar Mallik
Venue: Seminar Room, Ground Floor, Academic Building

Plenary Lecture	Speaker	Topic of the talk	Time
PL-1	**Prof. Isabelle Chataigner**	**Dearomatization of Electron-Poor Arenes**	**10.45-11.30 am**
PL-2	**Prof. Ashutosh**	**Hetero-metallic complexes: Facile strategy for**	**11.30-**

	Ghosh	synthesis, diversity in structures and magnetic properties, and effectiveness in catalysis	12.15 pm

Technical Session-1

(12.15-1.30 pm.)
Chair Person: Prof. Debasis Das
Venue: Seminar Room, Ground Floor, Academic Building
(Sponsored by ETHER EDGE)

Technical Lecture	Speaker	Topic of the talk	Time
TL- 1	Prof. Blanca Martin Vaca	Cooperative effects in catalysis: from metal-ligand cooperation in cycloisomerization reactions to organic catalysis in ring-opening polymerization	12.15-1.00 pm
TL-2	Prof. Jacques Maddaluno	Intramolecular carbometallation of alkynes: an overview	1.00– 1.30 pm

Lunch Break: 1.30-3.00 PM

Technical Session-2

(3.00-3.30 pm.)
Chair Person: Prof. Chittaranjan Sinha
Venue: Seminar Room, Ground Floor, Academic Building
(Sponsored by TECHNO WORLD EDUCATION)

Technical Lecture	Speaker	Topic of the talk	Time
TL-3	Prof. Prasanta Kumar Mukherjee	Spectral properties of inert gas atoms under a fullerene cage	3.00-3.30pm
TL-4	Prof. Debasis Das	Nanoscale Coordination Polymers: Green Synthesis to Real Life Implementations	3.30-4.00 pm
TL-5	Prof. Kumaresh Ghosh	Design-based molecular architectures in aggregation, ion sensing and dye removal	4.00-4.30 pm

Valedictory Session: 4.30-5.00 p.m.

Chair Person: Prof. Sujit Mondal, Dean Faculty of Science
(*Sponsored By: Systronicx, Hitachi, Indo Scientific, TKG Scientific*)
Prize and Certificate distribution
Cultural programme by DHWU Students

Concluding Speech: Convener

*Parallel Session

Poster presentation for display (PP)

Session-1	10.15 am-2 pm	PP-01 to PP-41
Session-2	2 pm -4.30 pm	PP-42 to PP-84

(NB: A parallel exhibition from different sponsors will continue throughout the day)

Poster Presenters

Poster Number	Author	Title	Institute
P-01	**Anowar Hossain**	Structural Elucidation with Theoretical Rationalization of Phthalic Acid and Aminopyrazine Ligand Based Coordination Polymers: On the Importance of N–H$\cdots\pi$ Interactions	*Department of Chemistry, Jadavpur University, Kolkata 700032, India*
P-02	**Dr. Arabinda Mandal**	Radical Scavenging Activity of thiol Drugs	*Department of Chemistry, Bidhannagar College, Kolkata 700 064, India*
P-03	**Arjun Kumar**	Studies on Complexation of Zinc by Some Chelating Organic Acids and Acidic Azo Dyes	*Department of Chemistry, B.N. Mandal University Madhepura-852113, Bihar, India.*
P-04	**Arpan Mal**	Interaction of the Heme Protein (Myoglobin) with Sodium Salts of Cholic and Deoxycholic Acids in Phosphate Buffer: A Detail Survey on Physicochemical and Molecular Docking Investigation	*Centre for Surface Science, Physical Chemistry Section, Department of Chemistry, Jadavpur University, Kolkata-700 032, W. B., India*
P-05	**Dr. Arup Mandal**	Alternative of Pt-based anticancer drugs: Ruthenium analogues	*Department of Chemistry, Rammohan College, 102/1 Raja Rammohan Sarani, Kolkata-700009*
P-06	**Bidyut Debnath**	Counterion-binding and related phenomena in sodium alginate-methanol-water ternary systems: A conductometric study	*Basirhat College, North 24 Parganas, West Bengal 743412, India*
P-07	**Dr. Biswajit Panda**	Stereospecific Synthesis of Poly(methylene-E-vinylene) by ROMP of Spiro-Cyclopropene	*Department of Chemistry, City College, 102/1 Raja Rammohan Sarani, Kolkata-700009, India,*
P-08	**Chhandasi Guha Roy Sarkar**	Frontier Molecular Orbital Compositions, Spectroscopic and Cyclic Voltammetric Studies of a Series of Rhodium and Iridium Complexes in the light of Density Functional Theory	*Department of Chemistry, Hooghly Mohsin College, Chinsurah, Hooghly, West Bengal, India*

P-09	**Debdas Sikdar**	Preparation of highly reinforced natural rubber nanocomposite of iron (III) oxide (Fe_2O_3) nanoparticles using a very small amount of epoxidized natural rubber as compatibilizer	*Department of Chemistry, University of Kalyani, Kalyani, Nadia, 741235, India*
P-10	**Eshita Kar Mandal**	Structural studies of an immunoenhancing cytotoxic heteroglycan isolated from an edible mushroom *Calocybe indica* var. APK2	*Sevayatan Sikshan Mahavidyalaya, Sevayatan-721514, Jhargram, West Bengal, India*
P-11	**Gargi Nandi**	Ab Initio Calculation of Structure, Spectroscopic Constants and Thermal Properties of an Ozone Depleting Reaction: $X + O_3 \rightarrow XO + O_2$	*Diamond Harbour Women's University, Sarisha, West Bengal, India.*
P-12	**Habibar Chowdhury**	Syntheses, molecular and crystalline architectures and luminescence behaviours of two zinc(II)pseudohalido compounds containing Schiff base ligands: Control of coordination numbers varying donor sets	*Department of Chemistry, Kabi Nazrul College, Murarai, Birbhum, West Bengal, 731219, India*
P-13	**Mehebub Ali Khan**	A reversible and selective "OFF-ON-OFF" fluorescent sensor for Zinc(II) in semi aqueous medium with biological application	*Aliah University, Kolkata ,West Bengal, India.*
P-14	**Mumu Chakrobarty**	Dimeric Carbazole Alkaloids Isolated from the Genus *Murraya* – A Review	*Government Girls' General Degree College; 7, Mayur bhanj Road, Kolkata – 700023, West Bengal, India*
P-15	**Nabanita Naskar**	Adapting environmentally benign practice for separation of radioisotopes using PEG-based Aqueous Biphasic System	*Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata-700064, India*
P-16	**Dr. Pallab Bhowmik**	Two dimeric and a helical MOFs complexes of Cu(II) from Schiff base and pseudohalides [OCN^-, SCN^- & $N(CN)_2^-$]	*Department of Chemistry, Sundarban Mahavidyalaya, Kakdwip, W.B*
P-17	**Samit Pramanik**	Investigation of electrical conductance properties of a newly synthesized copper (II) metal complex and its non-covalent interactions and TDDFT calculation	*Department of Chemistry, Jadavpur University, Jadavpur, Kolkata, West Bengal, India.*

P-18	**Sanchari Dasgupta,**	Designing of Novel Zinc(II) Schiff Base Complexes Having Acyl Hydrazone Linkage: Study of Phosphatase and Anti-Cancer Activity	*Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata 700009*
P-19	**Sandip Kumar Rajak**	A Correlation of the Drug Activities (Anti-bacterial) in the Structure of Some hetero cyclic compound containing benzimidazole and beta-lactam moiety in terms of the Density Functional Descriptors– A QSAR and QSPR Study	*Dumkal College, Basantapur, Dumkal, Murshidabad, WestBengal-742406, India*
P-20	**Saugata Konar**	Photoresponse properties and DNA binding abilities of 4-(4 pyridinyl)-2-pyridone salts	*Department of Chemistry, Bhawanipur Education Society College, Kolkata 700020, India,*
P-21	**Dr. Shefali Saha(Halder)**	A selective chemosensor for Al^{+3} detection based on Coumarinyl Schiff base	*Department of Chemistry, Kalyani Govt. Engg. College, Kalyani-741235*
P-22	**Santosh Kumar Sethi**	Studies on a Reductive Nitrosylation of Molybdenum in Its Lower Oxidation States	*Department of Chemistry, B.S.S. College, Supaul, Bihar,India*
P-23	**Soumitra Mandal**	Structural analysis of an arabinan isolated from alkaline extract of the endosperm of seeds of *Caesalpinia bonduc*	*Fakir Chand College, Diamond Harbour-743331, South 24-Parganas, W.B.*
P-24	**S. Ghosh**	Theoretical investigation of structure and spectroscopic constants of molecular systems important in semiconductor devices	*Department of Physics, Diamond Harbour Women's University, Sarisha, West Bengal, India*
P-25	**Dr. Sukesh Patra**	Preparation of Cellulose Nanofibers from the Domestic-waste by Chemical Treatment and Ultrasonication	*Midnapore College (Autonomous), Midnapore, West Bengal, India*
P-26	**Sumitava Khan**	Atmospheric Co_2 Fixation By Zinc (Ii) Complex Containing A Tetradentate Amine	*Department of Chemistry, Burdwan Raj College, Burdwan 713 104*
P-27	**Tanmay Mathur**	Synthesis of Bi-Hetrocyclic *azo* Compounds and studies their Antimicrobial activities	*Department of Chemistry, Abhedananda Mahavidyalaya, Sainthia, Birbhum, W.B.*

P-28	**Tapas Kumar Mandal**	An Expeditious Synthesis Of *Cis*-2-Aroylmethyl-4-Phenylthiochromans By Iodine-catalyzed Combination Of Thiophenol With Cinnamylideneacetophenones	*Department of Chemistry, Fakir Chand College, Diamond Harbour, West Bengal, India*
P-29	**Tripti Mandal**	Perchlorate, chloride and tetrafluoroborate salts of an organic compound with 4-(4-pyridinyl)-2-pyridone backbone: their structures, supramolecular aspects and functional properties	*Department of Chemistry, Jadavpur University, Kolkata 700032, India*
P-30	**Titiksha Das**	Unusual transformation of Coumarin fragment upon treatment with Cu (II) to afford an unprecedented complex	*University of Kalyani, Nadia, West Bengal, 741235*
P-31	**Abu Taher**	Microwave assisted “Click reaction” by polymer supported Cu(I) catalytic species	*Department of Chemistry, Burdwan Raj College* *Department of Chemistry, Bankura University*
P-32	**Arpita Chandra (nee Banerjee)**	Metal-Assisted Oxazolidine/Oxazine Ring Formation in Dinuclear Zinc(II) Complexes: Exhibition of cytotoxicity against AGS cell line	*In Vitro Carcinogenesis and Cellular Chemotherapy Chittaranjan National Cancer Institute, 37, S.P. Mukherjee Road, Kolkata-7000026*
P-33	**Tapas Ghosh**	Liquid Crystals from Shape-Persistent Porphyrin Stars with Intrinsic Free Space	*Department of Applied Sciences, Maulana Abul Kalam Azad University of Technology, Institute of Organic Chemistry, & University of Würzburg, Würzburg 97074, Germany Haringhata-741249, W.B., India*
P-34	**Indrajit Saha**	Synthesis and Spectroscopic Properties of *meso*-Alkylidenyl Carbaporphyrinoids Bearing One Exocyclic C-C Double Bond	*Department of Chemistry, Ramakrishna Mission Residential College, Narendrapur, Kolkata-700103.*
P-35	**Averi Guha**	Developments And Scopes Of Nanoelectronics	*Department of Chemistry, Surendranath Evening College*

P-36	**Dr. Kazi Sabnam Banu**	Effect of contaminants and additives on Plastic and Polymer Based Materials	*Department of Chemistry, Netaji Nagar Day College, 170/436, Netaji Subhas Chandra Bose , Netaji Nagar , Kolkata-700092,*
P-37	**Dr. Sintu Ganai**	A facile synthetic approach to benzothiadiazine-1,1-dioxides: A precursor of RSV inhibitors	*Netaji Subhas Open University, DD-26, Sector-I, Salt Lake, Kolkata- 700 064*
P-38	**Dasarath Mal**	Crystallization of five new supramolecular networks with both bipyridyl and dicyanamide ligands	*Vijaygarh jyotish Ray College, 8/2, Bijoygarh, Jadavpur, Kolkata, West Bengal 700032*
P-39	**Dr. Chaitali Biswas**	Synthesis and crystal structures of three Cu(II) Schiff base complexes having partial cubane $[Cu_3O_4]$ core	*Department of Chemistry, Sarojini Naidu College for Women, Kolkata-28, W.B.*
P-40	**Dr. Debaprasad Panda**	Thermodynamics of Solubility of Non-polar Gases in 1-Alkanol at Ordinary Temperature.	*Jogamaya Devi College, Department of Chemistry, Kolkata-700026, West Bengal, India*
P-41	**Abani Sarkar**	Trinuclear Zn(II)/Cd(II) Schiff base Complex as a Selective Chemo Sensor for Mercury(II) Involving Hg^{2+}-induced Displacement of $Zn^{II}/Cd^{II}$and Subsequent Hydrolysis of the Imine moiety	*University of Calcutta, 92, A. P. C. Road, Kolkata-700009, India.*
P-42	**Amit Adhikary**	Mapping of Solvent Mediated Molecular Self-Assembly of Fe(III) Discrete Compounds: Exploring their Magnetic Behaviour and Phosphatase Like Activity	*Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata 700009, India.*
P-43	**Dr. Amit Mandal**	Surface Functionalization of Graphene by Ionic Liquid for Fabrication of High Performance Poly(vinylidene fluoride) Nanocomposite films	*Department of Chemistry, Behala College, Kolkata – 700060,*
P-44	**Aratrika Chakraborty**	Surfactant-Mediated Solubilization of Magnetically Separable Nanocatalysts for the Oxidation of Alcohols	*Department of Chemistry, University of Calcutta, 92 A.P.C. Road, Kolkata-700009*
P-45	**Arnab Mandal**	Cooperative Influence of Pseudohalides and Ligand Backbone of Schiff-bases on Nuclearity and Stereochemistry of Cobalt(III) Complexes: Experimental and	*University of Calcutta, 92, A. P. C. Road, Kolkata-700009, India.*

		Theoretical Investigation	
P-46	**Indranil Kundu**	The coumarin–pterocarpan conjugate – a natural product Inspired hybrid molecular probe For DNA recognition	*Department of Chemistry, B.P.C. Institute of Technology, Krishnagar 741101, West Bengal, India:*
P-47	**Jayshree Sadhukhan**	A comparative study of the photophysical behaviour of the low-lying excited states of fluorophenols in the gas phase: $^1\pi\pi*$ - $^1\pi\sigma*$ energy gap effect	*School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata 700032, India* *Department of Chemistry, Government General Degree College, Singur, Hooghly, West Bengal 712409, India*
P-48	**Kalachand Mahali**	*The effect of electrolytes on the solubility of amino acids in water at 298.15.K*	*Department of Chemistry, University of Kalyani, Nadia. Pin 741235, W.B, India.*
P-49	**Dr. Lakshmi Kanta Das**	Migration of thiocyanate anions to produce “coordination position” isomers and formation of bi-component cocrystal in tri-nuclear $Ni_2^{II}Zn^{II}$ complexes with salen type di-Schiff base ligand	*Department of Chemistry, Government General Degree College, Kharagpur-II, Ambigeria, Madpur, Paschim Medinipur-721149, West Bengal, India.*
P-50	**Manindranath Bera**	Structure, Property and Application of Multimetallic Iron (III), Copper(II) and Zinc(II) Complexes	*Department of Chemistry, University of Kalyani, Kalyani, Nadia, West Bengal-741235, INDIA*
P-51	**Mrinmoy Ghosh**	Azido bridged binuclear copper (II) Schiff base compound: synthesis, structure and electrical properties	*Department of Chemistry, Acharya Prafulla Chandra College, New Barrackpore, Kolkata-700131.*
P-52	**Rumana Parveen**	Supramolecular Gels by Design: Towards the Development of Topical Gels for Self-delivery Application	*Department of Chemistry, University of Calcutta, 92, A. P. C. Road, Kolkata-700009, India*
P-53	**Sekhar Gain**	Oxidation of thiourea by metal bound superoxide; $[(NH_3)(en)_2Co^{III}(O_2)Co^{III}[(NH_3)(en)_2](ClO_4)_5$; in presence of Ellman’s Reagent in aqueous acetate buffer medium: A kinetic and mechanistic studies.	*Department of Chemistry, Ramakrishna Mission Vidyamandira, Belur Math, Howrah 711 202, India.*
P-54	**Sili Hansda**	Catalytic promiscuity of two novel cobalt	*Department of Chemistry, University of Calcutta, 92 A.*

		(II) complexes derived from redox non-innocent Schiff base ligands: unraveling the role of methyl groups in the ligand backbone on catalytic efficiency	*P. C. Road, Kolkata 700009, India*
P-55	**Somali Mukherjee**	Green Synthesis of Self Assembled Nano-Spherical Dysprosium MOFs: Selective and Efficient Detection of Picric Acid in Aqueous and Gas Phase	*Department of Chemistry, University of Calcutta, 92 A.P.C Road, Kolkata-700009, India.*
P-56	**Soumyabrata Goswami**	Field-Dependent Magnetism and Slow Magnetic Relaxation Behavior in Mn (II) And Co (II) Coordination Polymers	*Department of Chemistry, Amity University Kolkata, Rajarhat, Newtown, Kolkata-700135, India.*
P-57	**Sourav Das**	Exploring The Interaction of Stem Bromelain with Bile Salt Surfactants & Conventional Anionic Surfactants at Phosphate Buffer Medium of pH 7.0	*Centre for Surface Science, Physical Chemistry Section Department of Chemistry, Jadavpur University*
P-58	**Subhas Chandra Debnath**	Green nanocomposites: Synergistic effect of nanoclay and short jute fiber on the mechanical properties of natural rubber	*Department of Chemistry, University of Kalyani, Kalyani, Nadia, West Bengal, Pin-741235*
P-59	**Suhana Karim**	A Dinuclear Iron Complex as an Efficient Homogeneous Electrocatalyst for Water Oxidation Reaction	*Department of Chemistry, University of Calcutta, India*
P-60	**Sumana Chatterjee**	Role of coagulase negative staphylococci in colonization and subsequent degradation of plastic packaging surfaces	*Department of Chemistry, Basanti Devi College, Kolkata, West Bengal, India*
P-61	**Dr. Sunil Kumar Bhanja**	Colorimetric detection of Th4+ ion using CuO nanoparticles prepared by grafted Tricholoma mushroom polysaccharide	*Government General Degree College, Kharagpur-II, Ambigeria, Madpur, Paschim Medinipur-721149, West Bengal, India*
P-62	**Susmita Mandal**	mTORC2 promotes propagation of GBM cancer stem cells by activating Hedgehog pathway through Gli2 nuclear translocation	*Diamond Harbour Women's University, Sarisha, West Bengal-743368, India, & CSIR-Indian Institute of Chemical Biology, Kolkata-700 032, India*
P-63	**Swarup Chattopadhyay**	Dithiocarbamato complexes of dirhenium (II,II): Spectroscopic, structural, cytotoxicity and computational studies	*Department of Chemistry, University of Kalyani, Kalyani, Nadia 741235, WB, India*
P-64	**Swastik Karmakar**	Metal-mediated Strategies toward Biologically Significant Small Molecules	*Department of Chemistry, Basirhat College, Basirhat 743412, West Bengal, India*
P-65	**Tania Chowdhury**	Unveiling the binding interaction of zinc (II)	*Department of Chemistry, University of Calcutta, 92, A.*

		complexes of homologous Schiff-base ligands on the surface of BSA protein: A combined experimental and theoretical approach	*P. C. Road, Kolkata-700009, India*
P-66	**Tonmoy Chakraborty**	Macrocyclic tetranuclear ZnII complex as receptor for selective dual fluorescence sensing of F- and AcO-: effect of macrocyclic ligand	*Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata 700009, India.*
P-67	**Krishanu Sarkar**	Hydrothermal synthesis of a novel hybrid mesoporous material and its potential application in fuel cell	*Department of Chemistry, Netaji Mahavidyalaya, Arambagh, Hooghly 712601, West Bengal, India*
P-68	**Trisha Mitra**	Pd-Catalyzed 3-Amino-1-Methyl-1H-Pyridin-2-one Directed C(sp2)-H Arylation and Methylation	*University of Kalyani, Kalyani, Nadia, West Bengal- 741235, India*
P-69	**Dr. Uday Das**	Crystal Structure Analysis Of (2s*, 3ar*,4s*,7as*)-2,3,3a,4,5,7a-Hexahydro-3a,4-Bis(Methylsulfonyloxymethyl)- 2-Vinyl-1h From Laboratory X-Ray Powder Diffraction Data	*Department of Physics, Hooghly Mohsin College, Chinsurah, Hooghly*
P-70	**Ujjwal Das**	Interaction of d^{10} metal ion with potential organosulfur complexes of Platinum	*Department of Chemistry, Sarsuna College, 4/HB/A, Ho-Chi-Minh Sarani, Kolkata-700061, West Bengal, India.*
P-71	**Tapas. K. Ghosh**	Examination of the reaction pathways of IO+BrO reaction	*Department of Physics Diamond Harbour Women's University, Sarisha, WB, India*
P-72	**Aparajita Pal**	Methylglyoxal conjugated with chitosan nanoparticles as a potential anticancer agent	*Diamond Harbour Women's University, Sarisha, West Bengal, India* *Bose institute, Centenary Building, Kolkata- 700 054, India*
P-73	**Biplab Bhowmik**	A treatise on free radical in the basis of human life	*Department of Zoology, Diamond Harbour Women's University, Diamond Harbour Road, Sarisha, South 24 Pgs (S), 743368, India*
P-74	**Dinesh Chandra Ghosh**	Kinetics of alkaline hydrolysis of methyl green: Effects of surfactants	*Department of Chemistry, Jadavpur University, Kolkata 700032, India*
P-75	**Koushik Dhara**	Development of Targetable 'Turn-On' Fluorogenic Probes for Carbon Monoxide	*Department of Chemistry, Sambhu Nath College, Labpur, Birbhum 731303,*

		Imaging in Living Cells	*West Bengal, India*
P-76	**Monirul Islam**	Kinetics and Mechanism of Chromic acid Oxidation of D-Galactose in the Presence Of 1,10-Phenanthroline Catalyst in Sulfuric Acid Micellar Media	*Department of Chemistry, Seth Anandram Jaipuria College, Kolkata, 700005, India*
P-77	**Raj K. Nandi**	Bio-orthogonal Chemistry: Ethynylation of cysteine-containing peptides	*Department of Chemistry, Diamond Harbor Women's University,* *LCSO, ISIC, ,Ecole Polytechnique Federale de Lausanne (EPFL) CH-1015 Lausanne, Switzerland*
P-78	**Shantanabha Das**	Differential Regulatory T-Cell Modulation in Early Infection Models of Antimony Sensitive and Resistant *Leishmania donovani* Parasites	*Diamond Harbour Women's University, D. H. Road, Sarisha, West Bengal - 743368*
P-79	**Subrata Kumar Saha**	Fluorescence Sensor for Lysosome-Targeting Cellular Imaging of Hg^{2+} in Living Cells	*Department of Physics, Sambhu Nath College, Labpur, Birbhum 731303, West Bengal, India*
P-80	**Tanmay Chattopadhyay**	Magnetically separable Pd(0)@Fe_3O_4@AHBA nanocatalyst: C-C coupling reactions	*Department of Chemistry, Diamond Harbour Women's University,* *Diamond Harbour Road, Sarisha, South 24 Pgs (S), 743368, India*
P-81	**Uday Chand Saha**	A New Turn-On Fluorogenic Probe for Carbon Monoxide Detection in Aqueous Medium	*Department of Chemistry, Indas Mahavidyalaya, Indas, Bankura 722205, West Bengal, India*
P-82	**Sabuj Kanti Das**	A new microporous Ln-MOF: CO_2 uptake and fixation under ambient	*School of Materials Sciences, Indian Association for the Cultivation of Science, Jadavpur, West Bengal, India*
P-83	**Rajesh Bera**	Single end-on azido bridged 1D chain copper (II) complex: Synthesis, X-ray crystal structure and catalytic efficacy in homogeneous epoxidation of cyclooctene	*Department of Chemistry Dinabandhu Andrews College, Garia, Kolkata-700084*
P-84	**Soma Naskar**	Examination of the structure, spectroscopic constants and reaction kinetics of the reaction $XO + O \rightarrow X + O_2$	*Department of Physics, Diamond Harbour Women's University* *West Bengal-743368, India*

Brief CV of Prof. Isabelle CHATAIGNER

Isabelle CHATAIGNER

Professor in Organic Chemistry
University of Rouen Normandie

www.lab-cobra.fr (Heterocyclic chemistry, Cycloadditions, High pressure chemistry)
www.lct.jussieu.fr/pagesperso/chataign (Computational chemistry)

CAREER:

01/14-	Prof. in organic chemistry – University of Rouen Normandie
09/99-12/13	lecturer then associate prof. – University of Rouen – chemistry dept.
06/98-08/99	Post-doctoral fellow -Universita' degli Studi de Milan (Italie) with Prof. C. GENNARI.
09/94-06/98	PhD in organic chemistry – University of Nantes With Dr. Jean VILLIÉRAS
09/93-06/94	DEA – Institute of Natural Substances Chemistry With ICSN Prof. H.-P. HUSSON.

EDUCATION :

2009 :	Habilitation à Diriger des Recherches (HDR) : University of Rouen
1994 - 1997	Ph.D. in organic chemistry (University of Nantes)
1990 - 1993	Chemical engineer in chemistry at the ECPMS (Strasbourg - France).

RESEARCH INTERESTS:

Cycloaddition reactions
High pressure and flow chemistry in organic synthesis
Computational chemistry

SCIENTIFIC PRODUCTION:

≈ 55 publications
≈ 60 communications & conferences
3 Textbooks in Organic chemsitry

MAIN RESEARCH GRANTS:

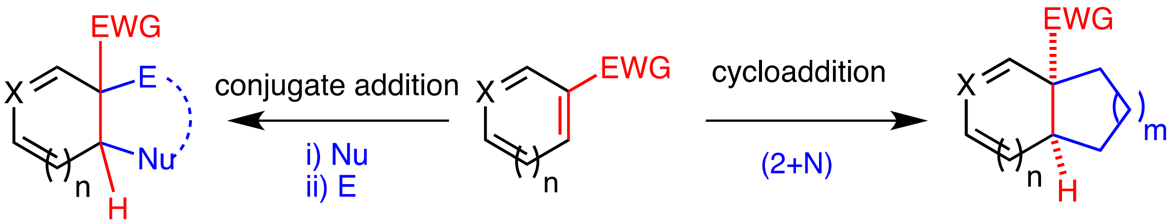
- European Grant (INTEREG V programme) – in collaboration with British universities and companies (2017-2021) Coordinator for the French side
- National Research grants (ANR) – 2017-2021 (P.I., PRC) and 2009-2013 (P.I. JCJC)
- 2 Invited Professorship positions in Japan (Tohoku University (Sendai) October 2016 (1 month), Osaka Prefecture University (Sakai) July 2018 (2 wweks))
- Director of 8 PhD students and 8 post-doctoral fellows since 1999

PL-1

Dearomatization of Electron-Poor Arenes

Batoul Rkein, Maxime Manneveau, Léo Birbaum, Muriel Durandetti, Michaël De Paolis, Julien Legros and **Isabelle Chataigner***
Normandie Univ, UNIROUEN, INSA Rouen, CNRS, COBRA, 76000 Rouen, France.
E-mail: isabelle.chataigner@univ-rouen.fr

Involving arenes in dearomatizing addition and/or cycloaddition reactions is a an attractive and convergent approach to construct complex polycycles from easily accessible substrates, however, challenging because of their intrinsic stability.
In this context, nitroarenes are interesting substrates, allowing to carry out various dearomatizing reactions when reacted with nucleophilic species, in cyclodditions or annulations for example.



Different aspects of these transformations, including (4+2) or (3+2) cycloadditions but also tandem processes such as (4+2)/(3+2) cycloadditions will be presented and commented on according to the proposed mechanisms.

(1) (a) Birbaum, L.; Gillard, L.; Gérard, H.; Oulyadi, H.; Vincent, G.; Moreau, X.; De Paolis, M.; Chataigner, I. *Chem. Eur. J.* **2019**, *25*, 13688–13693; (b) Pasturaud, K.; Rkein, B.; Sanselme, M.; Sebban, M.; Lakhdar, S.; Durandetti, M.; Legros, J.; Chataigner, I. *Chem. Commun.* **2019**, *55*, 7494 -7497; (c) Diab, S.; Noël-Duchesneau, L.; Sanselme, M.; Kondo, Y.; De Paolis, M.; Chataigner, I. *Eur. J. Org. Chem.* **2018**, 2048-2052; (d) Gérard, H.; Chataigner, I. *Chem. Eur. J.* **2017**, *23*, 13711-13717; (e) Andreini, M.; Chapellas, F.; Diab, S.; Pasturaud, K.; Piettre, S. R.; Legros, J.; Chataigner, I. *Org. Biomol. Chem.* **2016**, 14, 2833-2839; (f) Andreini, M.; De Paolis, M.; Chataigner, I. *Catal. Commun.* **2015**, *63*, 15-20; (g) Lee S.; Diab S.; Queval P.; Sebban M.; Chataigner I.; Piettre S. R. *Chem. Eur. J.* **2013**, *19*, 7181-7192; (h) Lee, S.; Chataigner, I.; Piettre, S. R. *Angew. Chem. Int. Ed.* **2011**, *50*, 472-476.

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Brief CV of Professor Ashutosh Ghosh

Professor Ashutosh Ghosh
Department of Chemistry
University of Calcutta

Educational Qualifications:

Ph.D. Indian Association for the Cultivation of Science, Kolkata, 1987
(Supervisor: Prof. N. RayChaudhuri)
M. Sc. (Chemistry), University of Calcutta, 1981
B. Sc. (Chemistry Honours), Presidency College, 1979

Post Doctoral Research/Visiting Assignments:

UNESCO Fellow: Charles University, Czechoslovakia; **MONBUSHO Fellow:** Nagoya University, Japan; **JSPS Fellow:** Tsukuba University, Japan; **Visiting Scientist:** University of Utah, USA; University of Dusseldorf, Germany.
Supervision of Ph.D. Thesis: Twenty students have been awarded Ph.D. degree

Field of Research: Synthesis, structural characterization, magnetic properties, and catalytic activities of homo- and heterometallic polynuclear complexes of 1st transition metal ions.

Award: Rheometric Scientific-ITAS Award (1995), CRSI Bronze Medal (2016), Professor Priyadaranjan Ray Memorial Award (2017)

Fellow: West Bengal Academy of Science and Technology (2013); Indian Academy of Science (2017)

Publications
277 papers published in the international journals.
h-index: 45, total citation received: ~ 6500*(Scopus)*

PL-2

Hetero-metallic complexes: Facile strategy for synthesis, diversity in structures and magnetic properties, and effectiveness in catalysis

Ashutosh Ghosh

Department of Chemistry, University College of Science, University of Calcutta, 92, A.P.C. Road,
Kolkata -700 009, India,
E-mail: ghosh_59@yahoo.com.

The symmetrical and unsymmetrical N_2O_2 donor salen type di-Schiff base complexes of Cu (II) and Ni(II) can conveniently be used as “metalloligands” as the oxygen atoms of the chelated Schiff base often coordinate to a second metal ion. Using the metalloligands, [CuL] or [NiL], we have synthesized several heterometallic complexes incorporating various metal ions along with some anionic coligands. The complexes are obtained in different shapes which have been determined mostly by the coordination modes of the anionic coligands. For example, the anionic co-ligands that bridge two adjacent metal centers invariably produce linear trinuclear complexes whereas both linear and bent structures are resulted when the anions are monodentate or noncoordinated. Interestingly, some fundamental solid state phenomena like “isomerism” (linear-bent, coordination position and supramolecular isomerism) “polymorphism”, “cocrytallization” are observed in such trinuclear complexes due to the flexibility in the coordination mode of the both metal and anionic co-ligands. Most of these heterometallic compounds satisfy non-zero spin ground state hence show ferrimagnetic exchange interactions. The coupling usually occurs through diphenoxido bridge between the metal centres. However, the anionic coligand can also take part in bridging to modulate the bridging angles and hence the coupling constant. By judiciously changing the counter anions, we varied bridging Cu-O-Mn and Ni-O-Mn angles in a wide range in search of ferro to antiferromagnetic crossover angles and succeeded to find experimentally this crossover angle in case of Ni-O-Mn bridge. We have also been able to use these hetero-metallic clusters as nodes to produce metal organic frameworks with the help of spacers 4,4’-bipy or dicarboxylates. Moreover, some of these compounds, consisting of $Cu^{II}_2Dy^{III}$, Cu_2Tb^{III} etc are found to behave like Single Molecule Magnets and the shapes of the molecule are found to have considerable effect on the SMM behaviours. The catalytic oxidase activities e.g. catechol oxidase and phenoxazinone synthase like activities of some of these heterometallic complexes are found to be very high presumably due to heterometallic cooperative effect.

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Brief CV of Prof. Blanca M. Martin Vaca.

Professor Blanca Martin Vaca. After a Maser degree in Inorganic Chemistry and a PhD in Organometallic Chemistry at the University of Oviedo (Spain). She completed then a post-doctorate and an assistant professor period at the University Pierre et Marie Curie (Paris 6, France), where she specialized in the application of Organometallic compounds to organic synthesis. She was recruited at the Paul Sabatier University as associate professor in 1998 and was promoted Full Professor in 2008. She is interested in organometallic derivatives by addressing their catalytic applications, in particular by exploring the cooperative effects that exacerbate their catalytic activity (Metal-ligand cooperation and dual catalysis). She is also interested in the preparation and applications of biodegradable polymers such as polyesters and polycarbonates, where she investigates organocatalyzed ring-opening polymerization of lactones and cyclic carboantes. She is involved in teaching chemistry at all levels of education (Bachelor and Master Degrees)

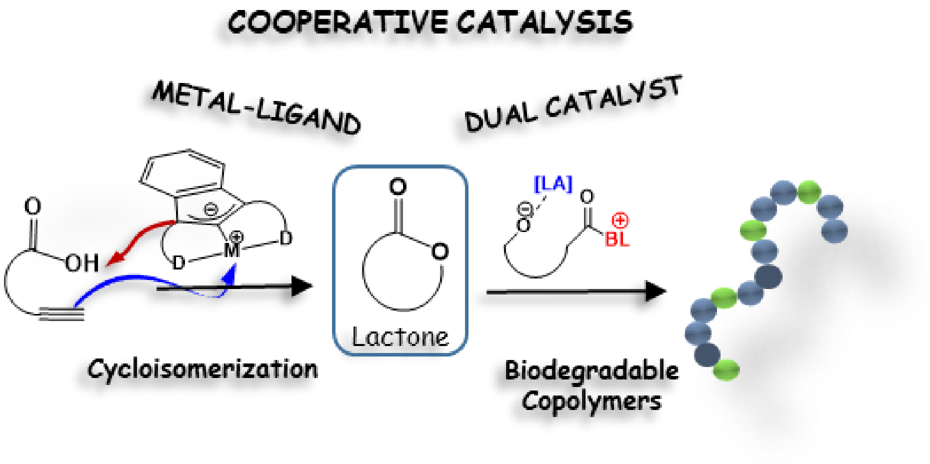
TL-1

Cooperative effects in catalysis: from metal-ligand cooperation in cycloisomerization reactions to organic catalysis in ring-opening polymerization

Professor Blanca Martin Vaca.

Paul Sabatier University, France
Email: bmv@chimie.ups-tlse.fr

Cooperative effects in catalysis are attracting more and more attention in order to improve catalysts performances. Over the past two decades, spectacular progress has been achieved in organometallic catalysis in the field of Metal/Ligand cooperative catalysis using pincer complexes. At the same time, organic and main group catalysis has allowed strong development of ring-opening polymerization reactions for the preparation of biodegradable polyesters. This conference will deal with both aspects.



Brief CV of Prof. Jacques Maddaluno

Prof. Jacques Maddaluno received an Engineer Degree in Chemistry from the Ecole Nationale Supérieure de Chimie de Paris (France) in 1983 and his Ph.D. degree from the University Pierre et Marie Curie in Paris (France) in 1986 under the guidance of Prof. J. d’Angelo. After spending two years as a postdoctoral fellow with Professors J. D. Barchas and Kym F. Faull at Stanford University (USA), he was appointed as CNRS Research Associate (Chargé de Recherches) in 1988 to do research in a joint laboratory with the University of Rouen (France). He was promoted to a CNRS Research Director position in 2000, still in Rouen. He received the French Chemical Society – Organic Chemistry Division award in 2012 and was nominated Distinguished Fellow in 2017. Between 2011 and 2017 he served as a Deputy Director of the CNRS Chemistry Department in Paris before being appointed as Director of this same department in June 2017. His current research interests include the development of new enantioselective reactions with carbanions as well as carbometallation reactions.

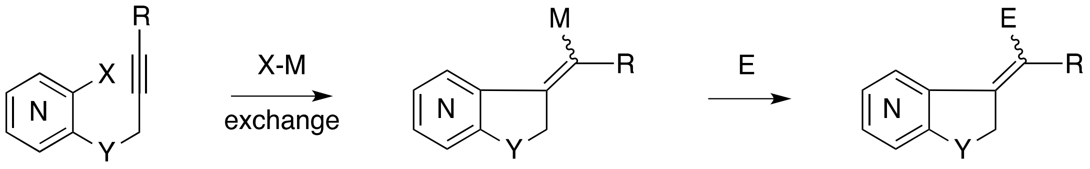
TL-2

Intramolecular carbometallation of alkynes : an overview

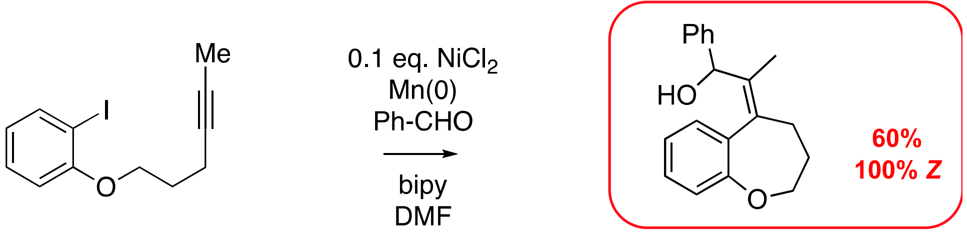
Jacques Maddaluno, PhD

UMR 6014 « COBRA »
CNRS, Université de Rouen & INSA de Rouen
76821 Mont St Aignan (France)
Email: jmaddalu@crihan.fr

The intramolecular carbometallation of alkynes is a cyclization reaction that can be easily implemented and provides a simple access to vinylmetals. These can be trapped by electrophiles and lead in turn to (binuclear) heterocycles bearing an exocyclic vinylidene pattern. In many cases, this latter function can be used before the double-bond isomerizes (and leads to the aromatization of the structure).



The cases of the carbolithiation and carbonickelation will be detailed. This methodology is relatively general and leads, in a single step, to functionalized systems of which access can be sometimes tricky, such as tetrahydrobenzoxepins.



Our results show that the terminal group R carried by the alkyne exerts a strong influence on the cyclization process. Experimental data and a theoretical DFT analysis of the mechanisms of this cascade reaction will be shown to shine light on the origin of these effects. We will also present some preliminary data on a related sila-palladation of alkynes.

Recent bibliography:
Lhermet, R.; Ahmad, M.; Hauduc, C.; Fressigné, C.; Durandetti, M.; Maddaluno, J. *Chem. Eur. J.* **2015**, *21*, 8105-8111. Rebih, F.; Andreini, M.; Moncomble, A.; Harrison-Marchand, A.; Maddaluno, J.; Durandetti, M. *Chem. Eur. J.* **2016**, *22*, 3758–3763. Ahmad, M.; Gaumont, A-C.; Durandetti, M.; Maddaluno, J. *Angew. Chem. Int. Ed.* **2017**, *56*, 2464–2468. Noël-Duchesneau, L.; Maddaluno, J.; Durandetti, M. *ChemCatChem* **2019**, 4154–4160.

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Brief CV of Prof. Prasanta Kumar Mukherjee

Prof. Prasanta Kumar Mukherjee
Ph D: 1972 CU and SINP
Specialisation: Atomic and Molecular Physics
Post Doc. SINP, AVH-Germany, JSPS-Japan
Retired from IACS Kolkata as Sr. Prof. Department of Optics
Current Affiliation: RKMVU & APC College
Fellowships: Alexander von Humboldt & JSPS
Visiting Scientist: Japan, Germany, Poland, Canada & Brazil
Number of Publication: 156

TL-3

Spectral properties of inert gas atoms under a fullerene cage

Prof. P. K. Mukherjee

Ramakrishna Mission Vivekananda Educational and Research Indstitute
Belur Math, Howrah
and
Physics Department
Acharya Prafulla Chandra College
New Barrackpore, Kolkata
Email: profpkmukherjee@gmail.com

Time dependent Coupled Hartree Fock theory and relativistic Coupled Cluster formalism have been applied to find low lying excited state properties of inert gas atoms He and Ne centrally confined under a fullerene cage. The structural properties like the total energy, ionization potential, static and dynamic polarizabilities, oscillator strengths and transition probabilities have been estimated for the first few dipole allowed excited states of dressed He and Ne. Calculations have been performed using the modified atomic potential due to the fullerene cage based on experimental findings. Neutral as well as charged fullerene cage were adopted. Interesting changes in the atomic structural properties have been observed. Coupled cluster method incorporates appreciable electron correlation effects on the structural properties which have been clearly noted.

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Brief CV of Professor Debasis Das

DR. DEBASIS DAS
Professor in Chemistry,
Department of Chemistry,
University Of Calcutta
92, A. P. C. Road, Kolkata-700 009, India.
E-mail: dasdebasis2001@yahoo.com
Mobile No.: 9830345023

Academic Records

B.Sc. & M. Sc. (Chemistry)	University of Calcutta (Presidency College); **Specialization**: *Inorganic Chemistry.*
Ph. D. (Science)	The Indian Association for the Cultivation of Science, Kolkata, Jadavpur University; **Advisor: Professor Nirmalendu Ray Chaudhuri**
Postdoctoral Research	National Tsing Hua University **Advisor: Professor C. P. Cheng.**

Professional Experience

July, 1999 – March, 2001	**Lecturer in Chemistry**, *Bangabasi Morning College*
April 2001– Nov., 2005	**Senior Lecturer in Inorganic Chemistry**, *Visva-Bharati*
Dec., 2005 – Nov. 2008	**Reader in Chemistry**; *University of Calcutta*
Dec. 2008 – Nov. 2011	**Associate Professor in Chemistry,** *University of Calcutta*
Dec. 2011- Till date	**Professor in Chemistry,** *University of Calcutta*
Nov. 2019 –Till date	**Registrar,** *University of Calcutta*

Activity as Ph.D. supervisor

Number of Scholars Obtained Ph. D.(Sc.) degree	**17**
Number of Research Scholars working at present	**8**
No. of Post-doctoral Fellow working at present	**3** (2 DSK PDF and 1 CSIR RA)

Publications

Total Number of Publications: **120**	Citation: **1885**
h-index: 23	**i-10 index: 67**

Awards

1. Recipient of **CRSI Bronze Medal (2019)** by The Chemical Research Society of India.
2. Honorary Reviewer of ACS, RSC, Wiley and Science Direct journals.

TL-4

Nanoscale Coordination Polymers: Green Synthesis to Real Life Implementations

Prof. Debasis Das
Department of Chemistry, University of Calcutta, 92, A. P. C. Road, Kolkata-700 009
Email: dasdebasis2001@yahoo.com

MOFs gain tremendous impetus due to it's enhanced applicability in various fields. However the major inconveniences associated with this, is it's low solubility in commonly known organic solvents. This restricts their usability in a number of desirable applications. Recent literatures suggest different techniques like solvothermal, nano-precipitation, surfactant mediated synthesis to prepare nano MOFs. Most of these are complicated and non eco-friendly. Therefore, a massive need still persist to design and fabricate eco friendly, reusable functionalized nano-MOFs to get enhanced applications.

To this end currently we are trying to develop eccentric green approaches to prepare nanoscale MOFs (NMOFs). We further have explored the utility of these NMOFs towards sticking environmental and biological issues like explosive detection, pollution control, drug therapy etc. Our produced Zn(II) based coordination Polymers show anti proliferative activity towards human colorectal carcinoma cell line.[1] We have designed novel Dy based NMOFs decorated with azide functionalities for selective and prompt detection of nitro explosive both in aqueous and vapour phase.[2] The applicability of luminescent NMOFs towards detection and sequestration of oxoanionic pollutants, degradation of industrial dyes have also been studied.[3] In this presentation some of our aforementioned research output will be presented and discussed.

*Reference***:**

1. Mukherjee, S.; Ganguly, S.; Manna K.; Mondal, S.; Mahapatra, S.; Das, D. *Inorg. Chem*. **2018**, *57*, 4050-4060.
2. Mukherjee, S.; Ganguly, S.; Chakraborty, A.; Mandal, R.; Das, D. Green Synthesis of Self Assembled Nanospherical Dysprosium MOFs: Selective and Efficient Detection of Picric Acid in Aqueous and Gas Phase. *ACS Sustainable Chem. Eng.* **2019**, *7*, 819−830.
3. Mandal, A.; Ganguly, S.; Mukherjee, S.; Das, D. *Dalton Trans.* **2019**, *48*, 13869-13879.

Brief CV of Prof. Kumaresh Ghosh

Prof. Kumaresh Ghosh

Professor of Chemistry, University of Kalyani

M.Sc in 1994, Indian Institute of Technology-Kharagpur, India

Ph.D (Under supervision of Prof. Shyamaprosad Goswami): 1999, Indian Institute of Technology-Kharagpur, India

Awards/recognition

- Chemical Research Society of India Bronze Medal award for the year 2018
- Appeared in the journal for CRSI Bronze Medal 2018; Angew. Chem. Int. Ed. 2018, 57, 2029-2030
- Elected as Fellow of West Bengal academy of Science and Technology in 2017.
- Dr. Basudev Banerjee Memorial award, 2007 (Given by Indian Chemical Society)
- Prof. D. K. Banerjee memorial Award, 2011 (Indian Institute of Science, Bangalore)
- Appeared in NJC Blog for publication in New Journal of Chemistry, 2011, 35, 1397.
- Award certificate form University of Kalyani for academic potentiality and excellence, 2014

Total Number of Publications:150

Editorial Board Member: Austin Journal of Organic and Bioorganic Chemistry
Mini reviews in Organic Chemistry

TL-5

Design-based molecular architectures in aggregation, ion sensing and dye removal

Prof. Kumaresh Ghosh

Department of Chemistry, University of Kalyani, Kalyani-741235, India.

Email: ghosh_k2003@yahoo.co.in; kumareshchem18@klyuniv.ac.in

Molecular architectures constructed based on a supramolecular approach are of increasing attention as new organic functional materials featuring aggregation, ion sensing and toxic removal. Thus synthesis of new molecular architectures, capable of forming dimensionally controlled aggregation in solution to form supramolecular gels *via* non-covalent interactions (hydrogen bonds, π-π stacking, electrostatic and van der Waals interactions, metal coordination etc.) draw attention in the area of supramolecular chemistry. In designing such architectures, choice of functional entities and their proper use in the scaffolds play essential role in establishing the non-covalent interactions leading to self organization. Understanding the complex interplay between molecular structure and supramolecular interactions that underpin the self-assembly into organogels is challenging. Over the past decade, such molecular architectures or gelators with various applications in biomedicine, drug delivery, sensing, reaction catalysis, tissue engineering, water purification, photophysics etc. have been of considerable importance as well-recognized class of "smart" materials.[1]

Importantly, the dynamic and reversible nature of non-covalent forces that encourage gelation can be controlled and even altered by some external stimulli like heat, light, redox, pH, ions etc., which induce gel-to-sol inter-conversion (or *vice versa*). Such gel-to-sol or sol-to-gel phase transition in the presence of chemical analyte is considered to be beneficial in developing molecular sensors, especially for detection of biologically relevant ionic species. In addition, the gelators with functional diversity are unique in heavy metal adsorption and water treatment for picric acid and dye removal. Our endeavour along this direction will be focused.[2]

References:

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P-01

Structural Elucidation with Theoretical Rationalization of Phthalic Acid and Aminopyrazine Ligand Based Coordination Polymers: On the Importance of N–H···π Interactions

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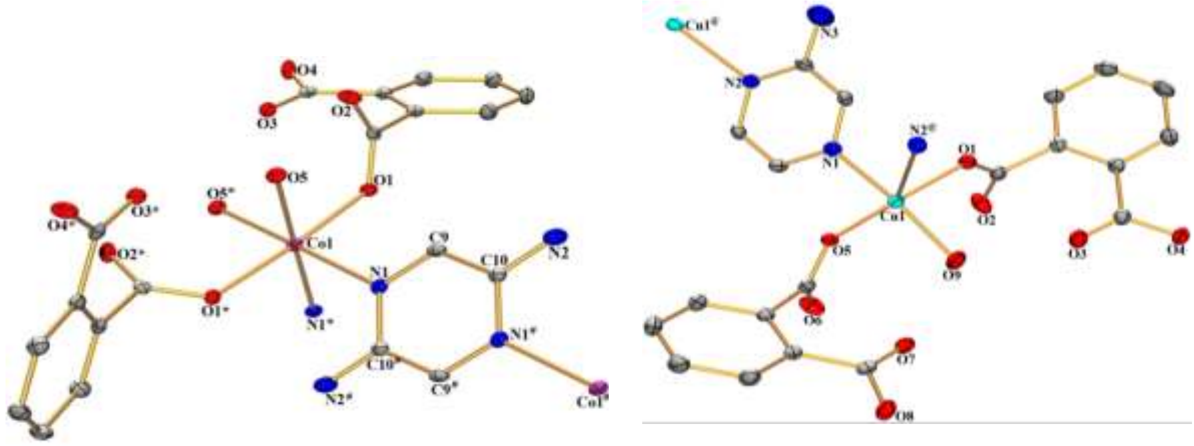
Two new coordination polymers, $\{Co(HL_1)_2(\mu\text{-}L_2)(H_2O)_2\}n$ (**1**) and $\{[Cu(HL_1)_2(\mu\text{-}L_2)H_2O]\cdot H_2O\}n$ (**2**) (H_2L_1 = Phthalic acid and L_2 = 2-aminopyrazine), have been synthesized by slow evaporation of solvent and characterized by IR spectroscopic, elemental, single-crystal X-ray diffraction and thermal analysis. X-ray results indicate that in both the polymers, phthalate acts as a monodentate ligand and the aminopyrazine ligand is responsible for the formation of the infinite one-dimensional chain structure. The solid-state structures are stabilized through hydrogen bonds and N–H···π interactions by generating two-dimensional layered structures. Finally, the non-covalent interactions have been studied energetically and using Bader's theory of atoms in molecules by means of Density Functional Theory (DFT) calculations.



(1) **(2)**

Figure 1. Central atom environments (ORTEP view) and atom numbering schemes of the title polymers **1** and **2**

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P-02

Radical Scavenging Activity of thiol Drugs

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In acid-media ($[H^+] = 0.01–0.06$ M), two of the marcaptan compounds, D-penicillamine (PEN, L_PH_2) and captopril (CAP, L_CH_2) exist in several proton-dependent forms which can reduce the superoxo complex, $[(en)(dien)Co^{III}(O_2)Co^{III}(en)(dien)]^{5+}$ (**1**) to the corresponding peroxo $[(en)(dien)Co^{III}(O_2)Co^{III}(en)(dien)]^{4+}$ (**2**) complex. The observed first-order rate constants, $k_{o,P}$ and $k_{o,C}$ for PEN and CAP increase with the increase in $[T_{PEN}]$ and $[T_{CAP}]$ (which are the analytical concentrations of the respective compounds) but decrease with increase in the media-acidity ($[H^+]$) and the media ionic strength (I). The protolytic equilibria in aqueous solution allow several potentially reducing forms to coexist for both PEN ($L_PH_3^+$, L_PH_2, L_PH^- and L_P^{2-}) and CAP (L_CH_2, L_CH^-, L_C^{2-}) but the kinetic analyses reveal that the order of reactivity for the species are $L_PH_3^+ \sim L_PH_2 <<< L_PH^-$ and $L_CH_2 < L_CH^- <<< L_C^{2-}$ respectively. The predominance and higher reactivities of the anionic species, L_PH^- and L_C^{2-} are supported by the negative slopes of the plots of $k_{o,P}$ or $k_{o,C}$ *vs.* I. Moreover, a large value of k_H/k_D for PEN suggests an inner-sphere electroprotic reaction pathway while the absence of such effect for CAP strongly supports an outer-sphere electron transfer reaction.

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P-03

Studies on Complexation of Zinc by Some Chelating Organic Acids and Acidic Azo Dyes

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Zinc is a biologically as well as industrially important metal. It is essential for plants as well as animals. Zinc is an essential component of a number of enzyme systems. Excessive quantities of zinc, however, are toxic for both plants and animals. Azo dyes are used in dyeing textile fibres. They are cost effective and have good fixative properties. Azo dyes also find application in complexometric titrations, as corrosion inhibitors; they also possess good pharmacological activity. However, azo dyes have also been found to be toxic to fauna and flora, when released into the environment through untreated effluents of dye and textile industries. They are resistant to natural degradation and have toxic potential such as genotoxic, mutagenic and carcinogenic effects. Coordination chemistry of zinc involving azo dyes as ligands, would be of academic as well as applied interest. As such, we have presently studied the complexation of zinc (II) by some chelating organic acids and some acidic azo dyes.

Complexes of Zinc(II) involving some chelating organic acids viz., salicylaldehyde, salicylic acid, anthranilic acid or 8-hydroxyquinoline and some acidic azo dyes viz., 5-(phenylazo)salicylic acid or 5-(phenylazo)-8-hydroxyquinoline, have been synthesised and characterised. Analytical results suggest the complexes to be of general formula, $[Zn\ L.L']$, where, L = deprotonated chelating organic acid and L' = unideprotonated acidic azo dye. Molar conductance values indicate the compounds to be non-electrolytic in nature. Infrared spectra of the compounds suggest that the -N=N- of the azo dyes did not coordinate to the metal. This may probably due to non-availability of a donor group at ortho position to the azo group, for chelation. Infrared spectra further evidenced the bonding of 5- (phenylazo)salicylic acid to the metal by deprotonation of COOH and coordination of OH group. 5-(phenylazo)-8-hydroxyquinoline was evidenced to bind to the metal by the deprotonation of OH and coordination of ring-N. The chelating organic acid ligands too have been evidenced to bind to the metal by deprotonation of COOH/OH and coordination of suitably oriented donor groups to form the chelate rings. ^{1}H NMR spectra of the compounds also suggested the above mode of bonding of the ligands to the metal.

P-04

Interaction of the Heme Protein (Myoglobin) with Sodium Salts of Cholic and Deoxycholic Acids in Phosphate Buffer: A Detail Survey on Physicochemical and Molecular Docking Investigation.

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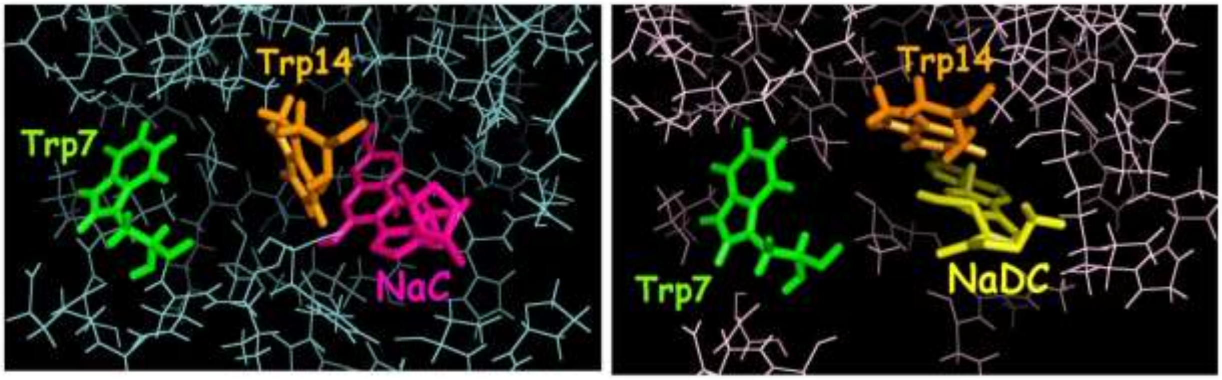
Previous investigation on protein-surfactant interaction has shown that cationic, anionic, nonionic, and gemini surfactants can nicely interact with myoglobin (Mb). The present study investigated the interaction of one heme protein myoglobin (Mb) with water soluble anionic surfactants like sodium cholate ((NaC) and sodium deoxycholate (NaDC) which acts also as bile salts. The interaction of NaC and NaDC with one heme protein myoglobin (Mb), has been probed by employing various physicochemical and spectroscopic techniques like tensiometry, UV–vis spectroscopy, fluorometry, time resolved fluorometry, circular dichroism(CD) spectroscopy, and microcalorimetry at physiological pH of 7.4 and 298 K. Tensiometric profile of NaC and NaDC show different nature in presence and absence of myoglobin. All the three break points in presence of heme protein supported from tensiometry, UV–vis spectroscopy, fluorometry, time resolved fluorometry, and microcalorimetry. The micelle of surfactants may be altered the conformational change of protein structure causing denaturation of the protein, and finally free micelles are formed on further addition of surfactant. Binding between surfactants with the tryptophan moieties present in the heme proteins described by the help of fluorescence life time measurement. The thermodynamic properties of each successively interaction process has been study from isothermal titration calorimetry (ITC). The interactive scenario between protein (Mb) with surfactants (NaC or NaDC) has been shown by the light of molecular docking analysis. In this report, the whole study describes a total survey of two anionic surfactants (biles salts) with heme protein interaction at pH=7.4 (Phosphate buffer) by employing various techniques.



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P-05

Alternative of Pt-based anticancer drugs: Ruthenium analogues

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The widespread use of platinum agents in the treatment of cancer began with the discovery of the antineoplastic activity of cisplatin by Barnett Rosenberg in the 1960s. But when cisplatin, the first discovered anticancer drug, failed to reach its maximum expectation then researchers were eager to find new analogues so that it can cover all the deficiencies shown by cisplatin. In this abstract, the target is to show how Ru-analogues had been introduced as alternatives.

Ruthenium complexes are very promising, especially from the viewpoint of overcoming cisplatin resistance with a low general toxicity. Ruthenium has found its way into the clinic, where its properties are exploited for very miscellaneous uses. The radio physical properties of Ru can be applied to radio diagnostic imaging. [1, 2] Ruthenium (II) and ruthenium (III) complexes have similar ligand-exchange kinetics to those of platinum (II) complexes. This property makes them the first choice in the search for compounds that display similar biological effects to platinum (II) drugs. [3, 4] The range of accessible oxidation states of ruthenium under physiological conditions makes this metal unique amongst the platinum group. One more property of ruthenium that makes it very appreciated in medicinal chemistry is its tendency to selectively bind biomolecules, which partly accounts for the low toxicity of ruthenium drugs.[3, 4] The ability of some ruthenium drugs to bind to transferrin has been proven.[5-9] Since rapidly dividing cells, such as microbially infected or cancer cells have a greater requirement of iron, they increase the number of transferrin receptors on their surfaces. This implies that the amount of ruthenium taken up by these infected or cancerous cells is greater than the amount taken up by healthy cells. This selectivity of the drug towards the diseased cells accounts for a reduction on its general toxicity.

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P-06

Counterion-binding and related phenomena in sodium alginate-methanol-water ternary systems: A conductometric study

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Counterion-binding and related phenomena of a naturally-occurring anionic polyelectrolyte sodium alginate in methanol-water mixed solvent systems have been explored using electrical conductivity as the probe. In particular, the variations of the counterion-binding behavior as a function of polyelectrolyte concentration and temperature were investigated. In order to understand the nature of polyion-counterion interactions, the conductivity vs. concentration data have been analyzed on the basis of scaling theory of polyelectrolyte solutions developed by Dobrynin *et al*. The fractions of free counterions in this system are found to be independent of polyelectrolyte concentration and temperature. The results indicate that the intra-chain charge-repulsion stretches the polyions to the maximum extent over the concentration range studied. The polyion equivalent conductivities are found to decrease with the increase in polyelectrolyte concentration manifesting an increase in polyion-counterion interaction with increasing polyelectrolyte concentration. Calculated polyion transport numbers indicate that the counterions get associated with the polyions and travel with them towards the positive electrode. The results further demonstrate that the monomer units experience more frictional resistance in solutions with higher methanol content, lower temperature and higher polyelectrolyte concentrations.

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P-07

Stereospecific Synthesis of Poly(methylene-E-vinylene) by ROMP of Spiro-Cyclopropene

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In addition to catalyzing the ring opening metathesis polymerization (ROMP) of cyclopropene derivatives, a first-generation Grubbs catalyst has been shown to differentiate E- and Z-double bonds in intermediates by distinct reaction patterns resulting in stereospecific poly(methylene-E-vinylene) synthesis. The intermediate with the Z double bond formed during the ROMP of cyclopropene is sensed by the catalyst, chopped by the catalyst and eliminated as the cyclohexadiene derivative, and a ruthenium−carbene species is regenerated for continued polymerization in the meantime. When a second-generation Grubbs catalyst is used, a cyclic polymer with all double bonds in the trans configuration is obtained as the sole polymeric product, in addition to the same cyclohexadiene derivative as described above. In the latter reaction, the degree of polymerization is independent of the loading of the catalyst. The formation of cyclic polymer is not common and the mechanistic pathway thereof remains unclear. One possibility would be a change in conformation of the alkenyl substituents on azetidine rings that would result in alteration of the folding nature of the polymer, leading to a cyclic polymer via ring closure metathesis.

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P-08

Frontier Molecular Orbital Compositions, Spectroscopic and Cyclic Voltammetric Studies of a Series of Rhodium and Iridium Complexes in the light of Density Functional Theory

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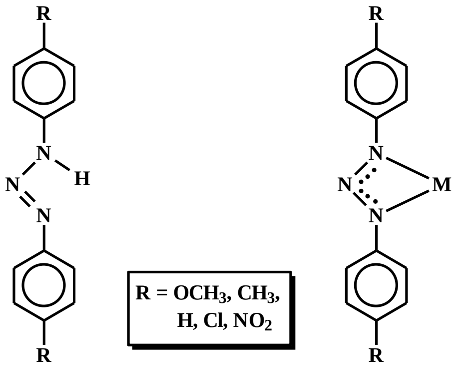
The chemistry of rhodium and iridium complexes has received continuous and sustained interest in the research arena for their interesting catalytic and biological properties.[1] The coordination environment around the central metal often influences these properties of the complexes. So, in this regard, choice of the ligand system is very important. Herein we have selected a group of 1,3-diaryltriazenes as the principal ligand. These ligands usually binds to a metal center (Figure 1), via dissociation of the acidic N-H proton (**1**), as monoanionic bidentate N,N-donor forming a four membered chelate ring (**2**).[2]



1 **2**

Figure 1

In the present work, chemistry of rhodium and iridium complexes with 1,3-diaryltriazene is reported with special emphasis on structure, spectroscopic and cyclic voltammetric properties of the complexes. The structures of the complexes are established with the help of X-ray crystallography. The frontier molecular orbital compositions and electron density of the complexes are obtained with the help of Density Functional Theory calculations using the Gaussian 03. The electronic spectral and cyclic voltammetric properties of the complexes are explained with the help of frontier molecular orbital compositions obtained by DFT calculations.

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P-09

Preparation of highly reinforced natural rubber nanocomposite of iron (III) oxide (Fe_2O_3) nanoparticles using a very small amount of epoxidized natural rubber as compatibilizer

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This research work reveals the preparation of iron oxide (Fe_2O_3) nanoparticles (IONs) by green sol-gel technique and its application in natural rubber (NR) nanocomposite as reinforcing filler. Epoxidized natural rubber (ENR) was used as a compatibilizer. The synergistic effect of 1 phr (parts per hundred parts of rubber) of IONs and 3phr of ENR can outstandingly increase the tensile strength by 40.83% and improve others mechanical properties of NR composite. The modulus at 100% & 300% elongation, elongation at break (%), the crosslink-density, cure rate index (CRI) and thermal aging were also considerably increased. The formation of ION was confirmed by FTIR, XRD and FESEM and the morphology of the naturally deep brown colored Fe_2O_3/NR/ENR nanocomposite was studied by scanning electron microscopy (SEM) which confirms the uniform distribution of IONs throughout composite matrix and the thermal stability was studied by thermogravimetric analysis (TGA).

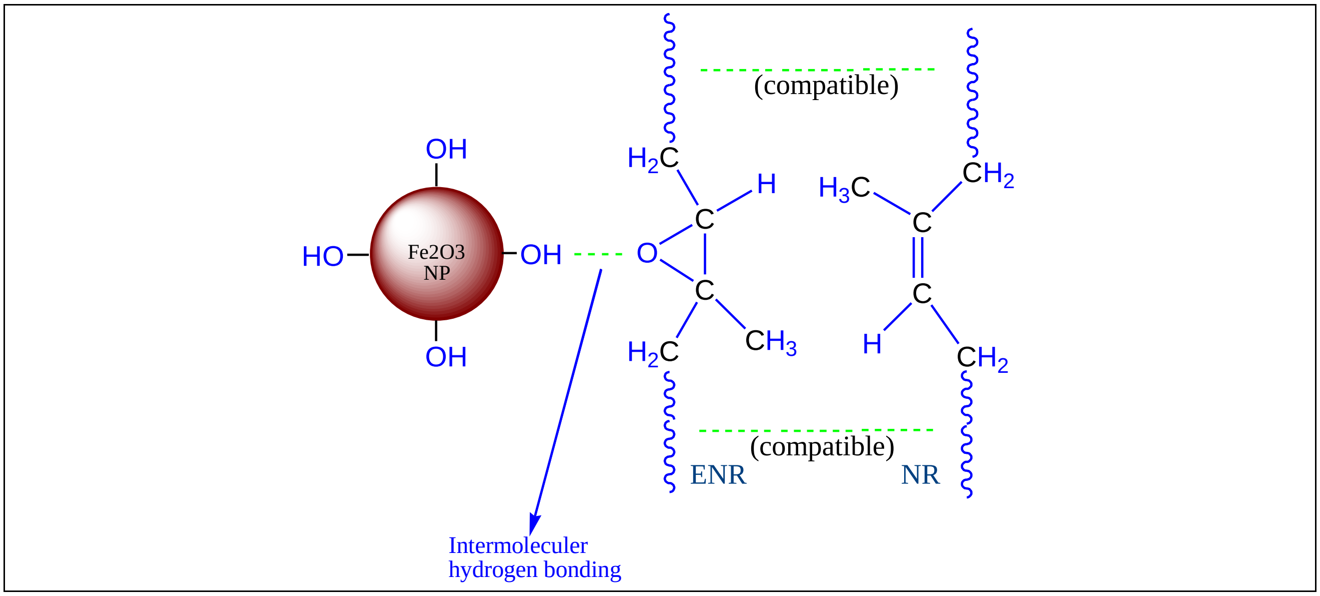

Figure: A probable representation of IONs-ENR-NR interactions in Fe_2O_3-NR/ENR nanocomposite

P-10

Structural studies of an immunoenhancing cytotoxic heteroglycan isolated from an edible mushroom *Calocybe indica* var. APK2

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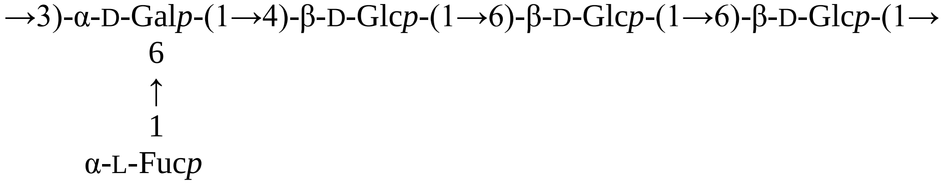
A water-soluble polysaccharide of an edible mushroom *Calocybe indica* var. APK2 showed immunoenhancing (macrophage, splenocyte, thymocyte, bone marrow activation) and cytotoxic activity towards HeLa cell lines and found to consist of D-glucose, D-galactose, and L-fucose in a molar ratio of nearly 3:1:1. On the basis of acid hydrolysis, methylation analysis, and NMR studies (^{1}H, ^{13}C, DEPT-135, TOCSY, DQF-COSY, NOESY, ROESY, HMQC, and HMBC), the structure of the repeating unit of the fuco-galacto-glucan was established as:



$$\begin{array}{ll}\rightarrow 3)\text{-}\alpha\text{-D-Gal}p & \text{-}(1\rightarrow 4)\text{-}\beta\text{-D-Glc}p\text{-}(1\rightarrow 6)\text{-}\beta\text{-D-Glc}p\text{-}(1\rightarrow 6)\text{-}\beta\text{-D-Glc}p\text{-}(1\rightarrow \\ \qquad\quad 6 & \\ \qquad\quad \uparrow & \\ \qquad\quad 1 & \\ \quad \alpha\text{-L-Fuc}p & \end{array}$$

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P-11

Ab Initio Calculation of Structure, Spectroscopic Constants and Thermal Properties of an Ozone Depleting Reaction: $X + O_3 \rightarrow XO + O_2$

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Recently, there is a scientific and public interest grown up about the climatic change and there by the environmental threat on the earth. The key factors responsible for the climate change and so the global warming is the excessive emission of Carbon Dioxide (CO_2), Chloroflurocarbons (CFCs), halogenated compounds, etc. The depletion of ozone layer in atmosphere occurs via the chain reaction:

$$X + O_3 \rightarrow XO + O_2$$
$$XO + YO \rightarrow X + Y + O_2 \text{ (X, Y= Cl, Br, I).}$$

The above mechanism of ozone destruction has been supported by the detection of XO complex in the stratosphere. Presently ab initio calculations have been done to investigate various minimum energy geometries and transition state geometries of the ozone depleting reaction $X + O_3 \rightarrow XO + O_2$ (X = Cl, Br, I) using an extensive correlation consistent basis set. Geometries and frequencies have been identified at the MP2 level of theory. The energetics has been studied at the Configuration Interaction level of theory. Several spectroscopic properties are calculated and are compared with the available experimental data. IRC calculations are going onq to find the reaction pathway.

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P-12

Syntheses, molecular and crystalline architectures and luminescence behaviours of two zinc(II)pseudohalido compounds containing Schiff base ligands: Control of coordination numbers varying donor sets

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Construction[1] of self-assembled coordination molecules and supramolecules of different nuclearities formed through strong metal-ligand covalent bonds[2] and weak non-covalent forces[3] has been the cynosure for isolation of different advanced functional materials.[4] One hexacoordinate zinc(II)azido complex $[Zn(L^1)_2(N_3)_2]$ (**1**) (L^1 = bidentate Schiff base) and one pentacoordinate zinc(II)thiocyanato complex $[Zn(L^2)(NCS)_2]$ (**2**) (L^2 = tridentate Schiff base) are isolated using one-pot synthesis of the building components. X-ray structural analyses reveal that zinc(II) center in **1** adopts a distorted octahedral coordination environment with a ZnN_6 chromophore ligated by four N atoms of two didentate Schiff base (L^1) and two N atoms of two terminal azide ions mutually in *cis* orientation (Fig.1), whereas metal(II) center in **2** adopts a distorted square pyramidal geometry with a ZnN_5 chromophore through coordination of three N atoms of one tridentate Schiff base (L^2) and two N atoms of two terminal thiocyanate ions (Fig.2).

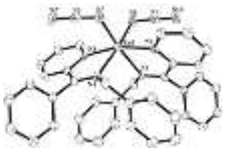

Fig.1

Fig.2

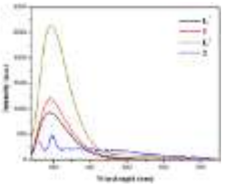

Fig.3

In the crystalline state, mononuclear units of **1** are engaged in weak cooperative intermolecular C-H…N hydrogen bonds and C-H$\cdots\pi$ interactions to form a 2D sheet structure along crystallographic *ab*-plane. In **2**, mononuclear units form non-ending linear 1D chains, which are stabilized through weak intermolecular C-H…S hydrogen bonds promoting to 2D sheet structure. Compounds **1** and **2** display intraligand π-π* fluorescence in DMF solution at room temperature (Fig.3).

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P-13

A reversible and selective “OFF-ON-OFF” fluorescent sensor for Zinc(II) in semi aqueous medium with biological application

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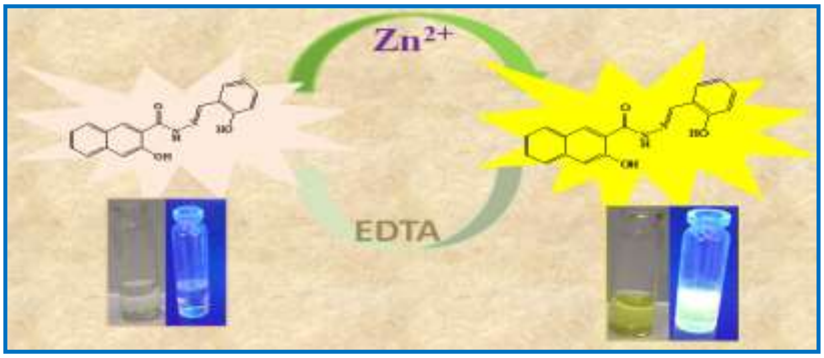
A simple Schiff base fluorescent sensor (**1**) was synthesized from the reaction of 3-Hydroxy-naphthalene-2-carboxylic acid hydrazide and 2-Hydroxy-benzaldehyde, and developed for selective detection of Zn^{2+} [1,2]. This

non-fluorescent sensor displayed obvious fluorescence enhancement after binding to Zn^{2+} ions with high sensitivity and selectivity, accompanied by obvious fluorescence emission enhancement (510 nm for Zn^{2+}). The detection limits were found to be and 1.24 $\times 10^{-7}$ M for Zn^{2+}. The binding mechanisms between **1** and Zn^{2+} ions were supported by IR, UV-visible and Emission Intensity. Furthermore, the fluorescent sensor was successfully used to recognize Zn^{2+} in living cells, suggesting that this simple biosensor has great potential in biological imaging applications.[3]



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P-14

Dimeric Carbazole Alkaloids Isolated from the Genus *Murraya* – A Review

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The genus *Murraya* belongs to the family Rutaceae of the order Rutales and is in the subtribe Clauseneae, subfamily Aurantoidae. It consists of shrubs or small trees distributed from Southeast Asia to Australia. About 8 species occur in India, *viz*., *Murraya koenigii*, *Murraya euchrestifolia*, *Murraya paniculata*, *Murraya exotica*, *Murraya siamensis*, *Murraya gleinei*, *Murraya omphalocarpa* and *Murraya altarnans*. *Murraya* species have been used in different folk medicines in India, Australia and South Africa.

Murraya koenigii Spreng (*M. koenigii*) occurs widely in East Asia and is a small tree. It is popular in India as the curry leaf plant and the leaves are widely used as a flavoring agent. Different parts of the plant have been used in traditional or folk medicine for the treatment of headache, toothache and stomachaches, influenza, rheumatism, traumatic injury and insect and snake bites, and as an antidysentric as well as an astringent. The EtOH extract of the root bark of *Murraya euchrestifolia* Hayata exhibits significant cytotoxicity ($ED_{50} < 20\ \mu g/mL$).[1]

J. Banerji *et al*.[2] has been published a review on chemistry and pharmacology of *Murraya koenigii* Spreng (Rutaceae) in 2010. The major classes of compounds isolated from different *Murraya* species are monomeric and dimeric carbazole alkalods, indole alkaloids, flavonoids and coumarins. The chief constituents of *Murraya koenigii* are various monomeric carbazole alkaloids, whereas *Murraya euchrestifolia* is very rich in monomeric as well as dimeric carbazoles. The present review is an attempt to compile and tabulate the spectral data and biological activities of the dimeric carbazole alkaloids isolated from the genus *Murraya* available in the literature till December 2010. This review will also include the one-pot synthesis of the dimeric carbazole alkaloid murranimbine from its monomer.[3]

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P-15

Adapting environmentally benign practice for separation of radioisotopes using PEG-based Aqueous Biphasic System

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Polyethylene glycol (PEG) based aqueous biphasic systems (ABS) are green analytical methods having extensive applications in separation science. With different inorganic salts, environment friendly reagent PEG forms ABS. Such systems enable partitioning of metal ions. At present, ABS is preferable for selective separation, pre-concentration and recovery of desired metal species (both stable elemental species and radioactive isotopes)[1]. Factors like lesser material cost, efficient phase separation, selectivity, low viscosity, etc. makes polymer/salt biphasic system more applicable and attractive. The trend in publication using ABS over last twenty years is appreciable and more research works are being carried out using this environmentally benign practice, as part of green chemistry endeavor.

ABS can be a separation tool for radioisotopes[2]. For example, various AB systems have been used to investigate the extraction behavior of ^{96}Tc, ^{97}Ru and ^{95}Nb radioisotopes in either PEG-rich/ salt-rich phase. Radioisotope ^{97}Ru with half-life of 2.83 d finds application in nuclear medicine and can be good radiopharmaceutical candidate. Natural Mo foil was irradiated at VECC cyclotron, Kolkata. This irradiation resulted in production of radioisotopes, ^{96}Tc ($T_{1/2}$=4.28 d), ^{97}Ru ($T_{1/2}$=2.83 d) and ^{95}Nb ($T_{1/2}$=35 d). Extraction/separation behavior of these radioisotopes was investigated using various polymer/salt combinations. Experimental samples were measured in gamma-spectrometry.

Since the matrix contained multiple radionuclides (^{96,99m}Tc, ^{97,103}Ru, ^{95,96}Nb) with similar chemical properties, probing their extraction in various ABS combinations became an interesting challenge. Various combinations of 2 M salt solutions (Na-tartarate, Na_2SO_4, $(NH_4)_2SO_4$, $NaHSO_3$, etc.) with 50% PEG (MW = 4000, 6000) showed differential extraction of ^{96}Tc, ^{97}Ru and ^{95}Nb. Hence, green chemistry proofs beneficial for separation of radioisotopes.

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P-16

Two dimeric and a helical MOFs complexes of Cu(II) from Schiff base and pseudohalides [OCN^-, SCN^- & $N(CN)_2^-$]

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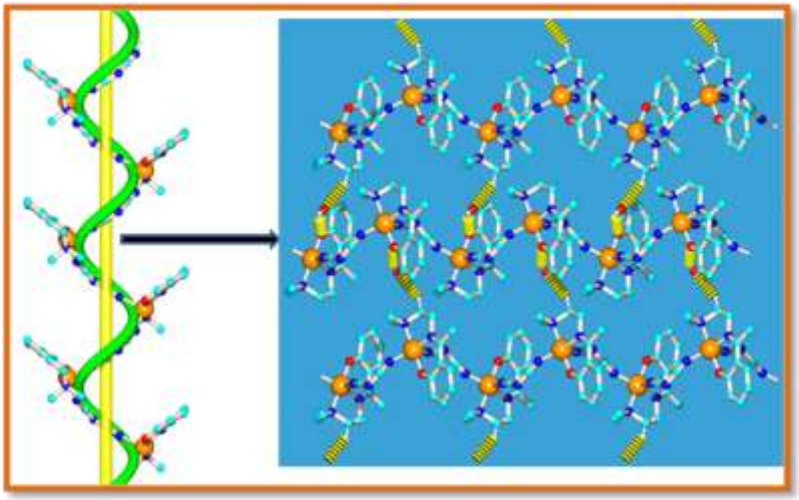
Three copper(II) complexes, [$Cu_2L_2(\mu_{1,1}$-NCO)(NCO)] (**1**), [$Cu_2L_2(\mu_{1,3}$-NCS)(NCS)] (**2**) and [CuL(μ1,5-dca)]n.nH_2O (**3**), where HL = 2-[1-(2-dimethylamino-ethylimino)-ethyl]-phenol, have been prepared and characterized by elemental analysis, IR and UV–Vis spectroscopy, single crystal X-ray diffraction studies and by cyclic voltammetry. Complexes **1** and **3** crystallize in monoclinic space group $P2_1/n$ and complex **2** in monoclinic $P2_1/c$. In complex **1**, OCN^- shows $\mu_{1,1}$ bridging mode; in complex **2**, SCN^- shows $\mu_{1,3}$ bridging mode whereas in complex **3**, $N(CN)_2^-$ shows $\mu_{1,5}$ bridging mode. The tridentate Schiff base ligand reacts with copper(II) to occupy its three equatorial positions. The coordination polyhedra around one of the copper center in compounds **1** and **2** are best described as an elongated (4 + 1) square pyramid, whereas the coordination polyhedral around other copper center is square planer. The copper atom in compound **3** has a slightly distorted square pyramidal environment. Significant C–H/π interactions are observed in both complexes **1** and **2**. Complex **3** is an example of MOFs containing penta cordinated Cu(II) ions linked together by $N(CN)_2^-$ to yield 1D infinite P and M-helical chains.



Refarence: (1) P. Bhowmik, S. Chattopadhyay, M.G.B. Drew and A. Ghosh, *Inorganica Chimica Acta* **2013,** 395 , 24.

P-17

Investigation of electrical conductance properties of a newly synthesized copper (II) metal complex and its non-covalent interactions and TDDFT calculation

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The complex $[Cu(pydc)_2(apy)]\cdot 3H_2O$ (**1**) ($pydcH_2$ = pyridine-2,6-dicarboxylic acid; apy = 2-aminopyridine) has been synthesized and characterized by elemental analysis, IR spectroscopy and single crystal X-ray diffraction techniques. Crystallographic analysis tells that the complex **1** has distorted square pyramid geometry with $pydcH_2$ coordinated as a tridentate ligand to each metal ion through two oxygen atoms of each carboxylate group and the nitrogen atom of the pyridine moiety. Three non-coordinated water molecules are present in the asymmetric unit and all are involved in constructing a $(H_2O)_6$ cluster with chair conformation like cyclohexane. In addition, a new dimension to water clusters research has been explored where the role of water has been shifted from its usual behavior of guest to that of a host. Apart from water cluster, the aromatic molecules are engaged in several non-covalent interactions like NH•••π, lone pair•••π, π•••π and hydrogen bonds.

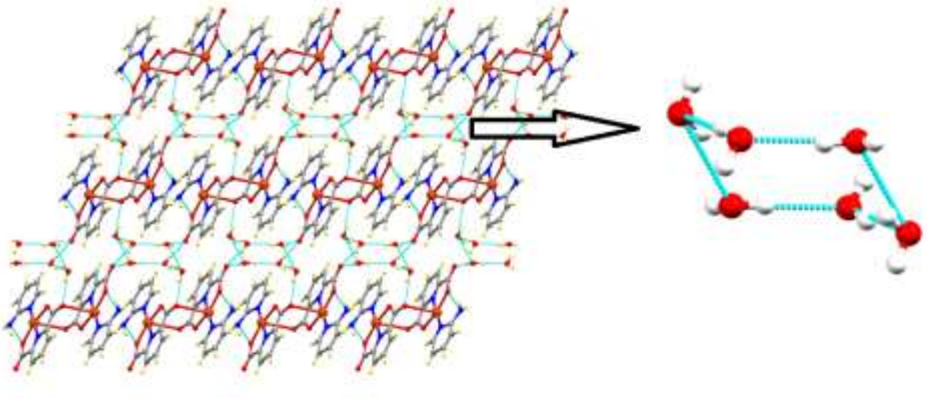

Fig.1. 2D architecture of H bonding interaction in **1**

The electrical conductivity in terms of current was measured at room temperature before and after annealed of the synthesized complex compound on thin film specimen of order 230 and 240 μA respectively with bias voltage 1 V. In addition, the electronic transitions of **1** were recorded and the electronic distribution of HOMO-LUMO was rationalized theoretically (through time-dependent density functional theory (TDDFT)).

P-18

Designing of Novel Zinc(II) Schiff Base Complexes Having Acyl Hydrazone Linkage: Study of Phosphatase and Anti-Cancer Activity

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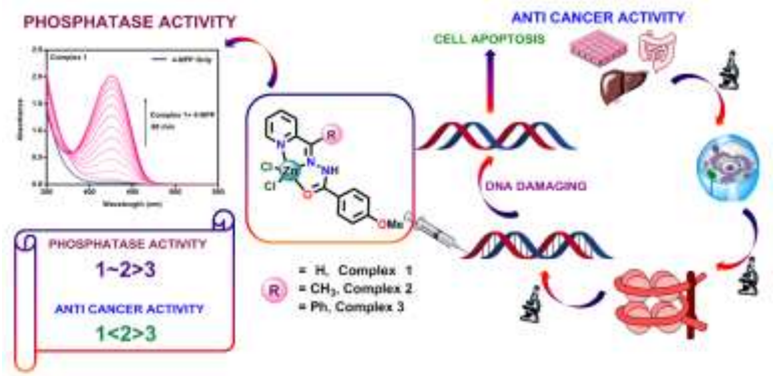
Hydrazone ligands and their transition metal complexes are celebrated class of compounds for their anti-oxidant, anti-inflammatory, antimicrobial, analgesic and anticancer property. The coordination of hydrazone to zinc(II) metal ion introduces the combine medical properties and hydrolytic properties in the complexes. In this present work three mononuclear zinc(II) complexes namely [Zn(L1)Cl_2](**1**), [Zn(L2)Cl_2](**2**) and [Zn(L3)Cl_2](**3**) were synthesized from three acyl hydrazone Schiff base ligands L1, L2 and L3 with the aim to explore their phosphatase activity and anti cancer activity.



All the complexes were able to hydrolyse the P-O bond of phosphate monoester in 90% (v/v) DMSO-water medium using 4-nitrophenylphosphate (4-NPP) as model substrate and the trend of their activity is; **1** ≈ **2** > **3** and complexes **1-3** were tested as potential therapeutic agents for cancer using HCT116 (human colorectal carcinoma), HepG2 (human hepato cellular carcinoma) and A549 (human non-small lung carcinoma) cells. Complex **2** showed the highest IC_{50} values for anti-cancer activity towards all three cell lines among three complexes. The internucleosomal degradation of DNA during apoptosis can detect by cell death detection ELISA. DNA fragmentation level that leads to cell death was examined and induced by complex **2** using HepG2 cells and significant level of DNA fragmentation was observed with regular interval of time.

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P-19

A Correlation of the Drug Activities (Anti-bacterial) in the Structure of Some hetero cyclic compound containing benzimidazole and beta-lactam moiety in terms of the Density Functional Descriptors– A QSAR and QSPR Study

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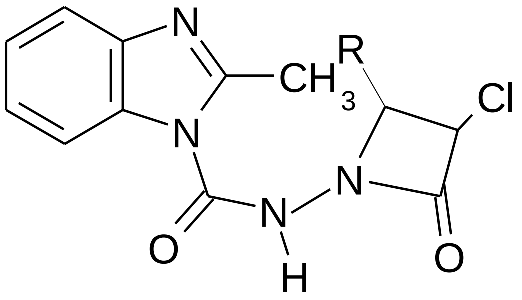
The benzimidazole ring is a significant pharmacophore in contemporary drug discovery[1,2]. Present study shows the correlation of activity[3] of as many as 13 Anti-bacterial (containing benzimidazole and beta-lactam moiety) drugs in terms of global reactivity descriptors under paradigm of QSPR/QSAR study. Investigation of antimicrobial activity of the compounds was done by using Gram-positive (*S. aureus, S. mutans and B. subtilis*) bacteria. The global descriptors nicely correlate the variation of activity with structures of the drug molecules.



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P-20

Photoresponse properties and DNA binding abilities of 4-(4 pyridinyl)-2-pyridone salts

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Three salts [perchlorate **(2)**, chloride **(3)** and tetrafluoroborate **(4)**] were synthesized from a 1-(2-aminoethyl)-6-hydroxy-2-oxo-1,2-dihydro-[$4,4'$ -bipyridine]-3,5-dicarbonitrile compound **(1)** and characterized by spectroscopic and single crystal X-ray diffraction methods. Various noncovalent interactions (e.g., anion•••π^+, π•••π, lp•••π) are explored in the solid state crystal structure of the salts. Optical band gaps of all the four compounds were determined from their solid-state UV-vis spectrum. Electrical properties like electrical conductivity, photosensitivity, etc. were calculated and the results revealed that they have potential to act as optoelectronic devices. The values of the electrical parameters increase several times when they are exposed to visible light rather than in dark conditions. The light sensing properties of the salts **(2–4)** are enhanced compared to that of the mother organic compound **1** but the magnitude of this enhancement is not same for the three salts.

P-21

A selective chemosensor for Al^{+3} detection based on Coumarinyl Schiff base

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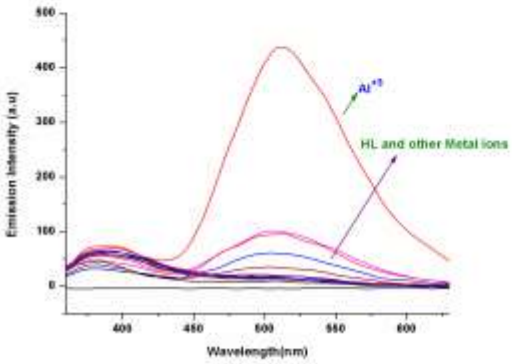
A novel Al^{+3}-selective chemosensor based on Coumarinyl Schiff base, 6-((Z)-(2-(2-(2-(((2-oxo-2H-chromen-5-yl)imino)methyl)phenoxy)ethoxy)benzylidene)amino)-2H-chromen-2-one, (**L**) has been synthesized and characterized by ^1H NMR, elemental analysis and ESI-mass spectrometry. The absorption and emission spectra of **L** have been investigated in the presence of different metal cations. Al^{+3} results in an instant color change of **L** from colorless to light green in THF. Due to binding of Al^{+3}, a significant fluorescence enhancement has been observed in in THF. Thus, **L** is expected to be used as an interesting Al^{+3} sensitive chemosensor. The 1:1 stoichiometry binding mode of **L** with Al^{+3} is supported by the Benesi-Hildebrand analysis. The binding constants in THF is found to be $1.84x10^4$ by the linear fitting of the Benesi-Hildebrand plot from the results of fluorescence titration.



Change in emission spectrum of L upon gradual addition of different metal ion in THF

P-22

Studies on a Reductive Nitrosylation of Molybdenum in Its Lower Oxidation States

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The activity of molybdenum in the natural systems is comprised of different oxidation states. The origin of the molybdenum activity involved in such reactions, essentially rests on the key role of Mo (IV). Probably the stability of this anion in a wider pH range may be suitable for biological activities of molybdenum in metalloproteins.

A number of molybdenum complexes in its lower oxidation states have been synthesized in aqueous medium. The compounds were characterized by infrared (FTIR), magnetic susceptibility, ESR, NMR, X-ray, photoelectron spectroscopy and single-crystal X-ray. Structural characterization of the prepared complexes has been made in the conformation with existing theories using these techniques. Emphasis has been made to understand the nitrosylation of molybdenum with concomitant reduction using hydroxylamine, especially for the dinitrosylation step.

P-23

Structural analysis of an arabinan isolated from alkaline extract of the endosperm of seeds of *Caesalpinia bonduc*

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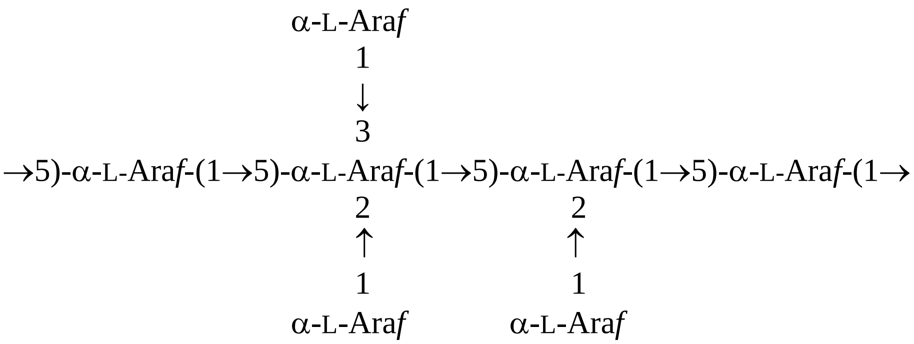
A water-soluble arabinan (M.W. ~2.0×10^{2} kDa) isolated from the alkaline extract of the endosperm of *Caesalpinia bonduc* was found to consist of T-Ara*f*, (1→5)-Ara*f*, (1→2,5)-Ara*f*, and (1→2,3,5)-Ara*f* in a relative proportion of approximately 3:2:1:1. On the basis of acid hydrolysis, methylation analysis, and NMR experiments (^{1}H, ^{13}C, TOCSY, DQF-COSY, NOESY, ROESY, HMQC, and HMBC), the structure of the polysaccharide was established. The proposed repeating unit of the polysaccharide has a branched backbone composed of (1→5)-α-L-arabinofuranose residues where branching occurs at *O*-2, *O*-3 positions of one residue terminated with two arabinofuranosyl residues and *O*-2 of another one terminated with same residue situated at adjacent position. The proposed structure of the repeating unit was established as:



$$\begin{array}{ccccc}
 & \alpha\text{-L-Ara}f & & & \\
 & 1 & & & \\
 & \downarrow & & & \\
 & 3 & & & \\
\rightarrow 5)\text{-}\alpha\text{-L-Ara}f\text{-}(1\rightarrow 5)\text{-} & \alpha\text{-L-Ara}f & \text{-}(1\rightarrow 5)\text{-} & \alpha\text{-L-Ara}f & \text{-}(1\rightarrow 5)\text{-}\alpha\text{-L-Ara}f\text{-}(1\rightarrow \\
 & 2 & & 2 & \\
 & \uparrow & & \uparrow & \\
 & 1 & & 1 & \\
 & \alpha\text{-L-Ara}f & & \alpha\text{-L-Ara}f &
\end{array}$$

References:

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P-24

Theoretical investigation of structure and spectroscopic constants of molecular systems important in semiconductor devices

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Among Group IV halides, divalent lead halides (PbX_2; X=F, Cl, Br & I) are well known because of their high iconic conductivity and applications in the development of discharge lamps, infrared and semiconductor devices. PbF_2 is useful because of its transparent nature into the near UV rays and plays a vital role for therapeutic application. $PbCl_2$ and $PbBr_2$ have strong application potential and they are used specially in infrared devices. PbI_2 is used in manufacture of solar cell, X-ray and gamma ray detectors. In addition, lead halides are decomposed by light at high temperature and this effect has been used in photographic processes.

At present, structure, vibration frequency, dissociation energies and various spectroscopic properties have been calculated for the above halides using an extensive basis set. Geometries and frequencies have been obtained at the MP2 level of theory. The energy values are obtained at the QCISD(T) level of theory at the MP2 optimized geometry. Various spectroscopic constants are calculated and compared with the available data. Theoretical calculations of these systems are limited, because of the concerned heavy atoms. In this sense, our calculated data may serve as future references.

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P-25

Preparation of Cellulose Nanofibers from the Domestic-waste by Chemical Treatment and Ultrasonication

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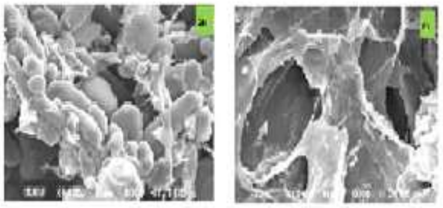
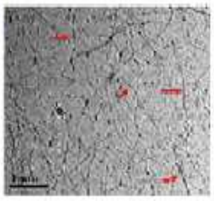
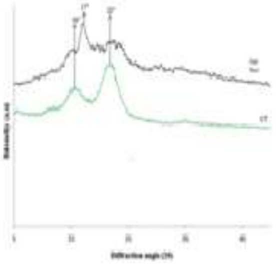
Agro-waste was explored as a source of raw material for production of cellulose nanofibers (CNFs). Cellulose nanofibers were isolated from peel of *cucumber*, *banana*, *pointed gourd* and *luffa* using alkaline treatment, bleaching and acid hydrolysis to eliminate non-cellulosic compounds and amorphous cellulose. The obtained chemically treated cellulose fibers werethen mechanically tailored and separated into nanofibers using high-intensity ultrasonication. Crystallinity of cellulose nanofibers was characterized by X-ray diffraction (XRD) and purity of cellulose was characterized by Fourier transformation infrared spectroscopy (FTIR.). SEM, FTIR and XRD results indicated chemical treatment employed was effec-tive in removing compounds other than cellulose fibers. The presences of nanofibers in all samples were confirmed by TEM. It has huge application as a reinforcement agent for the manufacture of bionanocomposites and can be considered as a renewable source of nanofibres which has an etymology to agro-waste.



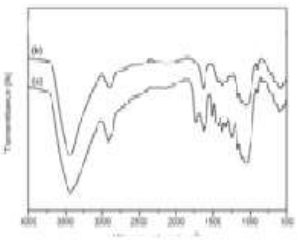
SEM



TEM



XRD



FTIR

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P-26

Atmospheric Co$_2$ Fixation By Zinc (Ii) Complex Containing A Tetradentate Amine

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The activation of CO_2 and its chemical fixation by metal complexes are of continued attention to control concentration of this greenhouse gas reducing several serious environmental problems. Development of effective chemical methods to absorb CO_2 and to convert it into useful materials by metal complexes is a challenge to the synthetic coordination chemists. In most cases, the carbonate complexes were obtained by addition of Na_2CO_3, $NaHCO_3$ or bubbling CO_2 to the reaction solution. Only a few examples of fixation of CO_2 from air are known at present. So our interest to develop a new system for effective fixation of atmospheric CO_2. In the present endeavor, we examine this behavior to Zinc (II) in combination with a tetradentate amine,N,N'-bis(3-aminopropyl)-1,2-ethanediamine (L). Successfully, we have isolated one trinuclear zinc(II) carbonato compound of the type $[Zn_3(\mu_3\text{-}CO_3)(L)_3](ClO_4)_4$ (**1**) by reaction of 1:1 molar ratio of $Zn(ClO_4)_2$. $6H_2O$ salt and L in open air at room temperature. Structural study reveals that a μ_3-carbonate binds three zinc(II) centers; each metal center in **1** adopts a distorted trigonal bipyramidal geometry with a ZnN_4O chromophore bound by four N atoms of the tetradentate amine (L) and one O atom of carbonate. The trinuclear units of **1** are engaged in N-H···O hydrogen bondings leading to 3D network structure.

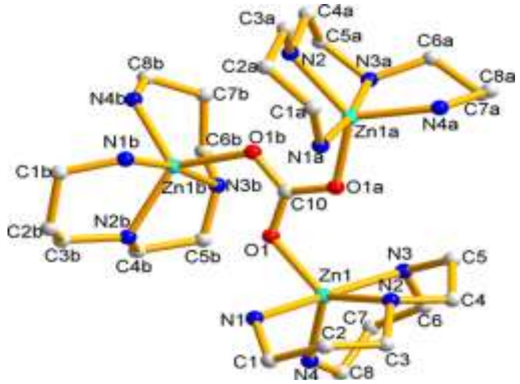

Fig.1. ORTEP of complex **1.**

P-27

Synthesis of Bi-Hetrocyclic *azo* Compounds and studies their Antimicrobial activities

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Compounds containing Azo-imine(-N=N-C=N-) group can control the different activities (photochromic, redox-active, PH -responsive and complex formation ability) on overall structure of the molecules. Various types of aryl-azo-heterocycles and symmetrical azo heterocyclic compounds containing Azo-imine group present in literature. Synthesis of some symmetrical bi-heterocyclic azo compounds also published in journals, e.g., in 4,4'-azobis(pyridine), 4,4'-azobis(2,2'-bipyridine), 5,5'-azobis(2,2'-bipyridine), 5,5'-azoxy bis(2,2'-bipyridine) and bis[2,6-bis-(2-pyridyl)-4-pyridyl-diazene], 2,2'-azobispyrazine. But reports on mixed unsymmetrical bi-heterocyclic azo compounds are scarce. Primarily thiazolyl-azo-imidazole compound appeared in literature where azo(-N=N-) binds with two heterocyclic rings thiazole and imidazole. N-heterocyclic rings containing pyridine, imidazole, benzimidazole, quinazoline and adenine derivative compounds exhibited so many biological activities like- Anticancer, Antibacterial, Antifungal, Anti-diabetic, Antiviral, Antihelmintic and also selective inhibitors. Designs of mixed unsymmetrical bi-heterocyclic azo compounds are the most important challenge to us. Our interest lies for the synthesis of N-heterocyclic ring containing pyridine, imidazole, benzimidazole, quinazoline and adenine Bi-heterocyclic Azo Compounds and also studing their biological activities.

P-28

An Expeditious Synthesis Of *Cis*-2-Aroylmethyl-4-Phenylthiochromans By Iodine-catalyzed Combination Of Thiophenol With Cinnamylideneacetophenones

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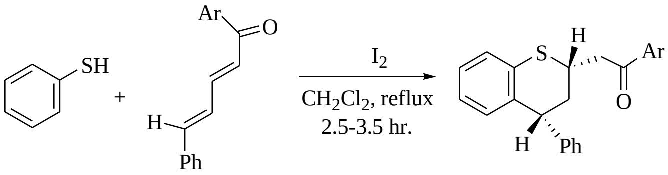
Numerous methods have been reported in the literature regarding the 1,4-addition of thiols to electron deficient olefins activated by different bases[1]. These reactions were also investigated using different Lewis acid[2] such as $Hf(OTf)_3$, $InBr_3$, $Bi(OTf)_3$, $Cu(BF_4)_2$. Conjugate addition of thiols to conjugated alkenes employing polyethylene glycol was developed by Kamal and others[3]. Another green procedure was developed by Khatik and others[4] where β-sulfido carbonyl compounds were formed at room temperature in short times and with excellent chemoselectivity Recently, various types of organo-catalyzed thiol addition to α,β-unsaturated carbonyl system were investigated[5]. The catalytic activity of iodine in organic transformations has been reported recently[6]. Therefore, development of new and facile synthetic routes leading to such heterocycles for assessing their biological potential is of considerable interest. Iodine-catalyzed cyclocondensation of cinnamylideneacetophenpone**(1)** and thiophenol, which results in formation of *trans*-2-phenyl-4-thiophenoxythiochroman**(2)** in excellent yield with high diastereoselectivity.



1 **2**

a: Ar = C_6H_5; **b**: Ar = C_6H_4-Cl-*p*; **c**: Ar = C_6H_4-Br-*p*
d: Ar = C_6H_4-Me-*p*; **e**: Ar = C_6H_4-OMe-*p*; **f**: Ar = C_6H_4-NO_2-**m**

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P-29

Perchlorate, chloride and tetrafluoroborate salts of an organic compound with 4-(4-pyridinyl)-2-pyridone backbone: their structures, supramolecular aspects and functional properties

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Three salts (perchlorate, chloride and tetrafluoroborate) were synthesised from a common 1-(2-aminoethyl)-6-hydroxy-2-oxo-1,2-dihydro-[4,4'-bipyridine]-3,5-dicarbonitrile mother compound and their solid-state crystal structures were established.[1] The asymmetric units of the three salts consist 4-(4-pyridinyl)-2-pyridone moiety with one protonated pyridine ring along with different anions and solvent water molecules (Fig. 1). Though the core organic moiety of the three salts is same, the main difference between the structures is in *bis*-arene torsion angle and the orientation of the ethylammonium group that strongly influences the solid-state architecture of the salts. Various non covalent interactions like, hydrogen bonding interactions, lp···π, anion···π^+ and/or π···π stacking interaction are explored in detailed from the solid-state structure of the salts.

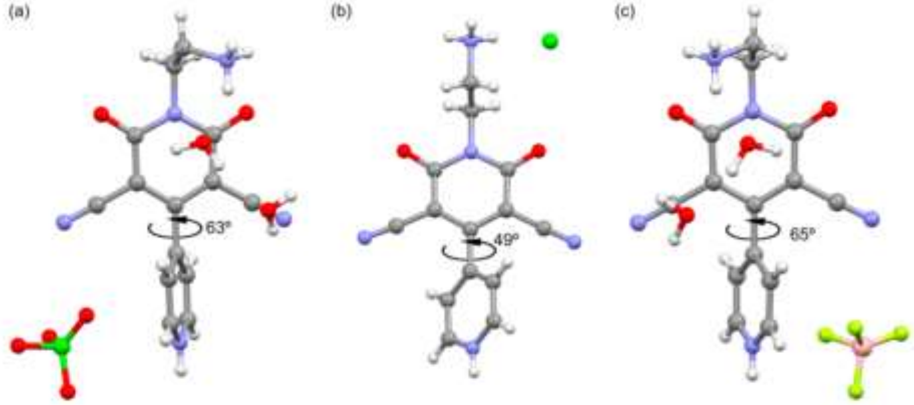

Fig. 1 X-ray structures of (a) perchlorate, (b) chloride and (c) tetrafluoroborate salts of 1-(2-aminoethyl)-6-hydroxy-2-oxo-1,2-dihydro-[4,4'-bipyridine]-3,5-dicarbonitrile compound with the indication of the bis-arene torsion angle.

Optical band gap of all the four compounds (three salts and the mother compound) were determined from their solid-state UV-vis spectrum and the values were found to be in the semiconductor range. Motivated from this result the electrical characteristics of the synthesized compounds were further studied. Salt formation substantially improved the electrical properties over the mother compound though the value of optical band gaps and electrical parameters differ from salt to salt. The difference in torsion angles in synthesized salts is also responsible for variation in the electrical conductivity of the salts. However, the values of electrical parameters of all compounds increase several times when they are exposed under visible light.

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P-30

Unusual transformation of Coumarin fragment upon treatment with Cu (II) to afford an unprecedented complex

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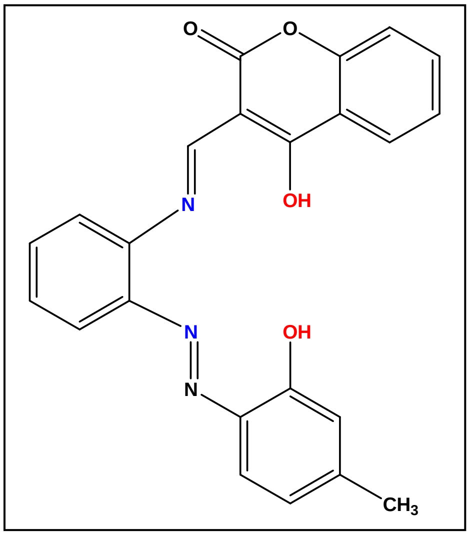
Coumarin and its derivatives are potential therapeutic agents. Appropriately designed ligands incorporated with coumarin fragment have been utilized to study the aspects ofcoordination chemistryof transition metal ions. In this presentation the design and synthesis of new coumarin containing ligands,**1**, and their transition metal complexes have been described. Although Ni(II) formed the desired complex with the new ligand but Cu(II) afforded a complex with concomitant unusual transformation of the coumarin fragment. The results are shown in this poster but studies on unveiling the reaction pathway and mechanism is in progress.



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P-31

Microwave assisted “Click reaction” by polymer supported Cu(I) catalytic species

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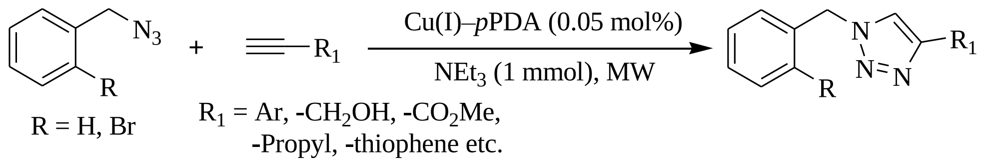
Copper(I) is the recommended catalyst for ‘Click reaction’ and most of the reaction protocols involved either by direct addition of a Cu(I) salt or in situ reduction of Cu(II) by sodium ascorbate.[1] In an effort to achieve a reusable heterogeneous catalytic nature, Cu(I) catalysts have been immobilized onto polymers.[2] Copper nanoparticles and nanostructured CuO have also successfully demonstrated as a catalyst for this reaction.[3] Polymer coated Cu_2O nanoparticles have been reported as a catalyst for click reactions in water.[4] The demand of green and sustainable synthetic method is a significant challenge to the chemical community.



Here Cu(I)–poly(phenylenediamine), Cu(I)–*p*PDA, complex using in situ polymerization and composite formation (IPCF) route has been synthesized in one-step under ambient conditions. The resultant material serves as an effective catalyst for a 1,3-dipolar cycloaddition reaction between terminal alkynes and azides to synthesize 1,2,3-triazoles with excellent yields using a microwave irradiation technique in the absence of any solvent. The composite has also been found to be an effective catalyst for the multicomponent synthesis of 1,2,3-triazoles from organic halides, sodium azide and terminal alkynes under the identical conditions.

Microwave irradiation technique for the current cycloaddition reactions dramatically decrease the time of the reaction and that consequently increase the turnover number of the reaction. It is also important to mention that the copper nanoparticles are also very active catalyst for the microwave assisted 1,3-dipolar cycloaddition reactions which was confirmed during the recyclability study for the current experiment.

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P-32

Metal-Assisted Oxazolidine/Oxazine Ring Formation in Dinuclear Zinc(II) Complexes: Exhibition of cytotoxicity against AGS cell line

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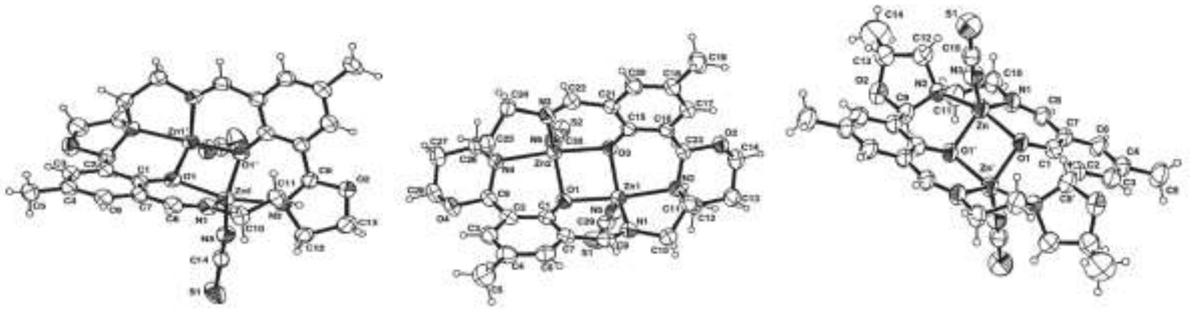
Bimetallic complexes have drawn wide attention for their interesting properties arising out of close proximity of the two metal centres. In various biological reactions dinuclear transition metal centres are known to play a central role. Dinuclear zinc complexes have attracted particular interest as synthetic structural mimics of the active site of a range of metalloenzymes, such as zinc-dependent aminopeptidases, metallo-β-lactamases, and alkaline phosphatases. The role and behaviour of zinc in all such bioinorganic processes are modulated by its coordination environment. Biological substrates, in principle, can bind to zinc by the substitution of coordinated water or by association. Many features of zinc, such as its ability in assisting Lewis activation, nucleophile generation, fast ligand exchange, and leaving group stabilization, make Zn ideal for the catalysis of hydrolytic reactions, including DNA cleavage, which is an important property for use as anticancer drugs. DNA is generally the primary intracellular target of anticancer drugs, which cause DNA damage in the cancer cells, blocking the division of cancer cells, and resulting in cell death. Here three novel dinuclear Zinc complexes of cresol-based compartmental macrocyclic ligands namely **1**, **2** and **3** have been synthesized and characterized. Synthesized 18-membered macrocycles are noted to be structurally unique, and their formation proceeds with the generation of two oxazolidine side rings in complexes **1** and **3** and two oxazine side rings in **2**. The formation of these unusual macrocycles is considered to be zinc-mediated. Preliminary studies with the complexes show that all of them exhibit an inhibitory effect, on the cell proliferation of human stomach cancer cell line AGS, though with different degrees, where complex **3** shows the highest efficiency.



1 **2** **3**

ORTEP diagram of **1**, **2** & **3**.

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P-33

Liquid Crystals from Shape-Persistent Porphyrin Stars with Intrinsic Free Space

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Star-shaped shape-persistent molecules allow a rational design of mesogens incorporating different chromophores in the arms and the core and are known for their excellent film forming properties.[1] Recently, shape-persistent stars with an oligo(phenylenevinylene)scaffold (OPV) have been prepared and showed void, which could be filled with various guests.[2] An OPV/Fullerene system exhibited nanosegregated donor-acceptor morphology with a remarkable increase in the mesophase stability.[3] Such nanomorphologies are of general interest for bulk-heterojunction (BHJ) materials and photovoltaic applications. Porphyrin derivatives are important natural products, which take over essential functions like catalysis, oxygen transport or light harvesting for photosynthesis.[4]

Shape-persistent star-mesogens based on a symmetrically *meso*-substituted zinc porphyrin core with arms based on phenylene, thienyl and ethenyl building blocks were successfully prepared. The formation of columnar liquid crystal phases for this class of mesogens is extremely sensitive to the conjugated arm structure, not least because of the need to fill the intrinsic free space. Transition temperatures to the isotropic phase are below 200 °C, owing to the out-of-plane rotation of the aromatic coupling units. The thermotropic behaviour and mesomorphic structures are investigated by POM, DSC and X-ray scattering and fibre simulation.

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P-34

Synthesis and Spectroscopic Properties of *meso*-Alkylidenyl Carbaporphyrinoids Bearing One Exocyclic C-C Double Bond

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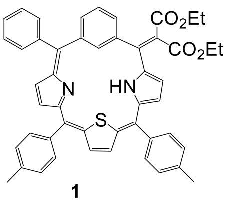
In recent years, the chemistry of porphyrins and their congeners including isomeric porphyrins, aromatic and non aromatic analogues and expanded porphyrin has drawn immense attention owing to their unique photophysical properties. In this regard, various porphyrinoids have been reported describing their spectroscopic properties in conjunction with macroaromaticity. However, porphyrinoids bearing exocyclic double bonds at *meso*-positions have not been studied extensively. The unusual features of these modified porphyrinoids inspired us to synthesize new *meso*-alkylidenyl-porphyrinoids bearing one exocyclic C-C double bond.[1] Such systems would be excellent model system to probe the relationships between global aromaticity and stabilizing/destabilizing effect of substituents. We have reported, for the first time, a generic synthesis of *meso*-alkylidenyl-thia(*m*-benzi)porphyrin **1** containing one exocyclic carbon-carbon double bond.[2] This process also resulted in the formation of a core-modified phlorin type compound **2** that contains one sp^3 hybridized *meso*-carbon atom. Phorins are hybrid class of molecules (porphyrinoids) that have intermediate structural features of porphyrins and calixpyrroles, and could be regarded as Calixphyrin. In contrast to the other conventional porphyrinoids, phlorins exhibit multi-electron redox chemistry. The presence of sp^3 carbon atom disrupts extended macrocyclic π-conjugation as a result of which electronic properties of phlorin also differ from porphyrin. Recently, we have synthesized new class of phlorin analogue **3** containing one exocyclic double bond. The detailed structural characterization and spectroscopic properties of **1**, **2** and **3** will be presented.



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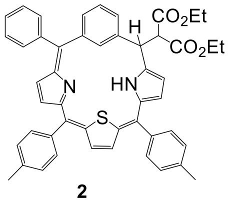

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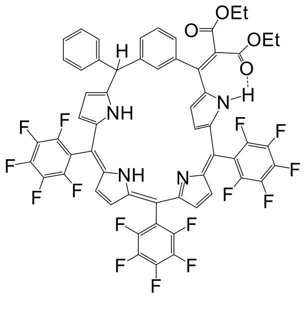

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P-35

Developments and Scopes of Nanoelectronics

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The application of nanotechnology in producing electronic devices leads to a new dimension of research area called nanoelectronics. Discovery of carbon nanotubes exhibiting unique electrical, mechanical, and chemical properties opened the new era in electronics technology. Nowadays, transparent conductive electrodes (TCEs) have been widely used in the field of organic photovoltaics (OPVs), organic light emitting diodes (OLEDs), liquid crystal displays (LCDs), touch screens, solar cells, and flexible displays. [1-3] Indeed some limitations in the conventional TCEs, interest has been shown in researching alternatives which [4-7] basically includes the use of nanomaterials, such as carbon-based nanomaterials and graphene networks, metal nano-wire networks and conductive polymers.

Currently there is a demand for nanoelectronics in medical diagnostics, environmental and food monitoring, detection of chemical, biological weapons. However with the increase in population density, the demand of electricity is increasing day by day and economic growth in many parts of the world has maintained a strong pace because of the availability of energy by the extraction of “cheap oil” (fossil fuels) which meet the current consumption at accessible prices. Today, third-generation devices, such as organic solar cells (OSCs) and dye-sensitized solar cells (DSSCs or dye cells) are being developed that use nanomaterials to convert solar light into electricity at significantly lower costs than those of conventional silicon cells.

With rapid industrialization, organic dyes from textile and fabric industries lead to water pollution which can be decomposed by UV illumination although is not at all cost effective for large scale. But if we use solar radiation (natural and abundant in most of the countries), the processing can be low-cost as well as large-scale purification of dye polluted water. Therefore, the focus has been shifted towards visible/solar light assisted photocatalysis [8, 9].

The electronics technology has evolved rapidly over the last decades and presently the manufacturing of compact lightweight and flexible devices bearing high speed and greater biocompatibilty is the need of the hour.

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P-36

Effect of contaminants and additives on Plastic and Polymer Based Materials

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Each polymer –based material (PBM) consists of a mixture of their representative polymer/s and their different chemical additives. Polymers becoming increasingly more important are biodegradable polymers, natural rubber and the major polymer types are polyvinyl chloride , polypropylene and polyethylene. Additives are effective chemicals which make polymers resistant to photodegradation and biodegradation, enhancing polymer properties and prolonging their lives. Its a very logical approach to design of chemical amiplification resists (additives) that can fight to airborne contamination of polymers. Manytimes microorganisms forming a biofilm that colonize on the surfaces of many polymers causing deterioration of polymeric materials. These biofilms consists of biofilms embeded in polymeric matrix are very effective contaminats to polymeric materials that damage the structure and function of many polymers in various ways. Among these: 1)leaching out of additives and monomers from polymer matrix by microbial degradation ii) by contaminating to adjacent media as water by released microorganism by biofilms iii) by coating the surface and masking surface properties iv) by attack by enzymes or radicals of biological origin to polymers are most important. Globally sourced brands of bottled water also showed some sign of microplastic contamination. A very common airborne contaminat is N-methyl pyrrolidine(NMP).So there should have been much extensive studies for the measured rates of absorption of different contaminants by chemical amplifier resists and polymer film .For this it is very necessary to design rationally the polymers for chemically amplifier resists which are insensitive to airborne chemical contaminats.

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P-37

A facile synthetic approach to benzothiadiazine-1,1-dioxides: A precursor of RSV inhibitors

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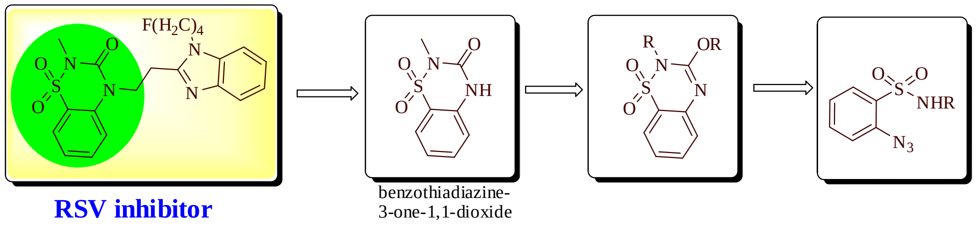
Sultams have gained popularity among the scientific community especially to the synthetic and medicinal chemists because this basic moiety is present in many natural products and biologically active substances.[1,2] Among various sultums, benzothiadiazine-1,1-dioxide derivatives have been reported to display various potent activity[3] including *Respiratory Syncytial Virus* (RSV) inhibitory activity[2].

In this context, I want to present some results to synthesize 1,2,4-benzothiadiazine-1,1-dioxide derivatives using intramolecular aza-Wittig reaction as the key step.[4] Reaction of o-azidobenzenesulfonamide with ethyl carbonochloridate afforded the corresponding amide derivatives, which subsequently gave 3-ethoxy-1,2,4-benzothiadiazine 1,1-dioxides through an intramolecular aza-Wittig reaction. The reactions of all the substrates having electron deficient group at 2-position proceeded smoothly providing excellent yields whereas the substrates having electron donating group gave relatively lower yields. Acid-catalyzed hydrolysis of 3-ethoxy-1,2,4-benzothiadiazine 1,1-dioxides furnished the 2-substituted benzothiadiazine-3-one 1,1-dioxides in good yields and high purity, which is the core moiety of RSV inhibitors. The detailed study will be presented during the poster session.



Outline to achieve RSV inhibitor from *o*-azido-*N*-substituted benzenesulfonamide

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P-38

Crystallization of five new supramolecular networks with both bipyridyl and dicyanamide ligands

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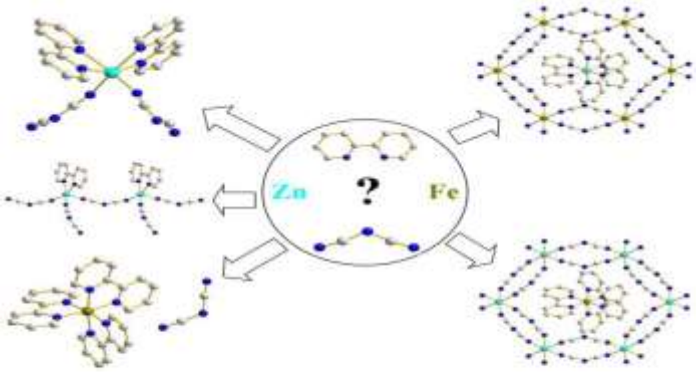
Supramolecular materials are important due to their distinct physical and chemical properties. Here we report synthesis and structural determination by single-crystal X-ray diffraction of five new supramolecular networks, $\{[Fe(bpy)_3OH][dca\cdot 4H_2O]\}n$ (**1**), {[Fe(bpy)3][Zn(dca)3]2}n (**2**), {Zn(bpy)2(dca)2}n (**3**), {Zn(bpy)(dca)2}n (**4**) and $\{[Zn(bpy)_3][Fe(dca)3]2\}n$ (**5**), where bpy = bipyridyl and dca = dicyanamide.



Compound **1** is made up of $[Fe(bpy)_3OH]^+$ cation layer and $[dca\cdot 4H_2O]$- anion layer. Water clusters are present in anionic sheet that link the adjacent layers of supramolecular assembly of compound (**1**). The anionic layer consists of random orientated dca anion and water clusters while the cationic layer has random occupied OH groups. Compounds **2** and **5** have similar molecular connectivity to previously reported structure but different combination of metal centres. They have a twodimensional $\{[M'(dca)^{3-}\}_n$ network which provides perfect hexagonal pockets for $[M(bpy)_3]^{2+}$ cations. Compound **3** has the neutral distorted octahedral monomeric units and these monomeric units are connected through intermolecular hydrogen bonding, forming a 3D network. One of anionic dca ligands in compound **3** is also random orientated. Compound **4** possesses *zig-zag* 1D chain structure and the 3D framework is generated through the weak interaction between aromatic rings of adjacent layers. All five compounds contain both bpy and dca. The crystallization of these compounds depends highly on the experimental conditions.

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P-39

Synthesis and crystal structures of three Cu(II) Schiff base complexes having partial cubane [Cu_3O_4] core

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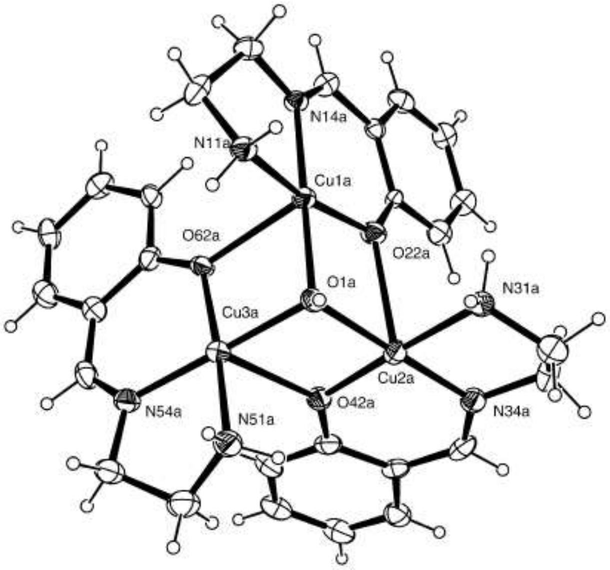
Three new trinuclear copper(II) complexes, $[(CuL^1)_3(\mu_3\text{-OH})](ClO_4)_2.3.75H_2O$ (**1**), $[(CuL^2)_3(\mu_3\text{-OH})](ClO_4)_2$ (2) and $[(CuL^3)_3(\mu_3\text{-OH})](BF_4)_2.0.5CH_3CN$ (**3**) have been synthesized from three tridentate Schiff bases HL^1, HL^2, and HL^3 (HL^1 = 2-[(2-amino-ethylimino)-methyl]-phenol, HL^2 =2-[(2-methylamino-ethylimino)-methyl]-phenol and HL^3=2-[1-(2-dimethylamino-ethylimino)-ethyl]-phenol). The complexes are characterized by single-crystal X-ray diffraction analyses, IR, UV–vis and EPR spectroscopy. All the compounds contain a partial cubane [Cu_3O_4] core consisting of the trinuclear unit $[(CuL)_3(\mu_3\text{-OH})]^{2+}$ together with perchlorate or fluoroborate anions. In each of the complexes, the three copper atoms are five-coordinated with a distorted square-pyramidal geometry except in complex **1**, in which one of the Cu^{II} ions of the trinuclear unit is six-coordinate being in addition weakly coordinated to one of the perchlorate anions.



P-40

Thermodynamics of Solubility of Non-polar Gases in 1-Alkanol at Ordinary Temperature.

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Gas solubilities are used in a wide variety of application from industrial to biochemical to oceanographic to environmental pollution control to the study of the properties of solution. Cavity Formation Energy (CFE) which is equivalent to the free energy cast of insertion of a solute in solvent is very important for predicting solubility of gases in liquid using Scale Particle Theory(SPT) .The CFE of solvent of normal 1-alkanols $C_nH_{2n+1}OH$ ($1\leq n \leq 12$) such as Methanol to 1-dodecanol at 293.15K has been determined. The solubility (in terms of Henry's law constant), Gibb's free energy of solution and (ΔG_s^0), the thermodynamical quantities for the solvation process defined by Ben-Naim and Marcus (ΔG_s^*) of non-polar gases like Hydrogen, Oxygen, Nitrogen, Helium, Neon, Argon, Krypton, Xenon etc in above liquid solvents at 293.15K also been calculated with this cavity formation energy using normal formalism of Scale Particle Theory (SPT). The calculated result then compare with experimental results. It yields good agreement with experimental results. The calculation shows importance of CFE in determining the solution properties and to determine other physico-chemical properties. The aim of this research is to

- to understand the equilibrium solubility of sparingly soluble gases from thermodynamics and statistical mechanical first principle
- to understand interaction of gases with 1-alkanols molecules.

P-41

Trinuclear Zn(II)/Cd(II) Schiff base Complex as a Selective Chemo Sensor for Mercury(II) Involving Hg^{2+}-induced Displacement of Zn^{II}/$Cd^{II}$and Subsequent Hydrolysis of the Imine moiety

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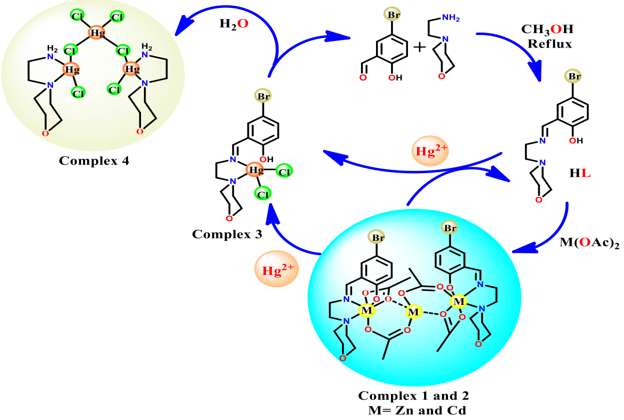
During last few decades the development of cation chemosensors is more important for some essential metal ions like Zn^{II}, Mg^{II} and Ca^{II} and some nonessential as well as toxic and carcinogenic metal ions such as Cd^{II}, Hg^{II}, and Pb^{II}.[1]

Scheme:



A series of group 12 (Zn, Cd and Hg) complexes have been prepared by using N_2O donor Schiff base ligand. Time dependent density functional theoretical (TD-DFT) computations revealed that the UV-Vis bands in the complexes originate from π→π* transitions and also supported red-shift in UV-Vis and PL band upon moving from Zn→Cd→Hg complexes .Interestingly **Zn** and **Cd** complrex are acting as impressive Hg sensor by the hydrolysis of imine moiety.[2] The DFT studies also indicated that the hydrolysis of imine moiety is thermodynamically favorable upon addition of Hg^{2+} to the prepared Zn and Cd complexes.

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P-42

Mapping of Solvent Mediated Molecular Self-Assembly of Fe(III) Discrete Compounds: Exploring their Magnetic Behaviour and Phosphatase Like Activity

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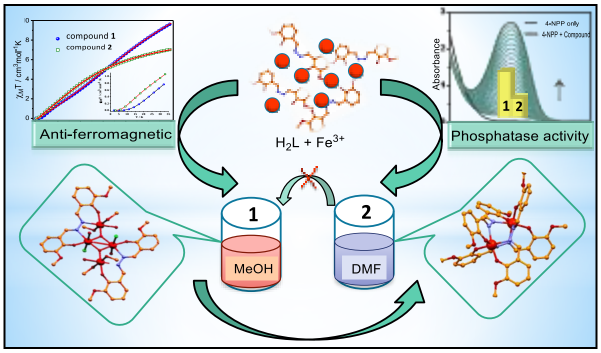
Transition metal based discrete complexes of different nuclearity can be formed *via* self-assembly process.[1-5] Mapping the self-assembly is very crucial to understand the natural algorithm for the formation of these structure. Two newly synthesized Fe(III) based complexes,$[Fe_4L_2(\mu_3\text{-}O)_2(Cl)_2(MeOH)_4(H_2O)_4](ClO_4)_2\cdot 4H_2O\cdot MeOH$ (**1**) and $[Fe_2L_3]\cdot 4DMF$ (**2**) were isolated using the reaction of iron(III) perchlorate with the ligand Compound **1** was self-assembled in MeOH but when solvent was changed to DMF, compound **2** was harvested. Further, compound **1** was converted to compound **2** just by dissolving compound **1** in DMF. Sequential self-assembly and conversion of compound **1** to **2** were monitored by UV-Vis spectroscopy and ESI-Mass spectroscopy in solution phase.



Magnetic studies revealed antiferromagnetic interactions for compound **1** and **2**. The spectrophotometrical investigation on their phosphatase like activity revealed remarkable hydrolytic efficiency for both the complexes.

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P-43

Surface Functionalization of Graphene by Ionic Liquid for Fabrication of High Performance Poly (vinylidene fluoride) Nanocomposite films

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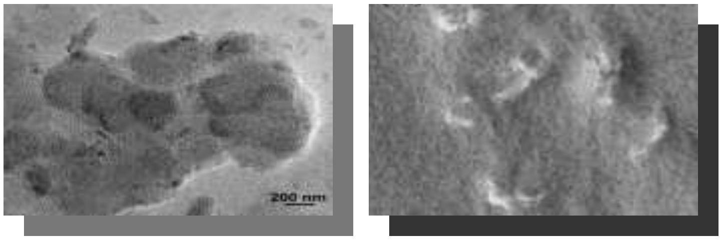
Multifunctional polymer nanocomposite films fabrication have drawn considerable research interest both in academic and industrial purpose because of new developments in thermal, mechanical, conductive and electroactive properties.[1-2] In high performance polymer nanocomposites, to achieve effective reinforcement property the nanofillers must follow high aspect ratio, homogeneous dispersion, good alignment and strong interfacial load transfer etc. Graphene, is a promising material for construction of a novel multifunctional materials, e.g. supercapacitors, photovoltaic devices, biosensor, biomedical devices etc.[2,3] This is because of their excellent thermal, mechanical, electrical, gas barrier and optoelectronic properties. In the chemical functionalization, the properties of the composite materials is comparatively less due to loss of its structure. The covalent functionalization of graphene with ionic moiety might improve the mechanical and conducting properties due to its strong interfacial interaction and easier transport of charges.[4]

Room-temperature ionic liquids (RTILs), consisting of imidazolium cations with counter anions are considered as “green solvents” are used in chemical industry and other purpose. The low flammability, thermal stability and high ionic conductivity are key properties of ILs for electrochemical and different nanotechnological applications.[4-5] Imidazolium-ion based ionic liquids is useful agents for dispersion of graphene etc because it may interact with the π-electronic surface of the graphene by means of cation-π and/or π-π interactions. This functional materials incorporated into polymer matrix Poly(vinylidene fluoride) (PVDF) to fabricate the nanocomposite films rendering homogeneous dispersion.[5] The newly developed materials shows the excellent thermal, conductive and electroactive properties which should be useful in different technological applications.



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P-44

Surfactant-Mediated Solubilization of Magnetically Separable Nanocatalysts for the Oxidation of Alcohols

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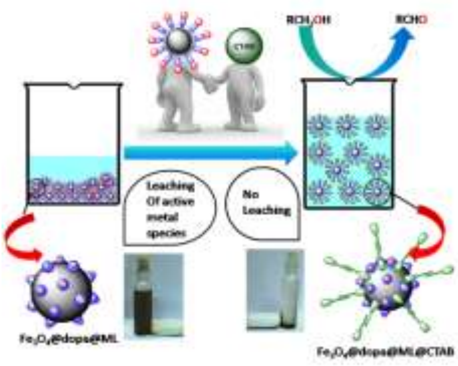
In this work we describe the fabrication and full characterization of water soluble iron (III) and manganese(III) Schiff base and complexes immobilized on dopamine stabilized Fe_3O_4 magnetic nanoparticles (HCAT-1 and HCAT-2) bearing a CTAB micelle structure (CTAB/Fe_3O_4@dopa@FeL(CHCAT-1) and CTAB/Fe_3O_4@dopa@MnL (CHCAT-2)). These water soluble nanocatalytic systems affords efficient oxidation of alcohols with the aid of a green oxidant, H_2O_2, thereby rendering the present approach a much economical, safer, and environmentally benign option. Apart from improving the reaction conditions, we have assumed that hydroperoxo intermediates have a relevant role in the reaction mechanism and we have characterized them by theoretical calculations based on density functional theory. The UV-Visible and ESI-MS studies also support the formation of hydroperoxo species

It is worthy of mention that the synthesized CTAB-coated magnetically separable nanocatalysts can be magnetically recovered from the aqueous reaction mixture after more than five cycles, which renders this approach as a sustainable and accessible one.



P-45

Cooperative Influence of Pseudohalides and Ligand Backbone of Schiff-bases on Nuclearity and Stereochemistry of Cobalt(III) Complexes: Experimental and Theoretical Investigation

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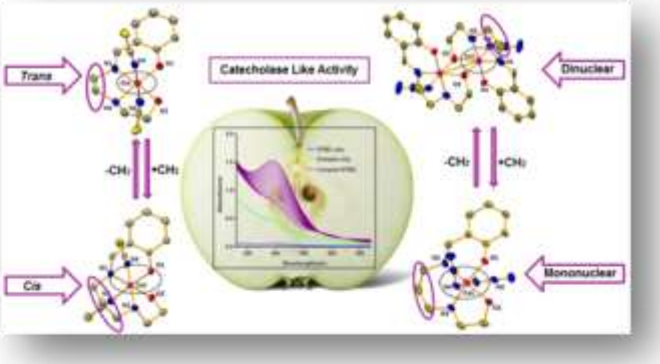
In the past few decades, cobalt(II/III) complexes of Schiff-base ligands having different nuclearity have drawn immense attention because of their potential application in the field of catalysis for the oxidation of organic functionalities.[1-2] As far as the nature of the ligand is concerned the crucial contributing factors are backbone flexibility, denticity, steric and electronic factors of the chelate ring, cavity size (for cyclic ligands) etc.[3-4]

Scheme:



Four cobalt(III) complexes(**1-4**), were synthesized from two Schiff-base ligands $\mathbf{H_2L^1}$ and $\mathbf{H_2L^2}$ respectively. Depending on flexibility of the ligand backbone subtle structural differences are observed in the synthesized complexes. Catecholase like activity of all the four complexes were performed in N,N-dimethylformamide (DMF) using 3, 5 -di-*tert*-butylcatechol (3,5-DTBC) as model substrate. Complex **2** was found to exhibit the highest activity.

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P-46

The coumarin–pterocarpan conjugate – a natural product Inspired hybrid molecular probe For DNA recognition

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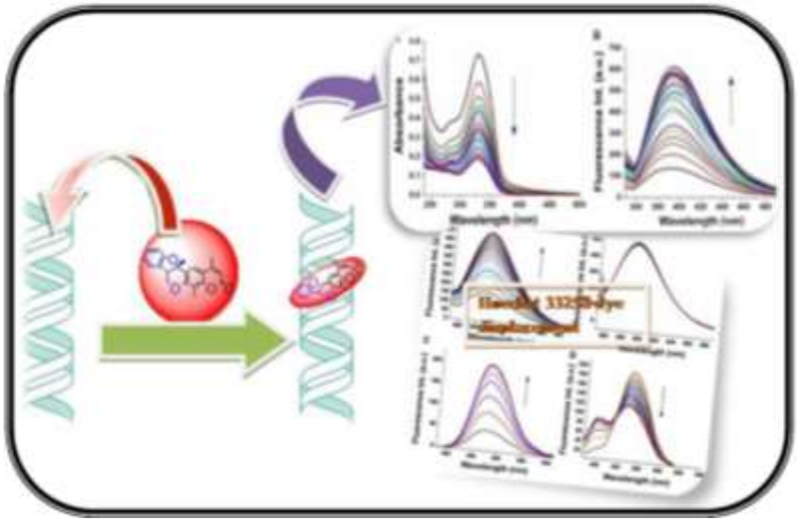
Thermally induced cascade sigmatropic rearrangement of a butynyloxycoumarin derivative has led to a quick access to the coumarin–pterocarpan hybrid molecules. Biophysical studies together with molecular modelling show that this nature-inspired hybrid molecule is capable of binding to the minor groove of DNA as a non-conventional entity. These conjugate molecules can recognize DNA at micromolar concentration. Mode of binding of these ligands was also studied. Accommodation of the pterocarpan derivative in the minor groove was also studied by molecular modeling.



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P-47

A comparative study of the photophysical behaviour of the low-lying excited states of fluorophenols in the gas phase: $^{1}\pi\pi*$ - $^{1}\pi\sigma*$ energy gap effect

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The basic light absorbing chromophore of the aromatic amino acid tyrosine is a phenol derivative, and excited state hydrogen detachment (ESHD) has been recognized to be a key mechanism for non-radiative dynamics of this class of molecules. A characteristic feature of the excited state dynamics of such molecules refers to low quantum yield of fluorescence of the strongly UV absorbing first excited $\pi\pi*$ state, which is partly altered upon forming hydrogen bonded complex with a water molecule in the gas phase environment, occurrence of X-H (X=O, N, S) bond dissociation upon $\pi\pi*$ excitation has been demonstrated[1,2], and an interplay between $\pi\pi*$ and $\pi\sigma*$ states has been proposed to be responsible for this. The same has been predicted by ab-initio calculation[3].Here the $^{1}\pi\pi*$ state is optically bright and bound in nature along the X-H dissociation coordinate. However it develops a conical intersection with dissociative $\pi\sigma*$ state at an intermediate X-H coordinate. At higher X-H stretching coordinate another conical intersection results between $^{1}\pi\sigma*$ and S_0 state owing to the dissociative and bound nature of the states, respectively. The introduction of Fluorine atom at different substitution position of phenol chromophore is expected to perturb the π electron cloud density differently and hence affect the potential barrier at the $^{1}\pi\pi*$ - $^{1}\pi\sigma*$ conical intersection thereby influencing the photodissociation dynamics of the molecule. In the present work, we have shown how Fluorine substitution at *m*- and *p*- position of phenol influence that dynamics. Our approach is to calculate using electronic structure method the relative energies of low-lying $\pi\pi*$ and $\pi\sigma*$ states and also locating the conical intersections. The calculations in ground and excited state electronic states have been performed using the complete-active-space self-consistent-field (CASSCF) method and TDDFT method using GAMESS package. The details of our findings will be presented in symposium.

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P-48

The effect of electrolytes on the solubility of amino acids in water at 298.15.K

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The standard free energies ($\Delta G_t^0(i)$) and entropies ($\Delta S_t^0(i)$) of transfer of amino acids in aqueous electrolytes solutions at 298.15 K are reported. The transfer energies have been determined from solubility measurements of each amino acid at different five equidistance temperatures range from 288.15 to 308.15 K by ‘gravimetrically’. The chemical parts of free energies ($\Delta G_{t,ch}^0(i)$) and entropies ($T\Delta S_{t,ch}^0(i)$) of transfer of the amino acids have been computed by subtracting the cavity effects and dipole-dipole interaction effects from the total transfer energies. The characteristics of the solvation thermodynamics of amino acids in aqueous electrolytes solutions studied earlier are also discussed here for comparison.

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P-49

Migration of thiocyanate anions to produce “coordination position” isomers and formation of bi-component cocrystal in tri-nuclear $Ni_2^{II}Zn^{II}$ complexes with salen type di-Schiff base ligand

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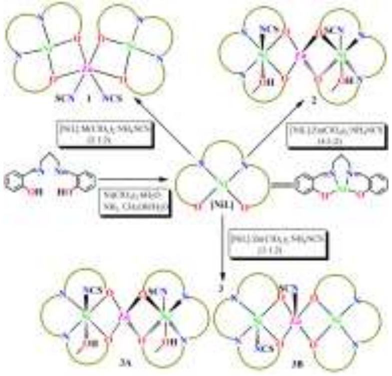
Isomerism and cocrystal formation are fundamental solid state phenomena. The “coordination position” isomerism occurs in multinuclear complexes with different arrangement of coordinating groups relative to the metal ions.[1] On the other hand, co-crystals are defined as solids that are crystalline materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio in the same crystal lattice.[2]



In this context, three trinuclear Ni(II)-Zn(II) complexes (**1**-**3**) have been isolated by reacting a “metalloligand” [NiL] (where H_2L = N,N'-bis(salicylidene)-1,3-propanediamine), Zn(II) and thiocyanate anion with different reactants ratios. All the complexes are structurally characterized by single crystal X-ray studies. In complex **1**, the two square planar nickel atoms and the octahedral zinc atom are arranged in angular shape where two monodentate thiocyanate ions bind to zinc atom. The chemical composition of **2** is the similar as that of **1** but here the zinc atom is tetrahedral and the thiocyanate ions coordinate to an axial position of each nickel atom making its geometry octahedral (the sixth position is occupied by methanol molecule). The migration of the thiocyanate ions from one metal center to other produces in the different metals coordination environments in **1** and **2**. Hence, these two are considered as “coordination position” isomers. Complex **3** consists of two linear isomeric trinuclear units **3A** and **3B**. In **3A**, the geometry of metals are identical to that in **2** while in **3B**, the square pyramidal zinc and one of the square pyramidal nickel atoms are coordinated by two terminally coordinated thiocyanate ions. Hence, these two “coordination position” isomers (**3A** and **3B)** result bi-component cocrystal of **3.**

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P-50

Structure, Property and Application of Multimetallic Iron (III), Copper(II) and Zinc(II) Complexes

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New tetranuclear iron(III), copper(II) and zinc(II) complexes, $[Fe_4(L)_2(phth)_2(OH)_2]\cdot 8H_2O$ (**1**), $Na_3[Cu_4(L)_2(\mu_4\text{-}PO_4)](OH)_2\cdot 14H_2O$ (**2**), $K_2[Cu_4(L)_2(\mu_4\text{-}AsO_4)](OH)\cdot 16^2/_3H_2O$ (**3**) and $[Zn_4(HL)_2(suc)]Br_2\cdot 12H_2O$ (**4**) have been prepared and characterized by utilizing a multidentate ligand, *N*,*N*'-Bis[2-carboxybenzomethyl]-*N*,*N*'-Bis[2-pyridylmethyl]-1,3-diaminopropan-2-ol (H_3L) along with exogeneous bridging groups such as phthalate (phth), phosphate (PO_4), arsenate (AsO_4) and succinate (suc). All four complexes have been characterized by single crystal X-ray crystallography. X-ray crystallographic analyses disclose that the metallic core of **1** consists of four distorted octahedral iron(III) ions with intraligand Fe--Fe separation of 3.656(2) Å. The metallic core of **2** and **3** contains four distorted square pyramidal copper (II) ions with intraligand Cu--Cu separation of 3.5221(16) and 3.5812(1) Å, respectively. Again, the solid state structure of **4** represents a tetra-metallic core containing four distorted trigonal bipyramidal zinc(II) ions with intraligand Zn--Zn separation of 3.472(2) Å. Complex **1** has a very interesting centrosymmetric structure involving in two crystallographically equivalent $[Fe_2(L)]^{3+}$ dinuclear units, connected together by a pair of *syn-syn* bridging phthalates and a pair of bridging hydroxides to generate a "dimer of dimers" structural motif. Both structures **2** and **3** contain two monocationic $[Cu_2(L)]^+$ units that are exclusively coordinated to either phosphate or arsenate in a unique mode. They exhibit a $\mu_4{:}\eta^1{:}\eta^1{:}\eta^1{:}\eta^1$ bridging mode of PO_4^{3-} or AsO_4^{3-} with each bridging among four copper(II) ions. In **4**, a succinate group connects two crystallographically equivalent $[Zn_2(HL)]^{2+}$ units in a *syn-syn* bidentate manner. The phosphatase-like activity of **1** and **4** has been examined using bis(*p*-nitrophenyl) phosphate (BNPP) as a model substrate. Low temperature magnetic studies of **2** and **3** show moderate antiferromagnetic interactions mediated among the copper(II) ions through alkoxide and phosphate/arsenate bridges.

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P-51

Azido bridged binuclear copper (II) Schiff base compound: synthesis, structure and electrical properties

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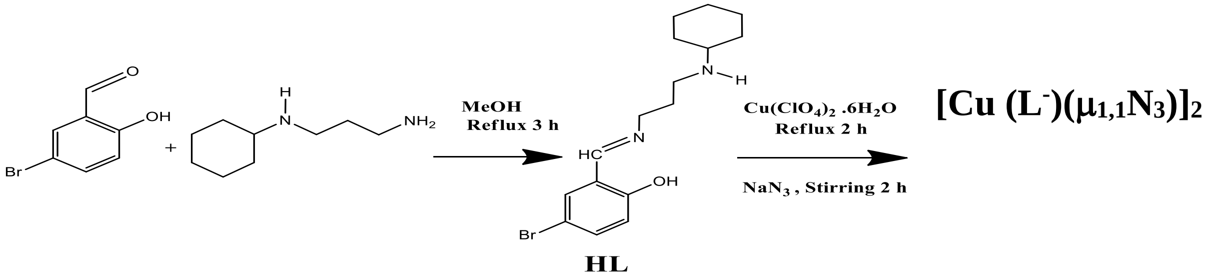
One azido bridged dinuclear Complex $[Cu(L^-)(\mu_{1,1}N_3)]_2$ (**1**) has been synthesized by 1:1 condensation of N-cyclohexyl-1, 3-propanediamine and 5-Bromosalicylaldehyde (HL).The complex **1** is subsequently characterized by elemental analysis, IR spectroscopy, single-crystal X-ray diffraction, FESEM, ESI-MS, and powder XRD successfully. The X-ray crystal structure of complex **1** reveals that, the Cu (II) ion exhibits a definite five-coordinate square pyramidal coordination arrangement with a centro-symmetric $\mu_{1,1}$-azido bridging in the end-on mode and forms a dimeric structure. The optical direct band gap of the complex **1** has been estimated **2.84** eV which has been supported by DFT study.[1] The current–voltage characteristics of Al/**1**/ITO structure have been analyzed considering the thermionic emission theory of Schottky barrier diode.[2,3] The transient behaviour of the test structure is found to be interesting by showing explicit frequency selective phenomena. In view of an application specific material's perspective, compound **1** can be exploited as an electronic material for the development of electronic filters.[4]

Synthesis outline:



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P-52

Supramolecular Gels by Design: Towards the Development of Topical Gels for Self-delivery Application

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Research activities pertaining to converting drug molecules into supramolecular gels has been intensified recently because of the various impediments such as synthetic limitation of carrier molecule, loading drug molecule and its sustain release, cytoxicity of the carrier molecule etc. associated with the conventional drug delivery system. Self- delivery[1] is an alternative option where modification of the drug molecule in such a way that the drug may be effectively delivered to the affected site without the help of a carrier molecule. Topical gel formation is one of the several possible routes for self-delivery.

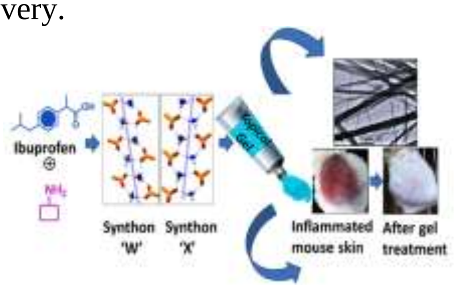

Figure 1: Topical gel of the organic salt of ibuprofen demonstrating to be useful both in vitro and in vivo to treat skin inflammation.

The present work deals with the development of supramolecular topical gels derived from a non-steroidal-anti-inflammatory drug (NSAID) – ibuprofen for delivering the drug to treat inflammated skin condition in a self-delivery fashion. In the present work, we have exploited a supramolecular synthon known as primary ammonium monocarboxylate (PAM) synthon to convert iburprofen to supramolecular gelators capable of forming topical gels with methyl salicylate (a common ingredients of commercially available topical gels) containing menthol by time-inexpensive non-covalent synthesis rather organic salt formation. While X-ray diffraction studies (SXRD and PXRD) establish the merit of supramolecular synthon based on which these gelators were designed, both in vitro and in vivo studies revealed that the simple and easily accessible gelator salts of ibuprofen were indeed useful in developing such topical gels for treating inflammation. Histological studies including immunohistology further probed the role of the gelator drug in treating inflammaiton. Cell imaging studies supported the cellular uptake of the gelator drug in such biomedical application.

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P-53

Oxidation of thiourea by metal bound superoxide; $[(NH_3)(en)_2Co^{III}(O_2)Co^{III}[(NH_3)(en)_2](ClO_4)_5$; in presence of Ellman's Reagent in aqueous acetate buffer medium: A kinetic and mechanistic studies.

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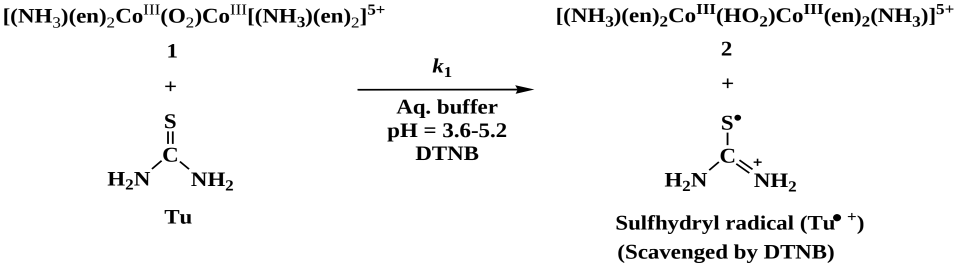
O_2- metabolism in the living organism are related to the alcohol induced oxidative stress and the O_2-derived species like superoxide ($O_2^{\cdot -}$) and hydrogen peroxide (H_2O_2) have often been implicated in the pathogenesis of acute and chronic tissue injury by activated phagocytes. Many of the living tissue damage done by O_2^- and H_2O_2 appear to arise by their metal-ion-dependent conversion into highly reactive oxygen radical. Thiourea and many of its derivative are very good direct scavenger of such radicals.



Besides this, thiourea and its derivatives have various important roles in agricultural and analytical field, which include applications in rubber industries as accelerators, in photography as fixing agents and to remove stains from negatives, and in agriculture as fungicides and herbicides. But in acetate buffer, reaction between $[(NH_3)(en)_2Co^{III}(O_2)Co^{III}[(NH_3)(en)_2](ClO_4)_5$ (**1**) and thiourea (T_{Tu}) followed complex kinetics and showed variable stoichiometry, moreover thiourea itself oxidised to produced sulfhydryl radical. In the presence of Eellman's reagent; 5, 5'-dithio-bis-(2-nitrobenzoic acid); DTNB, each mole of Tu quantitatively reduced one mole of the bridging superoxide ligand in $[(NH_3)(en)_2Co^{III}(O_2)Co^{III}[(NH_3)(en)_2](ClO_4)_5$ (**1**) and produced the hydroperoxo complex, $[([(NH_3)(en)_2Co^{III}(HO_2)Co^{III}[(NH_3)(en)_2]^{5+}$ (**2**). In the presence of Eellman's reagent the reaction became faster, and followed first order kinetics with a large excess of thiourea, over **1**. The observed first order rate constant (k_o) increases linearly with analytical concentration of thiourea (T_{Tu}). It was found that k_o increases with increasing $[H^+]$ but the linear plots of k_o against $[H^+]$ had definite intercepts. The solvent isotope effect is very small. This indicated a non-synchronous transfer of electron and proton from Tu to **1**. Therefore, in the above reaction the function of Eellman's reagent is to scavenge the sulfhydryl radicals.

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P-54

Catalytic promiscuity of two novel cobalt (II) complexes derived from redox non-innocent Schiff base ligands: unraveling the role of methyl groups in the ligand backbone on catalytic efficiency

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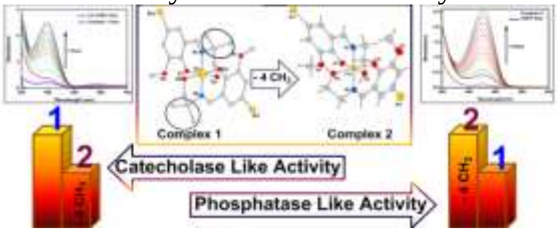
An important objective of bioinorganic chemistry is the development of coordination complexes that display catalytic activity analogous to the activity of enzymes. Over the course of time, designing of model catalysts exhibiting catalytic promiscuity *i.e.* bio-mimicking activity of different enzymes, draws emerging attention of bio-inorganic chemists.[1] A current approach for the development of bio-inspired catalysts by utilising first row transition metals is highly prevalent because of its low cost, global availability and reduced toxicity



Two Schiff base ligands namely (*E*)-4-bromo-2-(((1-hydroxy-2-methylpropan-2-yl)imino)methyl)-6-methoxyphenol($\mathbf{H_2L1}$) and (*E*)-4-bromo-2-(((2-hydroxyethyl)imino)methyl)-6-methoxyphenol ($\mathbf{H_2L2}$) were designed and synthesized by varying methyl groups to prepare cobalt(II) complexes $\mathbf{[Co(HL1)_2]}$(**1**) and $\mathbf{[Co(HL2)_2]}$(**2**) using cobalt(II) acetate as metal precursor. Complexes **1** and **2** were characterized by usual physicochemical techniques and solid-state structure of complex **2** was determined by X-Ray crystal structure analysis. The electrospray ionization-mass spectrometry (ESI-MS) analysis proved that complexes **1** and **2** were present as mononuclear entity in solution phase. The newly synthesized complexes were used to exploit their catalytic promiscuity. Catecholase like activity of both complexes**1** and **2** was carried out in *N*, *N*-dimethylformamide (DMF) medium using 3,5-di-*tert*-butyl catechol (3,5-DTBC) as model substrate(substrate: complex = 100:1)and the rate of the activity followed the trend,**1**>**2**. Phosphatase like activity was studied by using disodium salt of 4-nitrophenylphosphate(4-NPP) as model substrate in DMF-H_2O (substrate: complex = 20:1) mixture, indicating that the complexes were enormously accelerated the rate of phosphate monoester hydrolysis and the rate of the activity followed the reverse trend of catecholase like activity *i.e.* **2**>**1**. The role of methyl groups in the ligand backbone of $\mathbf{H_2L1}$ is supposed to be the determining factor to differentiate the catalytic efficiency of complexes **1** and **2** and the experimental observation has been supported by DFT calculations.

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P-55

Green Synthesis of Self Assembled Nano-Spherical Dysprosium MOFs: Selective and Efficient Detection of Picric Acid in Aqueous and Gas Phase

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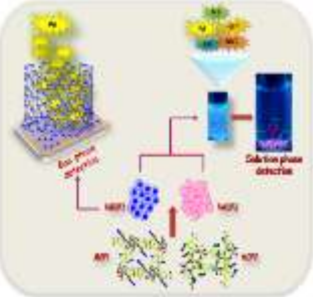
This work demonstrates solvothermal synthesis of two new lanthanide based MOFs namely, $[\{Dy(2N_3\text{-}TPA)_2(H_2O)(CH_3OH)\}]_\infty$ (**1**) and $[\{Dy_4(5N_3\text{-}IPA)_6(DMF)_3(H_2O)_4\}(DMF)(H_2O)_2]_\infty$ (**2**) derived from two carboxylate ligands namely, 2-azidoterephthalate ($2N_3$-TPA) and 5-azidoterephthalate ($5N_3$-IPA) respectively, with immobilized azide functionalities oriented towards the pore surfaces. Single Crystal X-ray Diffraction (SXRD) analyses reveal that **1** exhibit infinite 1D network while **2** display a 2D sheet structure with helical metal carboxylate chains. Both the compounds are found to exhibit excellent thermal and aqueous phase stabilities. A simple and convenient route has been adopted to reduce the particle size of the as synthesized compounds to prepare nanoscale Metal-Organic Frameworks (NMOFs). Unprecedentedly, nano spherical architectures are observed for both the cases under SEM and TEM analyses. These NMOFs are successfully exploited as fluorescent probe for the detection of various nitroanalytes such as nitrotoluene (NT), 2,6-dinitrotoluene (DNT), 4-nitrobenzoic acid (4-NBA) and picric acid (PA) etc. As suggested by the value of quenching constants, obtained from Stern-Volmer plots, the sensitivity of both the NMOFs towards PA sensing is exceptionally high. Furthermore, the time resolved fluorescence studies and theoretical calculations have been performed to speculate the excited state interaction of NMOFS with PA specifically. Moreover, selectivity towards PA sensing in presence of other structurally similar nitroanalytes and excellent reusability of the employed sensory platforms manifest great potentials of these materials for real life applications.



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P-56

Field-Dependent Magnetism and Slow Magnetic Relaxation Behavior in Mn(II) And Co(II) Coordination Polymers

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Coordination polymers (CPs) are inorganic or organometallic coordination compounds with repeating coordination entities composed of metal ions linked by ligands that form an extended array in one, two or three dimensions.[1] They are widely explored because of their structural tunability and find wide applications in molecular magnetism, heterogeneous catalysis, sensing, electrical conductivity etc.[2-4] In this presentation, we report four new Mn^{II}- and Co^{II}-containing magnetic CPs (**1** and **3**: Mn-containing; **2** and **4**: Co-containing) that have been synthesized at room temperature, using 5-bromo isophthalic acid (*Br-H₂isa*) and two different N-donating ancillary ligands [*bpe*: 1,2-bis(4-pyridyl)ethylene and *4-bpmh*: N,N'-bispyridine-4-yl-methylenehydrazine].[5] The complexes have been characterized by single crystal X-ray diffraction and other physicochemical techniques. Structure determination reveals two-dimensional (2D) coordination networks for all the complexes. In **1**, **3**, and **4**, Mn^{II} and Co^{II} dinuclear units are connected via Br-H_2isa ligands to form infinite 1D chains. The ancillary N,N'- donor spacer ligands interconnect the 1D chains into 2D coordination layers. Complex **2** can be viewed as being composed of cationic $[\{Co(bpe)\}_4]^{8+}$ square units that are joined by anionic Br-isa^{2-} bridges into a 2D grid-like framework. Complexes **1** and **3** (Mn) show a field-dependent change in magnetic behavior which is confirmed from the susceptibility measurements at varying fields, field-dependent magnetization measurements, as well as from hysteresis data. Complex **2** (Co) exhibits a slow magnetization relaxation phenomenon manifested by the AC susceptibility measurements at different temperatures and frequencies. Finally, complex **4** (Co) exhibits a magnetic feature that can be interpreted as antiferromagnetic exchange interactions between two syn-syn carboxylate-bridged Co^{II} atoms.

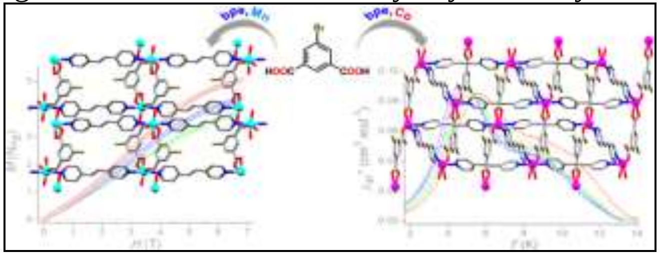

Figure 1. Schematic representation of the synthesis, structure and magnetic properties of the CPs.

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P-57

Exploring The Interaction of Stem Bromelain with Bile Salt Surfactants & Conventional Anionic Surfactants at Phosphate Buffer Medium of pH 7.0

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Stem bromelain (BM), a proteolytic enzyme isolated from pineapple (ananus cosmosus) stem belongs to cysteine proteinase family. This protein belongs to α + β protein class (like other crystalline proteinases, one such example is papain) with 23% helical structure, containing five (5) tryptophan (Trp.) units, whose characteristic absorbance (~280 nm) and emission (~354nm) varies with solvent polarities, determine the exposure of Trps in different environments, mediated by the interaction with surfactants. In this present study, we have used two Bile salt surfactants NaC and NaDC along with two anionic surfactants SDDS and SDBS, which interact with BM (0.005%) at phosphate buffer medium of pH 7. Tryptophan (Trp.) absorbance decreases initially with no shifting of absorbance peak at low concentration of SDDS, but at higher concentration, the native bromelain structure disrupts. Another anionic surfactant, SDBS shows the increment of Trp. absorbance at very lower concentration and then the absorbance peak gradually disappear with the increment SDBS absorbance peak (at 252 nm). In presence of bile salt NaC and NaDC, Trp. absorbance initially decreases at low concentration and after increases at high surfactant concentration. However the emission spectra were quite interesting shows the quenching and enhancement in the Trp. fluorescence for both the conventional anionic surfactants (SDDS and SDBS) with significant red/blue shift. In case of NaC, fl. Intensity of Trp. initially decreases at low NaC concentration and then intensity increases at high NaC concentraion with blue shift. NaDC only quench the fl. Intensity of Trp. Surface tension shows the interaction pattern of BM with surfactants, both in pre and post miceller region. The study of circular dichroism (CD) spectroscopy reveals the structural change of BM in presence of surfactants. Time resolved fluorescence spectroscopy (TCSPC) has also been performed. Several physicochemical parameters have been calculated from the outcome of these experiments.

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ISCTC-2020@DHWU

P-58

Green nanocomposites: Synergistic effect of nanoclay and short jute fiber on the mechanical properties of natural rubber

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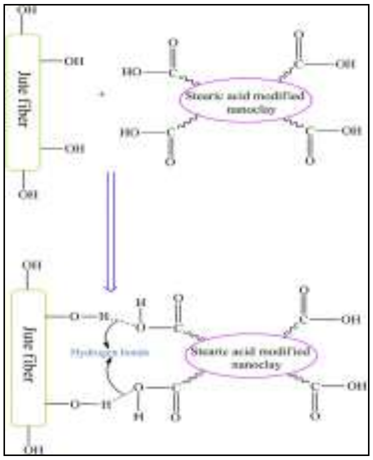
Green rubber composites can be tailored made to suit applications with desired properties by incorporating particulate natural fibers and clay into the natural rubber (NR) matrix. The effects of jute fiber on the mechanical as well as dynamic mechanical properties of the composites were studied. Effort has been given to investigate the synergistic effect of expanded nanoclay and jute fiber on natural rubber in the light of mechanical and dynamical properties and thermal properties. Synergistic interaction between short jute fiber and modified nanoclay increased the value of cure rate index (CRI) and tensile strength of NR composites successfully. The jute powder reinforced natural rubber composites were characterized by FTIR spectroscopy, scanning electron microscopy (SEM), dynamic and static mechanical property evaluation, thermo gravimetric analysis and evaluation of accelerated ageing properties. The presence of nanoclay has decreased the scorch time and optimum cure time of the rubber composite. The incorporation of jute has increased the modulus and tensile strength but marginally decreased the elongation of the jute-rubber composites. Incorporation of jute has shown very good ageing resistance of the rubber composite. Utilization of nanoclay and jute fiber has potentially enhanced the properties of natural rubber composites in a synergistic way.



The probable mechanism of interaction between jute fiber and stearic acid modified nanoclay

P-59

A Dinuclear Iron Complex as an Efficient Homogeneous Electrocatalyst for Water Oxidation Reaction

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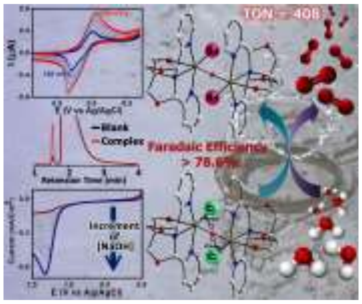
Among the current technologies for hydrogen production as an environmentally friendly fuel, water splitting has attracted great attention. However, the efficiency and turn over number of water electrolysis is severely limited for the oxygen evolution reaction (OER). To overcome this issue,the development of efficient electrocatalyst for the OER has drawn much attention.



Herein, we report a simple synthetic procedure and characterization technique for a newly prepared dinuclearoxo-bridged iron complex $[(FeLCl)_2O](FeCl_4)_2]$(L=(2-(pyridin-2-yl)oxazolidi-ne-4,4-diyl) and its electrocatalytic activity towards water oxidation reaction in acetonitrile medium with added sodium hydroxide solution. Experimental results show the catalyst is stable and produced molecular oxygen from water electrochemically with appreciable turnover number (408) along with high Faradic efficiency (>78.6%). Mechanistic investigation revealed by DFT calculations are performed.

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P-60

Role of coagulase negative staphylococci in colonization and subsequent degradation of plastic packaging surfaces

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Bacterial interaction with various polyethylene (PE) based packaging materials that include two varieties of biodegradable and three varieties of conventional PE carrier bags has been studied. Two different staphylococcal strains,BP/SU1, *Staphylococcus epidermidis* (MTCC, Chandigarh accession no. 9538) and BP/SU2, *Staphylococcus haemolyticus* (MTCC, Chandigarh accession no. 5731) are utilized for the study. The topography and wettability of a plastic surface along with the cell surface hydrophobicity of the bacterial strain are the determining factors in bacterial colonization. It has been found that the surface properties of the plastic packaging material dictate the propensity of bacteria to adhere. Reuse of these plastic carrier bags make it more hydrophobic and better bacterially assimilated irrespective of whether it is marketed as biodegradable or not.

P-61

Colorimetric detection of Th^{4+} ion using CuO nanoparticles prepared by grafted Tricholoma mushroom polysaccharide

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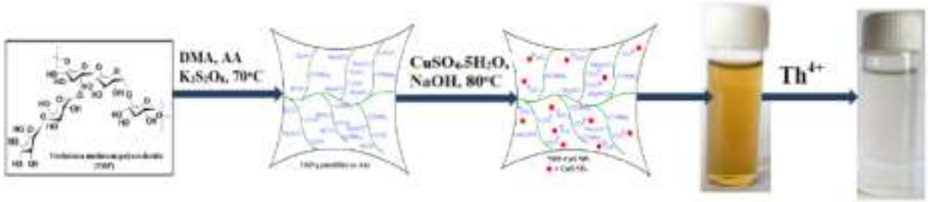
Natural polysaccharide based graft copolymer has gained considerable importance because of their eco-friendly behaviour. Over the last few years, the preparation of metal nanoparticles of different shape and size is an important area of research in the field of material sciencefor their various applications such as catalyst, toxic metal sensing, etc. The use of graft copolymers based on natural polysaccharides has been recognized to be the most promising hosts for the synthesis of metallic nanoparticles (MNPs) because of their outstanding biocompatible and biodegradable properties. Mushrooms are the potential source of different polysaccharides. A number of polysaccharides have been isolated from the mushrooms of different genus. Structural investigation of polysaccharides showed the presence of different types of glucans and heteroglycans. A natural polysaccharide (TMP) was isolated and purified from an edible mushroom *Tricholoma crassum* (Berk.) Sacc, that belongs to the family of Tricholomataceae having no toxicity, cultivated abundantly in the Asia region. The Tricholoma mushroom polysaccharide (TMP) is used for the synthesis of graft copolymer TMP-g-poly(DMA-co-AA) with a mixture of N,N-dimethyl acrylamide (DMA) and acrylic acid (AA) in presence of potassium peroxydisulphate ($K_2S_2O_8$) as the radical initiator. The synthesised graft copolymer TMP-g-poly(DMA-co-AA) is used for the preparation of TMP-CuO-composite nanoparticles [TMP–CuO NPs] by an eco-friendly approach. The ^{1}H-NMR, FTIR spectroscopy, FESEM analysis are performed for the characterization of the graft copolymer. TMP-CuO NPs are well characterized by UV-Visible and FTIR spectroscopy, XRD, EDAX, HRTEM, FESEM, and DLS analysis. The prepared TMP-CuO NPs have a unique property for sensing of toxic Th^{4+} in water medium, which is investigated by colorimetric method



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P-62

mTORC2 promotes propagation of GBM cancer stem cells by activating Hedgehog pathway through Gli2 nuclear translocation

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Glioblastoma multiforme (GBM) represents the most common form of malignant brain tumors in adults. The survival rate is extremely low because of its high grade status and aggressiveness. The heterogeneity of GBM is maintained by a small subset of the cell population defined as cancer stem-like cells (CSCs). CSCs undergo asymmetric division and are mainly responsible for the propagation, invasion, metastasis and recurrence. Mammalian target of rapamycin complex 2 (mTORC2) is aberrantly activated in cancer and therefore is considered to be an important therapeutic target. Hedgehog pathway that also often hyperactivated in CSCs, regulates transcription of several genes associated with angiogenesis, metastasis, cellular proliferation and cancer stem cell regeneration. However, contribution of mTORC2 towards Hedgehog pathway activity, yet not been explored. Here we have addressed the molecular crosstalk between mTORC2 and Hedgehog pathway activities in the context of GBM, using as a model system. We observed that higher mTORC2 activity enhanced expression of a few Hedgehog pathway molecules (Gli1, Gli2 and Ptch1) and amplified its target genes (Cyclin D1, Cyclin D2, Cyclin E, Snail, Slug and VEGF) both in mRNA and protein levels as reflected by increased metastasis, angiogenesis, cellular proliferation and stem cell regeneration. Inhibition of mTORC2 formation by a carbazole alkaloid, mahanine as a mTORC1/2 inhibitor, decreased Hedgehog pathway activity and attenuated all these above-mentioned events, suggesting their crosstalk with each other. Further investigations revealed that mTORC2 inhibited ubiquitination of Gli2 by inactivating GSK3β and thus promotes stability to Gli2 and its nuclear translocation. Moreover, enhanced mTORC2 activity led to the increase clonogenic properties and $CD133^+$ cells (CD133, a surface marker for CSCs) indicating its role in CSCs regeneration. mTORC2 inhibitor directed reduction of Hedgehog pathway proteins and also reduced CSCs. Thus, our observations support a role for elevated mTORC2 activity in regulating angiogenesis, metastasis, cellular proliferation and CSCs regeneration via Hedgehog pathway activity. Taken together it provides a rationale for including mTOR2 inhibitor as part of the therapeutic regimen for CSCs.

P-63

Dithiocarbamato complexes of dirhenium(II,II): Spectroscopic, structural, cytotoxicity and computational studies

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The rich redox properties of the metal-metal bonded dirhenium complexes have fuelled the interest in developing the chemistry of dirhenium.[1-4] Several decades ago the dirhenium complex $Re_2Cl_4(\mu\text{-dppm})_2$ (**1**) where dppm is $Ph_2PCH_2PPh_2$, with a $\sigma^2\pi^4\delta^2\delta^{*2}$ electronic configuration has been prepared.[5] $Re_2Cl_4(\mu\text{-dppm})_2$ contains labile chloride ligands in combination with substitutionally inert dppm ligands, but none has yet been reported in which the dppm and the Cl ligands have been replaced by other chelating ligands. Of the great variety of dirhenium complexes that are reported, [1] few have been isolated that contain dithiocarbamato ligand in the coordination sphere. We are aware of only the $Re_2(\mu\text{–}S)_2(S_2CNR_2)_4$ and $[Re_2(\mu\text{–}SS_2CNR_2)_2(S_2CNR_2)_3]^+$ complexes.[6] We have recently reported dithiocarbamato bridged paramagnetic dirhenium (III,II) complexes formed by the reaction of $Re_2(\mu\text{–}O_2CCH_3)Cl_4(\mu\text{-dppm})_2$ with different dithiocarbamato ligands.[7] No other dithiocarbamato complexes of dirhenium are reported in the literature. It was important to explore the reaction chemistry of **1** with dithiocarbamato ligands in order to assess the stability of the Re_2^{4+} core of **1** to ligands of this type. In the course of this work it was observed that under refluxing condition in dry ethanol, **1** reacts with the sodium salts of three different dithiocarbamato ligands to afford the diamagnetic Re_2^{4+} complexes $Re_2(\mu\text{–dppm})(L_R)_4$ [L_R=dithiocarbamato ligands] where substitution of four chloride and one dppm ligands occurs and the four dithiocarbamato ligands are involved in the chelating coordination modes to the dirhenium core. This is, to our knowledge, the first example of dithiocarbamato chelated dirhenium complexes with a Re_2^{4+} core containing dppm ligand. The synthetic procedures, structure and properties of the resulting complexes are reported. Density function theory (DFT) and time-dependent-DFT studies have also been carried out. The cytotoxicity of the complexes to the human lung and cervical cancer cell lines A549 and HeLa respectively was also evaluated by MTT assay.

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ISCTC-2020@DHWU

P-64

Metal-mediated Strategies toward Biologically Significant Small Molecules

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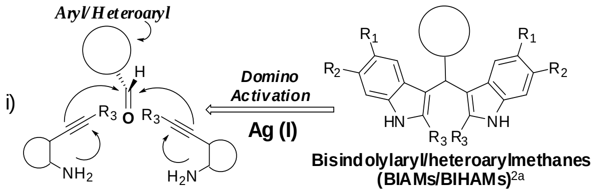
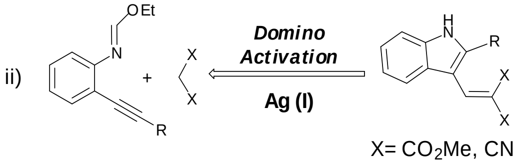
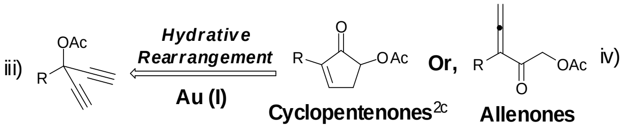
Since late twentieth century, metal catalyzed activation of alkene and alkyne unit plays an important role for the construction of biologically relevant small molecules.[1] Among various novel strategies, ring-closing olefin metathesis[1a], intramolecular Heck reaction[1b] and transition metal catalyzed cycloaddition/ cycloisomerization involving alkyne unit[1c] contribute significantly during synthesis of numerous biologically relevant heterocylic and carbocylic cores. Herein, some of our interesting approaches toward some biologically privileged moieties like indole,[2a,b] cyclopentenone[2c] and dihydrofuran[2d] would be presented.



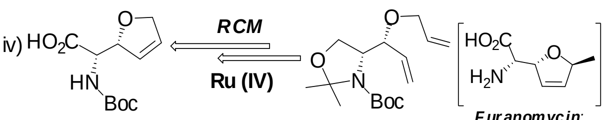
Novel 3, 3/-bisindolylmethane alkaloids (BIMs), isolated from various terrestrial and marine natural sources display remarkable biological activities.



Two derivatives[2b] are known to have antiproliferative activity on human MDA-MB 231 and MCF-7 breast cancer cells in a microplate assay



Many pharmaceuticals (e.g., Prostaglandins, Limaprost, Misoprostol, etc.) contain an alkyl substituent at the α-position of their cyclopentenone skeleton.



Dihydrofuranylglycine[2d]

***Furanomycin**: An important antibiotic (Isoleucine antagonist)*

References:

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P-65

Unveiling the binding interaction of zinc(II) complexes of homologous Schiff-base ligands on the surface of BSA protein: A combined experimental and theoretical approach

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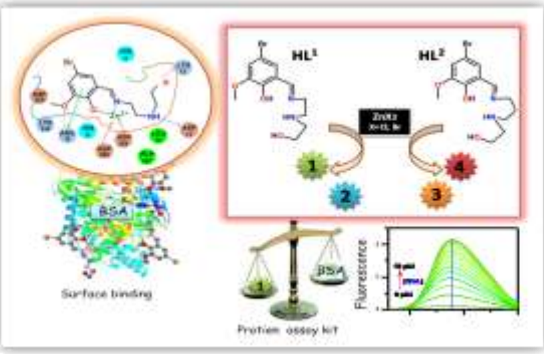
In the field of pharmacology not only synthesis of drugs is a matter of challenge but analysing their interaction with plasma proteins is also a major determinant of drug disposition, transportation and metabolism. Transport of metal based drugs through the blood stream requires the involvement of serum albumins among other proteins.



In this context we have synthesized four novel fluorescent Zn(II) complexes with two homologous ligands HL^1 and HL^2 with a purposeful intension to elucidate their mode of binding with Bovine serum albumin (BSA). Absorption, fluorescence, ITC, CD studies provide an evidence of strong 1:1 binding of the zinc(II) complexes with BSA protein having binding constant value in the range ~$0.94\text{-}4.51\times10^4$ M^{-1}. Complete thermodynamic profile (ΔH^o, ΔS^o and ΔG^o) have been evaluated that indicates presence of coordination interaction, Van der waals interaction occurring between our complexes and Asp254, Asp258, Asp13, Lys12, Arg10 amino acid residues of BSA. Elucidation of more conclusive information about the binding interaction has been achieved from molecular docking and dynamic studies. Binding of our complexes at the surface of BSA is the main potency of this work and that particular phenomenon has been exploited to measure unknown concentration of BSA protein. This is the first time to report zinc mediated Schiff base complex as a protein assay kit.

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P-66

Macrocyclic tetranuclear Zn^{II} complex as receptor for selective dual fluorescence sensing of F^- and AcO^-: effect of macrocyclic ligand

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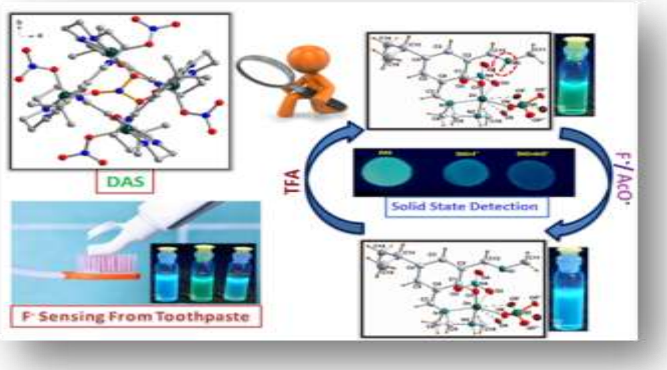
The design and synthesis of new specific receptors for the detection of biologically important cationic and anionic species with high selectivity in aqueous medium is still one of the greatest challenges in chemistry.[1] Nowadays a huge number of single ion responsive sensors that are selective for cations or anions have been reported.[2,3] Anions play a fundamental role in a wide range of chemical and biological processes, and numerous efforts have been devoted to the development of abiotic receptors for anionic species.



A 48-membered macrocyclic Zn^{II}-Schiff base complex **DAS** (Dual Anion Sensor) containing protonated imine has been synthesized and characterised. The single crystal X-ray structural analysis reveals a tetranuclear complex cation $[Zn_4(LH_3)(NO_3)_5]^{2+}$counterbalanced by a $[Zn(NO_3)_4]^{2-}$ anion. **DAS** acts as a dual anion sensor which can selectively detect fluoride and acetate in aqueous methanolic solution by change in UV-Vis spectra as well as by fluorescence enhancement. A probable mechanistic pathway has been proposed and DFT calculations corroborate well with the experimental data. Interestingly, **DAS** behaves as an **INHIBIT** logic gate with F^-/AcO^- and H^+ as inputs.

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P-67

Hydrothermal synthesis of a novel hybrid mesoporous material and its potential application in fuel cell

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Novel phosphate based hybrid materials[1] with dual porosity have been synthesized hydrothermally in absence of any structure directing agent in aqueous medium. The powder X-ray diffraction patterns for the hybrid material shows two intense peaks in the low angle diffraction pattern together with few other low intensity peaks. Transmission Electron Microscopy image of the sample confirms the micropores of *ca.* 1.5 nm in the specimen. The pore size distribution profile suggested the existence of large micropores of 1.4-1.6 nm pore width together with a very large mesopore having a broad peak maximum at 5.0 nm. The BET surface area[2] and the total pore volume for this sample were 215 m^2g^{-1} and 0.3 cm^3g^{-1}, respectively. The ^{13}C and ^{31}P MAS NMR spectrum confirmed the incorporation of phenyl group and it's attachment to the phosphonate moiety in this hybrid material. Field emission scanning electron microscopic images of this sample suggested the formation of very small nanocrystallites of 10-20 nm in size. Unique feature of this material is that the large micropores and mesopores[3] present in the framework was generated without the addition of any external structure directing agent. Phenyl groups attached to the P atoms at the pore mouth could repel the nearest phenyl groups of the neighboring P atom through Van der Waals force. This might be the origin of large micropore and mesopore. High sorption capacity of H_2 under cryogenic condition suggested the potential utility of this material in fuel cell.

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P-68

Pd-Catalyzed 3-Amino-1-Methyl-1H-Pyridin-2-one Directed C(sp^2)-H Arylation and Methylation

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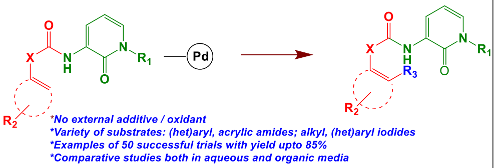
Over the past decades directing group mediated transition metal catalysed C-H bond functionalization has become a practical and robust tool for the preparation of different types of valuable organic molecules. C-H functionalization, catalyzed by palladium and other precious and non precious metal has found widespread use for the transformation of uncreative C-H bonds into carbon- carbon (C-C) and carbon- heteroatom (C-X) bond formation at both sp^2 and sp^3 carbon centers.[1] Practically, C-H arylation has become an effective alternative to traditional C-C cross-coupling reactions due to the minimization of stoichiometric metallic waste and the costs associated with the preparation of starting materials. Small molecules containing 2-pyridone unit has received much attention due to their significance in medicinal chemistry. Regarding this, development of novel methodologies *via* metal catalyzed carbon-carbon bond formation by chelation assisted C-H activation will be an attractive method to achieve therapeutically important 2-pyridone analogues and arylated acid synthons.



*No external additive / oxidant
*Variety of substrates: (het)aryl, acrylic amides; alkyl, (het)aryl iodides
*Examples of 50 successful trials with yield upto 85%
*Comparative studies both in aqueous and organic media

The development and utilization of bidentate directing groups in palladium-catalyzed transformations has come into limelight in recent years, considering bidentate directing groups are more encouraging tools to achieve transformations which were unsuccessful with conventional monodentate systems.[1b, 2] In this context, we report our studies on Pd(II)- catalyzed coupling reaction between methyl, aryl, heteroaryl iodides and sp^2 carbons both at β and γ positions using 3-amino-1-methyl-1H-pyridin-2-one (AMP) as an efficient, built-in bidentate *N*, *O*-directing group (DG) towards the synthesis of pyridone derivatives. The effect of temperature, solvent, reagent equivalence and substrate has been investigated for this DG mediated late stage functionalization reactions along with crystal structure of a selected analogue. Moreover, this DG has been applied successfully for ortho selective C(sp^2)-H activation in water as sole reaction medium in high yields to demonstrate the practicability of this methodology. I want to focus on a few results.

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ISCTC-2020@DHWU

P-69

Crystal Structure Analysis Of (2s*, 3ar*,4s*,7as*)-2,3,3a,4,5,7a-Hexahydro-3a,4-Bis(Methylsulfonyloxymethyl)- 2-Vinyl-1h From Laboratory X-Ray Powder Diffraction Data

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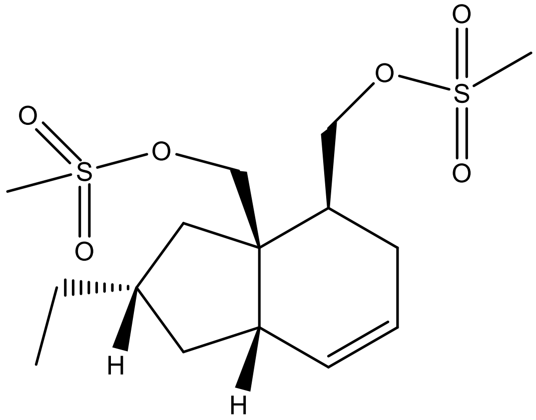
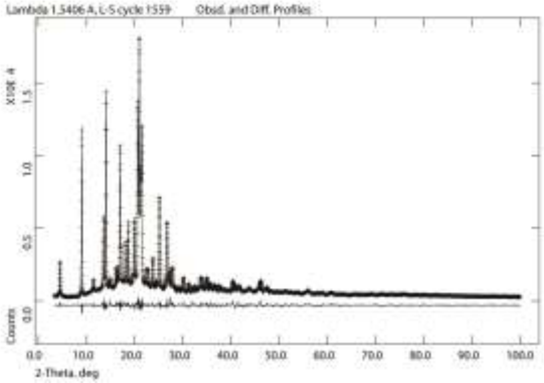
Hydrindane system with an angular substituent is frequently encountered in terpenoids. Cis-hydrindane derivative, (2S*, 3aR*,4S*,7aS*)-2,3,3a,4,5,7a-hexahydro-3a,4-bis(methylsulfonyloxymethyl)- 2-vinyl-1H-indene has been used as a precursor to the synthesis of biologically active diterpene umbellactal. The crystal structure of this hydrindane derivative has been solved from laboratory X-ray powder diffraction data using the direct space approach and refined through the Rietveld method to R_p=0.427 and R_{wp}=0595. The five- and six-membered rings in the title hydrindane derrivative assume a half-chair and an envelope conformations. The molecular conformation as established from crystallographic analysis agrees well with that obtained from the solid state DFT calculations. Intermolecular C-H...O hydrogen bonds link the molecules of the title compound into one-dimensional polymeric chains parallel to the [100] direction.



Chemical diagram



Rietveld plot.

P-70

Interaction of d^{10} metal ion with potential organosulfur complexes of Platinum metals.

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Recently Platinum metals incorporating organosulfur complexes of type $[M(L^S)ClP_2]$ (M = Ru, Os, Rh and Ir, P = PPh_3) behaves as a potential complexes as well as potential ligands in organometallic chemistry. These complexes has been synthesized following in situ $C(sp^2)$-H and $C(sp^3)$-S/C–hetero atom bond scissions,[1] of multidentate C^N^S ligand L^{SR} in the presence of analogous $MCl_3 \bullet 3H_2O$ and excess phosphines. The high electron density on the M-thiolato-S concerning superior nucleophilicity can be visualized through the formation of a number of S-centered derivatives, such as the oxygenation to sulfenato or sulfinato,[2] alkylation[3] and metalation[4] processes. Enormous interest has been paid to stabilize and characterize metal-bound thiyl complexes $(M(ArS^\bullet)L_n)$ since thiyl radicals have been used by nature in various biochemical processes.

Remarkable nucleophilic character as well as the high electron density on the M-thiolato-S can be envisaged through the formation of a number of S-centered derivatives. This observation has been corroborated with the nature of HOMO in M-thiolato, which assumes 50% of S_{3p}. From both the experimental and theoretical findings that of enhanced electron density on thiolato-S reveal to explore the reactivity of potential thiolato metalloligand toward soft thiophilic metal centers having closed-shell d^{10} configuration ($M' = Ag^+$, Au^+ and Hg^{2+})[5] with the aspiration of possible formation of S-bridged heterometallic aggregates. It should be noted that μ_2-S homo-dinuclear compound $[M^{III}(L^S)Cl(PPh_3)]_2$ is formed almost quantitatively from precursor M-thiolato in presence of soft metal ions. The exclusive formation of sterically encumbered syn-dimer instead of its anti analogue can plausibly be elucidated due to intramolecular noncovalent phenyl-phenyl along with *metallochelate-metallochelate* stacking interactions. In the course of synthesis of syn-dimer, a hexanuclear μ_3-S intermediate $[Ir^{III}Ag^I_2(L^S)Cl(NO_3)_2(PPh_3)_2(CH_3CN)]_2$ incorporating 8-membered $\{Ag_4S_2O_2\}$ metallacycle was isolated in excellent yield in the crystalline state. The stability of remarkable macrometallacycle can be attributed to the intramolecular argentophilic interaction[6] along with noncovalent Ag····C and Ag····O short contacts besides the classical covalent bonding of μ_2-bridged S and O atoms.

The organosulfur compounds exhibit rich spectral properties including inherent physicochemical properties[7], luminescence and they are very important in the stand point of supramolecular design.

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P-71

Examination of the reaction pathways of IO+BrO reaction

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In the lower stratosphere region, ozone plays a vital role in protecting harmful ultra-violet (UV) radiation in reaching to our earth and thereby decreases several hazardous effects on human life and civilization, like sunburn, skin cancer, global warming, effects on earth's environment, impact on vegetation, etc. Several natural occurring processes, factory outlets, preservation processes contain Chlorofluorocarbons (CFCs) and other chemicals containing halogens (Cl, Br or I) those are generally grouped as Ozone Depleting Substances (ODS). These ODS chemically react with the ozone in the stratosphere and there by deplete the ozone layer.

However, experimental investigations on these systems are available, theoretical investigations in this line are limited. The present report is focused on such an important ozone depleting key reaction of IO with BrO. This reactions proceed through different channels, viz.

$$\begin{aligned} \mathrm{IO + BrO} &\rightarrow \mathrm{Br + OIO} \\ &\rightarrow \mathrm{I + BrOO} \rightarrow \mathrm{I{+}Br{+}O_2} \\ &\rightarrow \mathrm{IBr + O_2} \\ &\rightarrow \mathrm{I + OBrO} \end{aligned}$$

Here, *ab initio* calculations have been performed to investigate various minimum energy geometries and transition state geometries formed in course of the reactions, spectroscopic constants, heat of reaction and reaction pathways to the different channels. The data may be helpful in understanding their effectiveness in ozone depletion as well as future references.

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P-72

Methylglyoxal conjugated with chitosan nanoparticles as a potential anticancer agent

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Methylglyoxal (MG), a ketoaldehyde & normal metabolite has been known for its anti-cancer property exclusively in malignant cells. MG specifically kills cancer cells by inhibiting glycolysis and mitochondrial respiration without much adverse effect upon normal cells.

One of the major limitation of using MG as an anticancer drug is that MG is rapidly degraded by various enzymes present in the body. So any shielded nanoparticles drug delivery system that may prevent this degradation of MG *in vivo* would be more competent as an anticancer drug. Keeping this in mind nanoparticulated methylglyoxal (Nano-MG) was prepared by conjugation of MG with bio-polymer chitosan by Schiff's base formation and characterized. The average diameter of Nano-MG was ~ 60 nm and containing ≈ 100µg of MG/ml of prepared Nano-MG solution. Ehrlich ascites carcinoma (EAC) cells, human breast cancer cell line HBL-100, and lung epithelial adenocarcinoma cell line A549 were used as test systems to compare Nano-MG with bare MG in vitro. *In vitro* studies with Nano-MG showed higher cytotoxicity and enhanced rate of apoptosis in HBL-100 and A549 cell line in comparison with bare MG, but no detrimental effect on normal mouse myoblast cell line C2C12 at the concerned doses. *In vivo* studies were performed on both EAC cells inoculated and also in sarcoma-180-induced solid tumor-bearing Swiss albino mice to assess the anticancer activity of Nano-MG in comparison to bare MG with varying doses, times and administrative routes. Efficacy of Nano-MG was about 200 fold higher in EAC bearing mice and about 75 fold higher in Sarcoma-180 induced solid tumor bearing mice than its bare counterpart.

All these data suggest that Nano-MG may constitute a promising tool in anticancer therapy in near future.

P-73

A treatise on free radical in the basis of human life

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A chemical entity having an unpaired electron in its outermost shell is called free radical. It has an acute intension to capture electron from other molecule. Scientific knowledge about free radicals is very important for our biological system. Free radical mainly binds with lipid, protein and DNA in our body. They have some beneficial roles: (i) destroy of pathogen, (ii) kill cancer cells, (iii) keep brain active, (iv) keep muscles smooth, (vi) control of the internal organ etc. On the other hand, increase of concentration of free radical causes various disease such as Alzhimer’s because various disease such as Alzhimer’s perkinson’s, rheumoid arthritis, aging, cancer etc. There are different types of free radicals such as: a. Singlet Oxygen (O_2), b. Hydroxyl radical ($OH^{\cdot}$), c. Super oxide radical $(O^{-\cdot})_2$ d. Peroxyl Radical ($ROO^{\cdot}$). Diagnosis of free radical done by following techniques:
a. Electron spin resonance, b. Nuclear magnetic resonance using a phenomenon called CIDNP.

P-74

Kinetics of alkaline hydrolysis of methyl green: Effects of surfactants

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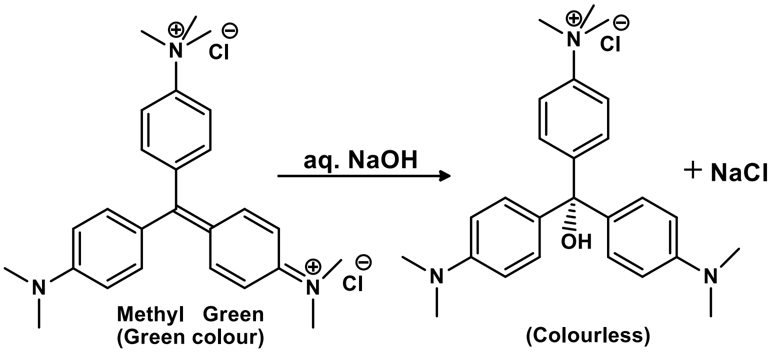
The alkaline hydrolysis of methyl green has been studied in presence of two anionic surfactants, viz., sodium dodecylsulfate (SDS) and sodium bis(2-ethylhexyl) sulfosuccinate (AOT) in the sub-micellar region in the temperature range 293 to 308 K. A decrease in the rate constant with increasing surfactant concentration has been observed reaching to a limiting minimum value. The inhibition effect has been explained in terms of different models of pre-miceller catalysis. The same reaction has also been investigated in the presence of aqueous solutions of different potassium salts such as chloride, bromide and iodide. The reaction rate has been found to be inhibited by all the halide salts. The decrease in reaction rate with increasing salt concentration may be explained on the basis of modified Bronsted-Bjerrum equation. Thermodynamic parameters and binding constant for substrate-surfactant interactions in the pre-cmc region have been evaluated.



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P-75

Development of Targetable ‘Turn-On’ Fluorogenic Probes for Carbon Monoxide Imaging in Living Cells

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Carbon monoxide (CO) has long been known as a toxic pollutant, often called the "silent killer" because of its tasteless, colourless, odorless and particularly hard to sense nature.[1,2] Despite its deadly status, it is evident from various studies that CO can be continuously produced in our human body *via* endogenous degradation of heme by a family of inducible (HO-1) and constitutive (HO-2) heme oxygenase enzymes.[3] CO, a gasotransmitter molecules, was considered to be an important versatile signaling bio-molecule with significant therapeutic potential protecting from inflammatory, vascular or even cancer diseases.[4,5] It has an essential controlling role in a variety of physiological and pathophysiological processes that take place within the nervous, cardiovascular and immune systems.[6] These have fascinated unparalleled attention for deepening research of CO in biology. Many chemical and biological aspects of CO remain elusive owing to having the lack of ways for selective monitoring of this transient small molecule. Thus, the development of the selective method for direct tracking of this small molecule in living systems is of great scientific concern.

In this research, for the first time, we have designed and developed simple and effective lysosome and nuclear cell compartment targetable fluorogenic probes based on *3-nitro naphthalimide* platform that can detect selectively carbon monoxide (CO) in HEPES buffer (pH 7.4, 37 °C). The probable detection mechanism was established through the transformation of nitro to the amino functionalized system in the presence of CO. Probes triggered a ‘turn-on’ fluorescence response to CO with a simultaneous increase of fluorescence intensity by more than 50-times. The responses are selective over a variety of relevant reactive nitrogen, oxygen, sulfur species and also various biologically important cationic, anionic and neutral species. Also, these fluorogenic probes serve as efficient candidates for monitoring intracellular CO in living cells and the fluorescence signals predominantly localize in the lysosomes compartment (MCF7) and nuclear-region (Raw 264.7, and A549 cells).

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P-76

Kinetics and Mechanism of Chromic acid Oxidation of D-Galactose in the Presence Of 1,10-Phenanthroline Catalyst in Sulfuric Acid Micellar Media

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In aqueous sulfuric acid media, Cr^{VI} oxidation of D-Galactose in the presence and absence of catalysts like1,10-phenanthroline (phen) have been carried out under the conditions, $[\text{D-Galactose}]_T >> [Cr^{VI}]_T$ at different temperatures. Under the kinetic conditions, the monomeric species of Cr^{VI} has been found kinetically active in the absence of phen catalysts while in the heteroaromatic N-base catalyzed path, the Cr^{VI}-phen complex has been suggested as the active oxidants. In the catalysed path, Cr^{VI}-L complex (L = phen) receives a nucleophilic attack by the substrate to form a ternary complex which subsequently experiences a redox decomposition through two electron transfer leading to the organic products and Cr^{IV}-L complex. Both the uncatalysed and catalysed paths show the first order dependence on $[\text{D-Galactose}]_T$ and $[Cr^{VI}]_T$. The uncatalysed path shows a second order in $[H^+]$. But the catalysed path shows a first order dependence on $[H^+]$. The heteroaromatic N-base catalysed path is first order in $[\text{phen}]_T$. These findings remain unchanged in the presence of externally added surfactants. The cationic surfactant i.e. *N*-cetylpyridinium chloride (CPC) inhibits the rate in catalysed paths. The observed micellar effects have been rationalized by considering the distribution of the reactants between the micellar and aqueous phases in terms of the proposed reaction mechanism.

P-77

Bio-orthogonal Chemistry: Ethynylation of cysteine-containing peptides

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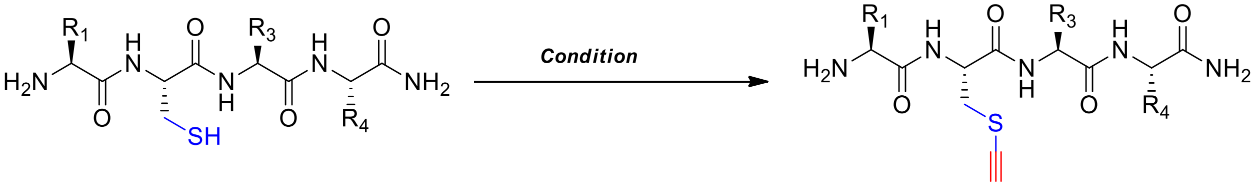
Regardless of their comparatively low profusion in proteins, cysteines are vibrant for cellular biochemistry. For example, cysteines form disulfide bridges, are actively involved in enzyme catalysis as nucleophiles and can be post translationally oxidized or modified through palmitoylation, prenylation or nitrosylation.[1a] Many of the so-called functional cysteines display noticeable hyperreactivity and these reactive hot spots can be precisely identified in complex proteomes with broad-range electrophilic probes.[1b] Such probes represent particularly useful tools for competitive activity-based protein profiling.



Small-molecule thiols are readily alkynylated by alkynyl benziodoxolones (EBX reagents).[1c] Ethynylation of cysteine is a big challenge as not only it is an easily oxidizable group but also lack of suitable ethynyl containing reagents. Taking account in mind in our laboratory we have developed a protocol to achieve ethynylation of cysteine-containing peptides. How this labeled protein can post functionalized using different chemistry of terminal alkyne segments have been demonstrated. I report recent work on ethynylation of cysteine-containing peptides and its application in biological systems by using hypervalent iodine reagents with our ongoing project on "umpolung strategy"[1d-i] and biorthogonal Chemistry.

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P-78

Differential Regulatory T-Cell Modulation in Early Infection Models of Antimony Sensitive and Resistant *Leishmania donovani* Parasites

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The disease Kala-azar caused by *Leishmania donovani* (LD) is characterized by the depression of host cellular immune response. In the Indian subcontinent LD parasites are mostly resistant to commonly used antileishmanial drug, like sodium antimony gluconate (SAG). It is known that infection with pentavalent antimony (Sb)-resistant parasites induce aggressive pathology.

Very limited information is available on the host-parasite interaction at the onset of disease. As a surrogate of early *in vivo* immunological scenario we studied the interaction between normal human peripheral blood mononuclear cells (PBMCs) with Sb-sensitive and Sb-resistant parasites. We exposed PBMCs from healthy human beings for up to 8 days, to either pentavalent antimony sensitive (SbS-LD) or resistant (SbR-LD) *Leishmania donovani* clinical isolates, in order to compare some of their immune signatures.

Towards the beginning of the experiments we found $CD4^{+}CD25^{-}CD127^{-}$ type-1 T-regulatory (Tr1) cell population to produce IL-10 in both antimony sensitive and resistant parasite exposed cultures. But, in contrast to SbS-LD, there was a pronounced increase in the IL-10 producing $CD4^{+}CD25^{+}CD127^{low/-}$ inducible T-regulatory cells (iTregs) in the PBMC cultures with SbR-LD parasites sampled at day 8. Assessment of suppression capacity of the sorted iTregs from different cultures on day 8 revealed that iTregs from SbR-LD exposed PBMCs had more pronounced suppressive ability compared to SbS-LD counterpart. Suppression function of SbR-LD induced iTregs were dependent on both IL-10 and TGF-β, whereas the SbS-LD induced iTregs mainly relied on IL-10 for their suppressive ability. This ability to trigger secretion of both IL-10 and TGF-β from SbR-LD induced iTregs was found to be dependent on the unique surface biochemistry of these parasites. These SbR-LD parasites have a unique surface glycan signature that modulates the host immune system more aggressively. Thus, giving rise to higher pathogenesis in case of antimony resistant *L. donovani* infection.

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P-79

Fluorescence Sensor for Lysosome-Targeting Cellular Imaging of Hg^{2+} in Living Cells

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A heavy-metal ion like mercury (Hg) is most toxic to the most living organisms.[1,2] Intake of any form of mercury is highly toxic and effectively perturbs brain, kidney, and immune systems as well as the nervous system at very low concentrations.[3,4] The toxic nature of Hg^{2+} has gathered unparalleled attention, deepening the research of mercury in biology. Various biological and chemical aspects of Hg^{2+} remain undisclosed owing to having a lack of a selective method for direct tracking of this ion in the cellular compartment. Thus, the development of the selective method for direct tracking in a targetable manner of this Hg^{2+} in living systems is of great scientific interest. So, there is a strong need to develop simply prepared fast responsive selective fluorescence sensors for Hg^{2+} that can work in an aqueous medium. To the best of our knowledge so far, to date, there has been no description of any targetable fluorescence sensor in the literature that can selectively detect lysosomal Hg^{2+} in living cells.

A new lysosome-targetable fluorescence sensor was designed and synthesized based on *4-methyl-2,6-diformylphenol* as a fluorophore. The fluorescent probe displays highly sensitive fluorescent detection of Hg^{2+} in HEPES buffer solution (10 mM, DMSO 1%) of pH 7.0 at 37 °C due to the formation of highly fluorescent formyl-functionalized derivative. The sensor triggered a "turn-on" fluorescence response to Hg^{2+} with a simultaneous increase of fluorescence intensity by 180-fold just after 10 min. The response is very selective over a variety of biologically relevant cations, anions, molecules, and competitive toxic heavy metal cations. The limit of detection (LOD) was calculated as low as 6.82 nM. Also, the sensor is able to monitor the subcellular distribution of Hg^{2+} specifically localized in the lysosome's compartment in the MCF7 human breast cancer cell line by fluorescence microscopy.

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P-80

Magnetically separable Pd(0)@Fe_3O_4@AHBA nanocatalyst: C-C coupling reactions

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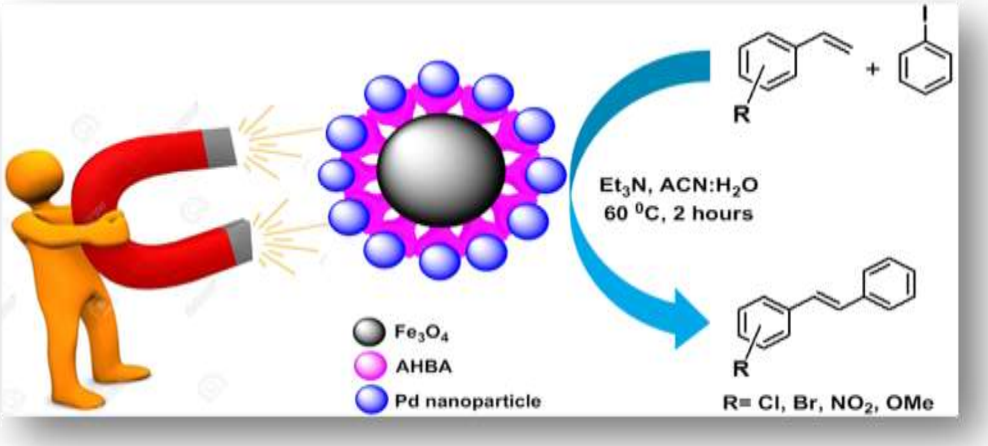
Here we have developed a new method to synthesize a novel magnetically separable Fe_3O_4@AHBA@Pd(0) [AHBA=3-amino-4-hydroxybenzoicacid] heterogeneous nanocatalyst via anchoring of palladium(0) on the surface of AHBA-coated Fe_3O_4 nanoparticles. The synthesized nanocatalyst was characterized by FT-IR, PXRD, ICP, XPS, FESEM, EDX, TEM, TGA, BET and FT-RAMAN analysis. X-Ray photoelectron spectroscopy (XPS) study prove the presence of Pd(0) on the surface of Fe_3O_4@AHBA. BET analysis exhibits high surface area of the prepared nanocatalyst which craft catalytic activity towards Heck coupling reactions with high turnover frequency (TOF) at 60 °C in water-acetonitrile solvent within 2 hours. The nanocatalyst can be easily recovered from the reaction mixture by using an external magnet and recycled up to six times without significant decrease in its catalytic activity. All the isolated products are obtained as solids or oils, fully characterized by ^{1}H-NMR spectroscopy.



P-81

A New Turn-On Fluorogenic Probe for Carbon Monoxide Detection in Aqueous Medium

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Carbon monoxide is a well-known toxic gas inhaled fromcommon sources e.g. smoke and car exhaust, however various studies have shown that mammalian cells continuously generate carbon monoxide (CO) gas via endogenous degradation of heme by a family of inducible (HO-1) and constitutive (HO-2) heme oxygenase enzymes.[1,2]Carbon monoxide has shown an essential regulatory role in a variety of pathophysiological and physiological processes that take place within the nervous, cardiovascular and immune systems.[3] CO produced in the vessel wall by heme oxygenase enzymes possesses vasorelaxing properties, and has been revealed to prevent vasoconstriction and also both acute and chronic hypertension through soluble guanylate cyclase stimulation.[4] CO gas has been described to facilitate potent anti-inflammatory effects at concentrations ranging from 10 to 500 ppm.[5] Many aspects of CO in chemical and biological systems remain elusive owing to having the significant signal dichotomy because of the lack of ways for selective monitoring of this transient small molecule.

In this context, we developed a coumarin-based fluorogenic probe, for the selective detection of CO in HEPES buffer of pH 8.0 at 37 ^{o}C. The detection of CO in a fluorogenic platform is achieved with a concomitant increase of fluorescence intensity by 150-times using Pd(0)-mediated chemistry through the intramolecular cyclization-elimination reaction. The probe represents a unique chemical tool that features a selective 'turn-on' response to CO over reactive oxygen, nitrogen, and sulfur species and can be used to image CO in living cells.

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P-82

A new microporous Ln-MOF: CO_2 uptake and fixation under ambient conditions

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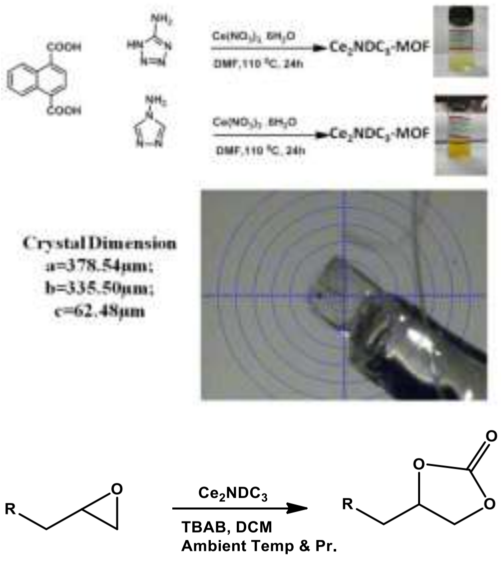
Metal organic frameworks (MOFs)[1] bearing multicarboxylate linkers are in great demand for designing robust heterogeneous catalysts as well as solid adsorbents for different gases.[2,3] A new microporous Ce(III)-based metal organic framework Ln-MOF (Ce_2NDC_3) has been synthesized under solvothermal conditions (Scheme 1), which showed CO_2 uptake as well as CO_2 fixation to produce cyclic carbonates. The material showed CO_2 uptake capacity of 1.64 and 1.22 mmol g^{-1} at 273 and 298 K respectively. The Ce_2NDC_3 showed high catalytic activity in CO_2 fixation reaction (epoxide to cyclic carbonate) for the synthesis of cyclic carbonates with a maximum yield of 92% at ambient temperature and pressure.[2] The Ce_2NDC_3 catalyst showed high recycling efficiency in CO_2 fixation reaction, together with retention of the MOF structure after several rounds of reuse. Presumably, the presence of acidic Ce(III) metal ions with vacant coordination sites and microporosity in the coordination polymer network are responsible for the high catalytic activity.



Scheme 1. Synthetis scheme of Ln-MOF, cyclic carbonate and crystal description

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P-83

Single end-on azido bridged 1D chain copper (II) complex: Synthesis, X-ray crystal structure and catalytic efficacy in homogeneous epoxidation of cyclooctene

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A new azido derivative of a NNO donor tridentate Schiff base copper(II) complex $[CuL(\mu_{-1,1}\text{-}N_3)]_n$ (HL = 1-(N-ortho-hydroxyacetophenimine)-2-(N-ethyl)aminoethane) containing single end-on $\mu_{-1,1}$-azido bridged 1D infinite chain has been synthesized and characterized. X-ray single crystal structure analysis reveals that the complex $[CuL(\mu_{-1,1}\text{-}N_3)]_n$ is a 1D chain in which neighboring Cu(II) chromophores are related by glide planes and linked by single azido bridges in the EO mode. No measurable magnetic interaction was evidenced in the complex $[CuL(\mu_{-1,1}\text{-}N_3)]_n$ through variable temperature magnetic susceptibility measurements (10-300 K). The complex was used as an active catalyst for the epoxidation of cyclooctene using *tert*-butyl-hydroperoxide as oxidant. The catalytic activity of the complex has been compared in a series of solvents. The results show that in acetonitrile medium, the epoxide was produced in high yield with high selectivity.

P-84

Examination of the structure, spectroscopic constants and reaction kinetics of the reaction XO + O → X + O_2

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The stratospheric ozone layer plays a vital role by absorbing ultraviolet rays coming from sun. Various greenhouse gases, like Carbon dioxide (CO_2), Carbon Monoxide (CO), Chloroflurocarbons (CFCs) etc. are depleting Ozone layer day-by-day and thereby causing skin cancer, eye damage, climate change etc. So, it has become an important task worldwide to know details about these complexes, their reactivity and their effectiveness in ozone depletion.

Both XOO and OXO (X=Cl, Br, I) play a pivotal role in the destruction of ozone layer in the stratosphere. These are formed by the reaction of X and XO radical with O_2 and O, respectively. So XO + O is one of the important reactions in atmospheric ozone depletion, which proceeds as:

$$XO + O \rightarrow OXO \text{ or } XOO \rightarrow X + O_2 \text{ (Cl,Br,I)}$$

This X now react with O_3 to form XO (viz. $X + O_3 \rightarrow XO + O_2$), which in turn proceeds a chain reaction.

Presently, ab initio calculations have been performed to investigate various minimum energy geometries, transition state geometries involved in the reaction, their spectroscopic constants and reaction kinetics of the above reaction. Using proper basis set, geometries and frequencies have been obtained at the Moller-Plesset perturbation theory (MP2). Energy values are obtained at the QCISD(T) method. IRC calculations are going on to obtain an idea of reaction pathways.

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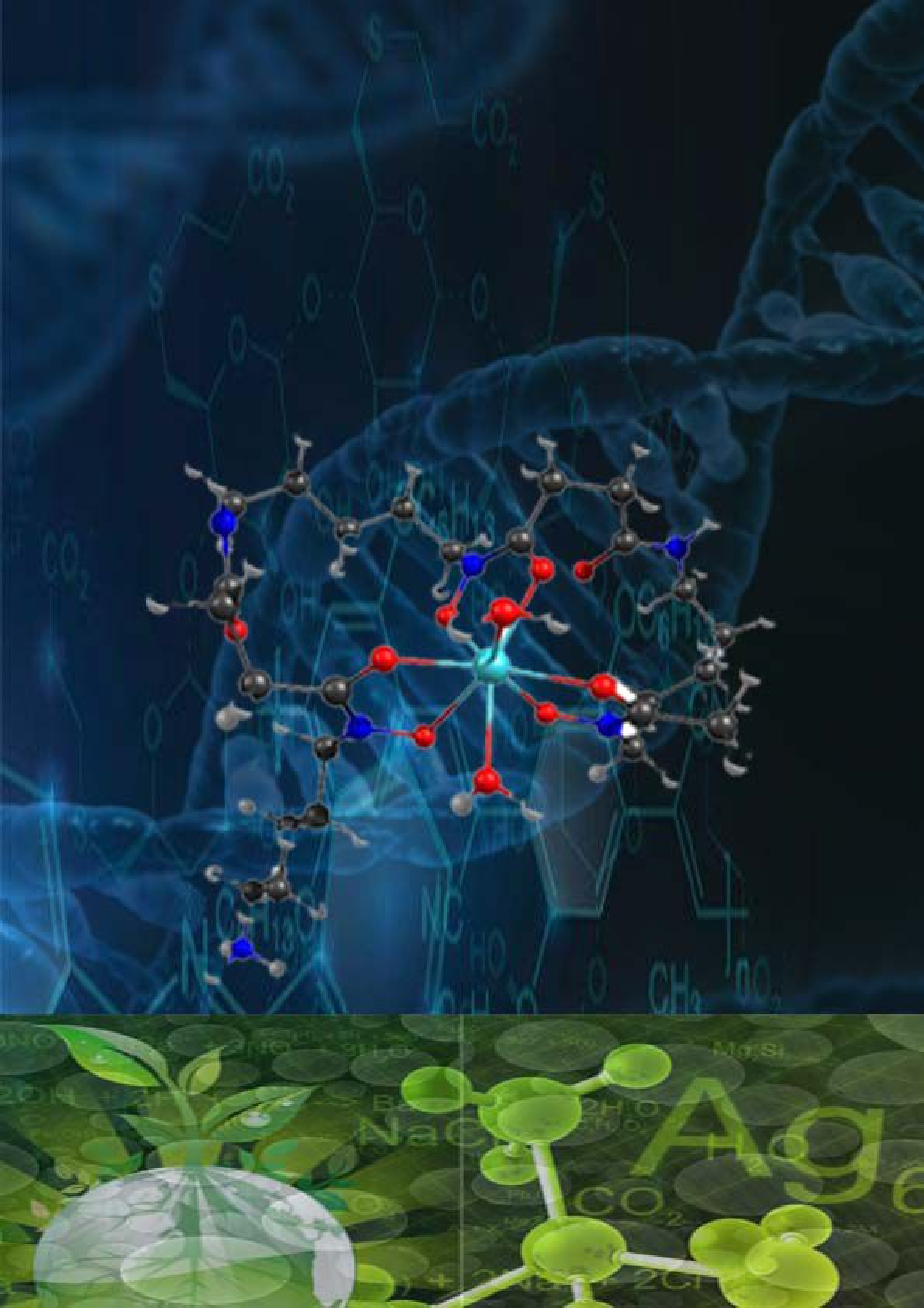
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