

# One Day International Conference on Chemistry in Daily life (ICCDL-2022)



**H** 1  
1.008  
  
Hydrogen

**Li** 3  
6.941  
  
Lithium

**Be** 4  
9.012  
  
Beryllium

**Na** 11  
22.990  
  
Sodium

**Mg** 12  
24.305  
  
Magnesium

**K** 19  
39.098  
  
Potassium

**Ca** 20  
40.078  
  
Calcium

**Sc** 21  
44.956  
  
Scandium

**Ti** 22  
47.867  
  
Titanium

**V** 23  
50.942  
  
Vanadium

**Cr**  
  
Chromium

**Rb** 37  
85.468  
  
Rubidium

**Sr** 38  
87.62  
  
Strontium

**Y** 39  
88.906  
  
Yttrium

**Zr** 40  
91.224  
  
Zirconium

**Nb** 41  
92.906  
  
Niobium

**Mo**  
  
Molybdenum

**Cs** 55  
132.90  
  
Cesium

**Ba** 56  
137.33  
  
Barium

Lanthanides and Actinides

**Hf** 72  
178.49  
  
Hafnium

**Ta** 73  
180.95  
  
Tantalum

**W**  
  
Tungsten

**Fr** 87  
223  
  
Francium

**Ra** 88  
226  
  
Radium

Actinides

**Rf** 104  
261  
  
Rutherfordium

**Db** 105  
262  
  
Dubnium

**Sg** 106  
263  
  
Seaborgium

24th November, 2022

Venue:

Diamond Harbour Women's University  
Sarisha, WB, India

Photographs show samples of the pure or nearly pure element except as follows: Al, Rn, Fr, Ac, Pa, and Np show radioactive

**Organised by : Department Of Chemistry  
Diamond Harbour Women's University  
(Sponsored by Higher Education Department, GOVT. OF W.B.)**

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Other sizes of this poster: [periodictable.com](http://periodictable.com)  
Real samples like these: [element-collection.com](http://element-collection.com)

**Ac**  
  
Actinium

**Th**  
  
Thorium

**Pa**  
  
Protactinium

**U**  
  
Uranium



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## Disclaimer

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**DIAMOND HARBOUR WOMEN'S UNIVERSITY**

**Prof. Dr. Sayeedur Rahman**

**Registrar**

**MESSAGE**

I am happy to know that Department of Chemistry of the University is going to organize one day International Conference on "Chemistry in Daily Life" on 24<sup>th</sup> November, 2022. The Program will consist of (i) Inaugural Lectures (ii) Key note Lecture (iii) Invited Lectures and (iv) Oral and Poster Presentations.

I extend my greetings and good wishes to the Hon'ble Speakers, Distinguished Guests, Students, Teachers and Non-teaching staff of the Department of Chemistry, Diamond Harbour Women's University for the success of the International Conference.

Date: 18-11-2022

Prof. Jayanta Maity  
Head of the Department  
Chemistry  
Diamond Harbour Women's University

  
Prof. Dr. Sayeedur Rahman

Registrar  
*Registrar*  
Diamond Harbour Women's University  
Sarisha, 24 Parganas (S), W.B.



# DIAMOND HARBOUR WOMEN'S UNIVERSITY

## Department of Chemistry

Ref. No:.....

Date:.....

24/11/2022

### FORWARD

With great pleasure we welcome you in the **International Conference on "Chemistry for Daily Life"** on **November-2022** is aimed to highlight the latest research in the field of Chemical Sciences and other interdisciplinary subjects like biological science, various engineering disciplines etc. from across the nation. With a very select group of invited talks and contributory papers, the conference promises to be a very informative and stimulating one.

The Chemistry Department started its journey in 2017. Right from the beginning of journey, the department is trying to provide one of the best academic environments in the nation. Also, the department is engaged in research activities on basic and contemporary areas of chemistry, relevant to the society. We hope that you will enjoy your stay at Diamond Harbour Women's University, Sarisha, South 24 Parganas, W.B. and the conference as well.

Dr. Jayanta Maity

*J Maity 24/11/22*

HOD, Chemistry Department  
Diamond Harbour Women's  
University, Sarisha, South 24  
Parganas, W.B



**HEAD**  
Dept. of Chemistry  
Diamond Harbour Women's University  
Diamond Harbour Road  
Sarisha, South 24 Parganas  
West Bengal, 743368



# ICCDL-2022@DHWU

## **Organizing Committee**

### **Chief Patron:**

Prof.(Dr.) Soma Bandyopadhyay  
Hon'ble Vice Chancellor, DHWU

### **Patron:**

Prof.(Dr.) Sayeedur Rahman  
Registrar, DHWU

### **Organising Chairman:**

Prof.(Dr.) Dilip Das,  
Dean, Faculty of Science, DHWU

### **Treasurer:**

Dr. Pujarini Banerjee

### **Conveners(Joint):**

Prof. Jayanta Maity  
(Professor and HOD, Chemistry  
Department,DHWU)

&

Dr. Tanmay Chattopadhyay  
(Assistant Professor,Chemistry  
Department,DHWU)

### **Members:**

All Research scholars and students of  
Department of chemistry, DHWU

### **Organising Secretary:**

Dr. Raj Kumar Nandi

&

Dr. Ria Sanyal (Assistant Professor DHWU)



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## One Day International Conference on Chemistry in Daily Life

(ICCDL-2022)

Organized by

Department Of Chemistry

Diamond Harbour Women's University

24<sup>th</sup> November, 2022

### Programme Schedule

Registration : 9.00 am to 10.25 am.

#### Inaugural Session

- Welcome Address: 10.25 -10.30 am
- Inaugural Speech: Prof. Soma Bandhopadhyay, Hon'ble Vice Chancellor ,DHWU. Time:(10.30-10.45)am

Address by Prof.(Dr.) Sayeedur Rahman,Registration,DHWU. Time(10.45-10.50)am

Address by Prof.(Dr.) Dilip Das ,Dean,Faculty of Science,Time:(10.50- 10.55)am

- Vote Of Thanks: (10.55-11.00 )am

#### Technical Session

- Key Note Address: Prof. Susanta Lahiri,Emeritus Scientist,DHWU,WB . Time:(11.00-11.30) am
- Plenary Lecture: Prof.Ennio Zangrando, University of Trieste, Italy. Time:(11.30-12.15)pm



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- **Invited Lecture-1:** Prof.Tapas Chakraborty, Director, IACS,WB. Time:(12.15-1.00 )pm
- **Invited Lecture-2:** Prof. Dilip K.Maiti, FRSC,University of Calcutta,WB. Time:(1.00-1.45)pm

### Lunch and Poster Session

#### PP-01 to PP-45

- **Oral Presentation:**OP1-OP8 (5minutes Presentation and 2 minutes Discussion)Time: (3.00-4.00)pm
- **Valedictory Session:**( 4.00-4.30) pm

### Oral Presenter (OP01-OP08)

Poster Number	Author	Title	Email id	Institute
OP-01	Tania Chowdhury	Antioxidant and Anti-microbial drugs and our contribution to chemistry	tania.chowdhury1994@gmail.com	Department of Chemistry, Calcutta University, 92,A.P.C road Kolkata,700009
OP-02	Pamela Pal	Synthesis of Heterocycle-annulated pyridine derivatives via Povarov reaction	Palpamela1995@gmail.com	Department of Chemistry, Diamond Harbour Women's University Sarisha,West Bengal,743368, India
OP-03	Ananya Chaudhuri	Simple Technique to Prepare Robust, Durable, Water-repellent Thin Coating on Textile Surface	jayantajune@gmail.com	Department of Chemistry, Sidho-Kanho-Birsha University,Ranchi Road, 723104
OP-04	Suhana Karim	Atmospheric Water Induced Reversible Structural Transformation of a Two-dimensional Ni(II) based Ferromagnetic	Suhana.k13@gmail.com	Department of Chemistry, Calcutta University, 92,A.P.C road Kolkata,700009



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		MOF:A Highly Efficient Water		
OP-05	Sayanti Show	An approach to nature resourced compound curcumin in radiochemical experiments	sayantishow@gmail.com	Diamond Harbour Women's University, Sarisha, 743368, West Bengal, India.
OP-06	Sudeshna Ghosh	Bond dissociation energies of $\text{GeX}_2$ and $\text{GeX}^{\pm}_2$ ( $X= \text{F}, \text{Cl}, \text{Br}, \text{I}$ )	Sudeshna.dhwu.physics@gmail.co	Department of Physics, Diamond Harbour Women's University
OP-07	Riya Mondal	Application of nanoparticles against parasites of fishes as a novel tool of diseases control	panchakotbb@gmail.com	Department of Zoology, Diamond Harbour Women's University, Sarisha, West Bengal, India.
OP-08	Aniruddha Mondal	Study of surface morphology with electrical and optical properties of GO and rGO	Aniruddha,chem007@gmail.com	Department of Chemistry

### Poster Presenter (PP01-PP45)

Poster Number	Author	Title	Email id	Institute
PP-01	Puja Samanta	Conformations of linalool investigated through FTIR spectroscopy and electronic structure calculations	Spuja821@gmail.com	Diamond Harbour Women's University
PP-02	Prasenjit Mistry	SYNTHESIS OF POTENTIALLY BIOACTIVE URACIL DERIVATIVES BY THE USE OF TRANSITION-METAL CATALYSED REACTIONS	prasenjit.mistry@gmail.com	Department of Chemistry, University of Kalyani, Kalyani-741235, India
PP-03	Priya Roy	A comprehensive study of ROS mediated filaricidal and mosquitocidal activities	royprya12@gmail.com	Department of Zoology, Diamond Harbour Women's University, Sarisha-743368, India





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		of silver nanoparticles		
PP-04	Rimpa Mondal	Experimental and Theoretical Investigation of the Catalytic Performance of Reduced Schiff Base and Schiff Base Iron Complex: Transformation to Magnetically Retrievable Catalyst	rimpamondal1956@gmail.com	Diamond Harbour Women's University, Sarisha, West Bengal, India.
PP-05	Rinku Ghanta	Triton X-100 functionalized Cu(II) dihydrazone based complex immobilized on Fe <sub>3</sub> O <sub>4</sub> @dopa: A highly efficient catalyst for oxidation of alcohols, alkanes, and sulfides and epoxidation of alkenes	rinkughanta96@gmail.com	Diamond Harbour Women's University, Sarisha, West Bengal, India.
PP-06	Gargi Nandi	Ab initio calculation of ozone depleting reactions $1 \text{ Br}^- + 3 \text{ O}_3 \rightleftharpoons 1 \text{ BrO}^- + 3 \text{ O}_2$ and $3 \text{ Br}^- + 1 \text{ O}_3 \rightleftharpoons 3 \text{ BrO}^- + 3 \text{ O}_2$	garginandiindia@gmail.com	Department of Physics, Diamond Harbour Women's University
PP-07	Soma Naskar	Ab initio study for the reaction mechanism of ozone with bromine ion	somanaskar1993@gmail.com	Diamond Harbour Women's University, Sarisha, West Bengal, India.
PP-08	T. K. Ghosh	A comparative study of the mechanism of the reaction $\text{ClO} + \text{O} \rightarrow \text{Cl} + \text{O}_2$	tapaskrg@yahoo.com	Department of Physics, Diamond Harbour Women's University, Sarisha, West Bengal, India
PP-09	Tanmay Chattopadhyay	Development of an efficient magnetically separable nanocatalyst : application for various organic Transformations	tanmayc2003@gmail.com	Diamond Harbour Women's University, Sarisha, West Bengal, India
PP-10	Dr. Kazi Sabnam Banu	Synthesis of Nano Materials and Challenges: A Brief Review	<a href="mailto:kazisabanam80@gmail.com">kazisabanam80@gmail.com</a>	Netaji Nagar Day College, Kolkata, West Bengal, India
PP-11	Dr. Puspendu Roy	New Rh(III) chloro complex of a tetradentate S-picolyl azo ligand of acetyl	royuspendu1991@gmail.com	Netaji Nagar Day College Kolkata-700092, West Bengal, India.



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		acetone: Synthesis, X-ray structure, spectral characterization, electrochemistry, DFT computation and interaction with DNA		
PP-12	Uday Das	Study of antibacterial activity of multiwalled carbon nanotubes synthesized by Spray pyrolysis method	udaydas_ju@yahoo.co.in	Department of Physics, Hooghly Mohsin College, Chinsurah, Hooghly-71210 West Bengal, India
PP-13	Swadhin Kumar Saha	Design and synthesis of biopolymer inspired gold nanoparticle as an efficient antifilarial agent	swadhin.chem@gmail.com	Department of Chemistry, Kazi Nazrul University, Asansol-713340, India
PP-14	Anamika Hoque	Hydroxy-naphthaldehyde and Biphenyl-containing amido Schiff base derivative as a turn-on fluorescent chemosensor for Al <sup>3+</sup> ion	anamikahoque35@gmail.com	Aliah University, Action area IIA/27, New Town, Kolkata-700160
PP-15	Soumadip Banerjee	Theoretical Exploration of Multi-Diels-Alder reaction on neutral & Li + - encapsulated C 60 fullerenes	banerjee.soumadip@gmail.com	School of Mathematical & Computational Sciences
PP-16	Sumitava Khan	Mononuclear cobalt(III) halide complexes with tetradentate Schiff base: Syntheses, structures and properties	mynamesumitavakhan@gmail.com	Department of Chemistry, Burdwan Raj College, Burdwan 713 104, West Bengal
PP-17	Abu Taher	Synthesis of sultam and sultone derivatives using domino-Knoevenagel hetero-Diels-Alder reaction	abuchem81@gmail.com	Department of Chemistry, Bankura University, Bankura, West Bengal, India
PP-18	Sukanya Das	A Transition Metal Catalyzed Cyclization-Alkynylation Strategy Towards fused Heterocycles using Hypervalent Iodine Reagent	sukanyadas01997@gmail.com	Department of Chemistry, Diamond Harbour Women's University, Sarisha-743368, West Bengal, India
PP-19	Eshani Paul	Coumarin-coupled new pyridyl azo phenol derivatives: Aggregation and selective sensing of F <sup>-</sup> and CN <sup>-</sup> ions	eshanipaul23@gmail.com	Department of Chemistry, University of Kalyani, Kalyani-741235, India.



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PP-20	Md Sanaul Islam	A isophthalohydrazide containing Schiff base derivative as a turn-on fluorescent chemosensor for Al <sup>3+</sup>	sanaulchm@gmail.com	Aliah University, Action area IIA/27, New Town, Kolkata-700160
PP-21	Samim Khan	Controlling Mechanical Motion in 1D Coordination Polymers: Photosensitive to Non-Solvent Crystal	samimchm@gmail.com	Aliah University, IIA/2, Action Area-II, New Town, Kolkata-700160
PP-22	Papiya Sikdar	Regioselective Oxidative C-H Halogenation of Pyrazolo[1,5-a]pyrimidines in Water	papichem22@gmail.com	Department of Chemistry, University of Kalyani, Kalyani, India-741235
PP-23	Pijush Singh	Supramolecular Hydrogel from an Oxidized By-product of Tyrosine	singhpijush62@gmail.com	Department of Biochemistry & Biophysics, University of Kalyani, Kalyani, Nadia-741235, West Bengal, India.
PP-24	Subhasis Ghosh	Rhodamine-linked naphthalimide derivative as colorimetric probe for Cu <sup>2+</sup> and S <sup>2-</sup> detection	subhasis.ghosh95@gmail.com	Department of Chemistry, University of Kalyani, Kalyani-741235, India.
PP-25	Prithwiraj Byabartta	Copper(II)-Chloro-arylazoimidazole-triphenylphosphine complexes : Synthesis, Spectroscopic and redox study.	prbjccc@gmail.com	Department of Chemistry, Jogesh Chandra Chaudhuri College, 30- Prince Anwar Shah Road, Kolkata-700033;
PP-26	Dr. Sanju Das	Cyanide Selective Off-On Fluorescent Chemo-sensor with in-vivo Bio-imaging in pure Water	sanjudasju@gmail.com	Assistant Professor, Department of Chemistry, Maulana Azad College, Kol-13
PP-27	Sunita Jhulki	Paradoxical effects of Reactive oxygen species on human cancer	sunitajhulki416@gmail.com	Dept. of Zoology, Diamond Harbour Women's University, Sarisha, West Bengal, India.
PP-28	Dr. Prateeti Chakraborty	Exploration of pseudohalide mediated Weak Interactions in Schiff base complexes and study of their photophysical property	prateeti_17@yahoo.co.in	Department of Chemistry, Bangabasi College, Kolkata-700009, India,
PP-29	Dr. Jaydeep Adhikary	Mechanistic Pathway Investigation of Catecholase-like Activity of three Mononuclear Nickel (II)	adhikaryj86@gmail.com	a Department of Chemistry, Uluberia College, Uluberia, Howrah – 711315, West Bengal, India



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		Complexes of Schiff Base ligand 2-[(2-piperazin-1-yl-ethylimino)-methyl]phenol		
PP-30	Aparajita Paul	Reactive oxygen species: an intricate regulator of health and diseases	aparajita.zoology@gmail.com	Dept. Of Zoology, Diamond Harbour Women's University, Sarisha, West Bengal, India.
PP-31	Papia Datta	Photophysical, Photochemical, Biological & Photo voltaic properties of Novel Coumarylazoimidazoles	papiaju@yahoo.in	Department of Applied Science, RCC Institute of Information Technology, Beliaghata, Kolkata
PP-32	Arpita Dutta	Enhanced electrochemical performance of ZnO@rGO nanocomposite for supercapacitor application	duttaarpita1995@gmail.com	Department of Physics, Diamond Harbour Women's University, Sarisha, West Bengal, India
PP-33	Bipasa Dey	Behavioural response of earthworms as a tool for studying soil pollution	bipasadey2019@gmail.com	Parasitology Laboratory, Department of Zoology, Diamond Harbour Women's University, Diamond Harbour – 743368, West Bengal, India
PP-34	Sneha Biswas	Effect of O-substitution in imidazole based Zn(II) dual fluorescent probes in the light of arsenate detection in potable water: a combined experimental and theoretical approach	sneha.khardah@gmail.com	Department of Chemistry, University College of Science, University of Calcutta, 92 A. P. C. Road, Kolkata 700009, India
PP-35	Dr. Arabinda Mandal	Food as Poison: Disaster in daily life	watcharabinda@gmail.com	Department of Chemistry, Bidhannagar College, Salt Lake, Kolkata-700064, India
PP-36	Md Kalimuddin Mandal	Effect of P H on the Removal of Dyes from Water Body Using Okra Leaf	kalimuddin.mandal@gmail.com	Department of Chemistry, Aliah University, Action Area IIA/27, New Town,



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				Kolkata, India
PP-37	Susmita Mandal	Curry Leaves: Good Food & Better Life	susmita.dhwu@gmail.com	CSIR-Indian Institute of Chemical Biology, Kolkata- 700 032, India Diamond Harbour Women's University, Sarisha, West Bengal- 743368, India
PP-38	Patit Paban Malik	Preparation and studies of Cerium and uranium doped simulated radioactive waste glasses	patitbu99@rediffmail.com	Department of Chemistry, B.B. College, Asansol, West Bengal, India
PP-39	Pradip Kumar Tapaswi	Synthesis of New Aliphatic Dianhydride EDSA and its Low Dielectric Aliphatic Polyimides (APIs)	pradipkumartapaswi@gmail.com	Narasinha Dutt College, Howrah, West Bengal, India.
PP-40	Debrina Jana	Perovskite nanomaterials: new paradigm in photovoltaics and optoelectronics	debrina.chem@gmail.com	Gour Mohan Sachin Mandal Mahavidyalaya, Bireswarpur, South 24 Parganas, West Bengal, India.
PP-41	Rina Mandal	Chalcone Based Macrocyclic Epoxide and Interactions with beta Lactoglobulin Protein	rinamondal07@gmail.com	Department of Chemistry, Uluberia College, Howrah- 711315, India.
PP-43	Najirul Haque	Zn(II) metal embedded 3D-COF (Zn@RIO-1) for synthesis of valuable products via CO <sub>2</sub> fixation under solvent free condition	nazirulhaq95@gmail.com	Department of Chemistry, University of Kalyani, Nadia, 741235
PP-44	Mainak Sarkar	Metal free COF organocatalyst for conversion of Isocyanates to Urea Derivatives	ami.mainak1997@gmail.com	Department of Chemistry, University of Kalyani, Nadia, 741235
PP-45	Dip Kumar Nandi	<b>CO<sub>2</sub> FIXATION BY SYNTHESIS OF N-METHYLATED PRODUCTS USING NEWLY DESIGNED HETEROGENEOUS Zn(II) EMBEDDED POROUS ORGANIC POLYMER CATALYST</b>	iamdipnandi@gmail.com	Department of Chemistry, University of Kalyani, Nadia, 741235



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## Brief CV of Prof. Susanta Lahiri

Prof. Susanta Lahiri

Department of Chemistry

Diamond Harbour Women's University

**CSIR-Emeritus Scientist**

**&**

**Adjunct Professor of Physics**

**Sidho-Kanho-Birsha University, Purulia**

**&**

**Guest Faculty, Department of Chemistry, University of Calcutta**

**&**

**Guest Faculty, Department of Chemistry, Rani Rashmoni Green university**

**Academic Profile**

**Education:**

- **D. Sc, Chemistry, 2009, University of Calcutta**
- **Ph.D., Analytical Chemistry, 1994, University of Calcutta (Saha Institute of Nuclear Physics)**
- **M.Sc. Chemistry, 1987, University of Burdwan**

**Position Held:**

- **Lecturer, Department of Chemistry, University of Burdwan, 1994-1997**
- **Reader, Saha Institute of Nuclear Physics, 1997-2000**
- **Associate Professor, Saha Institute of Nuclear Physics, 2000-2004**
- **Professor, Saha Institute of Nuclear Physics, 2004-2012**
- **Senior Professor, Saha Institute of Nuclear Physics, 2012-2021**
- **Head, Chemical Sciences Division, Saha Institute of Nuclear Physics, 2019-2021**

**Honors/Awards**

- **Hevesy Medal Award 2015 (Highest International Honour in the field of Nuclear and Radiochemistry) (First and only Indian who received this award since its inception in 1964)**
- **J C Ghosh Memorial Lecture Award, Indian Chemical Society, 2014**
- **Associate Member of Third World Academy of Sciences (twice), 2000-2003, 2004-2006**

**Research Interests**

1. Nuclear and Radiochemistry
  - a. Accelerator production of clinically important neutron deficient radionuclides
  - b. Radiotracer technique
  - c. Naturally Occurring Radioactive Materials (NORM)
  - d. Superheavy elements, Accelerator Mass Spectrometry.
2. Green Chemistry
3. Trace Analysis and Biomonitoring

**Publications:** More than 260 publications in International peer-reviewed journals



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**Abstract of Key note address**

After the introduction of Green Chemistry in 1991, it is now commanding all branches of Science. Green Chemistry is a life long good practice. I shall discuss some aspects of Green Chemistry in daily life.



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## Brief CV of Prof. Tapas Chakraborty

Prof. Tapas Chakraborty

School of Chemical Sciences

Indian Association for the Cultivation of Science

**Senior Professor and Director (Additional Charge)**

### Academic Profile

#### Education:

- Ph.D., Laser Spectroscopy, 1992, IACS
- M.Sc. (Special in Physical Chemistry), 1987, Calcutta University
- B.Sc. (Honours in Chemistry), 1985, Calcutta University

#### Position Held:

- Postdoctoral Research Associate, University of Akron, USA, 1992-1994
- Assistant Professor, IIT Kanpur, 1994-2001
- Associate Professor, IIT Kanpur, 2001-2005
- Professor, IIT Kanpur, 2005-2007
- INSA Visiting scientist, Technical University of Munich, Germany, 1997
- Visiting Professor, University of Aarhus, Denmark, 2005
- Professor, IACS, 2007-Present

### Honors/Awards

- Young Scientist Medal Award, Indian National Science Academy, 1993
- DST Ramanna Fellowship Awards: 2007 and 2011
- Fellow, Indian Chemical Society and J C Ghosh Memorial Lecture Award
- Fellow of the [Indian Academy of Sciences](#) (FASc)

#### Research Interests

- **LIF spectroscopy and excited state dynamics of cold molecules and clusters in a supersonic jet expansion**
- **Laser-induced Proton/ H-atom transfer reactions in cold molecular clusters and probing by photo-ionization time-of-flight mass spectrometry**
- **Ion mobility mass spectrometry for structure and photochemistry of important biomolecules and molecular complexes in liquids and gas phase**
- **Atmospheric photochemistry and atmospheric simulation for anthropogenic and biogenic VOCs**
- **Matrix isolation infrared spectroscopy of molecular complexes under the cryogenic conditions (below 10 K)**

#### Publications:

Nearly 130 publications in renowned journals

#### Teaching:

Experienced teacher at both UG and PG levels





## ICCDL-2022@DHWU

### **Ion mobility mass spectrometry: A tool for determination of molecular structure**

Tapas Chakraborty

School of Chemical Sciences, Indian Association for the Cultivation of Science  
Jadavpur, Kolkata 700032

Mass spectrometry is an indispensable analytical tool in modern methods of chemical analysis, which allows accurate measurements of molecular masses up to many tens of kilodaltons with high degree of accuracy. In addition to molecular masses, valuable information about molecular structures is routinely obtained exploiting the MS-MS fragmentation in the collision cell of a mass spectrometer. However, identification of a completely unknown molecule by means of mass spectrometry alone is still a challenge. Spectroscopic methods, on the other hand, as used in different ranges of the electromagnetic spectrum, are versatile in addressing issues pertaining to molecular structures and conformations. However, as the size of the molecules becomes larger, retrieval of detailed structural information from spectroscopic data are constrained by many factors, and in particular due to spectral broadening, overlap and fast isomeric conversions, in addition to the inherent limitations of the lack of mass selectivity. In my talk, I shall present data from our recent studies to emphasize that much of the desired information pertaining to the structure of a complex molecule can be secured by combining gas-phase ion mobility method with high resolution mass spectrometry and liquid phase chromatography. Measurements of mobility of mass-selected molecular ions through a gas-cell filled with non-interacting gases (helium, nitrogen, carbon dioxide etc.) provide valuable information about global structure of molecules, and much effort has been put to investigate the conformational behavior of large molecules by such means in the recent years [1]. The collision cross-section values as obtained from mobility measurements are now used as molecular markers for different groups of compounds like carbohydrates, peptides, proteins etc. I shall discuss the finding of our recent studies about conformational preferences of a popular laser dye molecule (DCM) in methanol solution [2], and also the tautomeric distribution of curcumin, the yellow aromatic dye, which is the main constituent of turmeric, in water-methanol mixture [3].

#### **Reference:**

[1]. F. Lanucara, S. W. Holman, C. J. Gray and C. E. Eyers, "The power of Ion mobility mass spectrometry for structural characterization and the study of conformational dynamics", *Nature Chemistry*, **6** (2014) 281-294.



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### CV of Prof. Ennio Zangrando

Ennio Zangrando received the degree in Chemistry at University of Trieste in 1974 with full marks (*summa cum laude*). After four years as clinical chemist in a Paediatric Hospital, he joined the Department of Chemical Sciences at University of Trieste as an Associate Researcher (1983), prior to become Associate Professor (1998) and then Full Professor of General and Inorganic Chemistry (2012) within the Faculty of Pharmacy at the same University.

In 1988-89 he worked in Switzerland in the Laboratorium fur Kristallografie (University of Bern, Prof. Hans B. Burgi) on the use of statistical methods in the analysis of structural data.

In 2008-2010 he was President of the regional section of the Italian Chemical Society.

Since the retirement from academy he was appointed as "Senior Professor" from the University of Trieste and now he collaborates in research activity with colleagues from different labs.

Prof. Zangrando has authored more than 400 papers on international chemistry journals.

His research interest deals with X-ray crystallography, using conventional RX sources as well as synchrotron radiation. His work was dedicated to the structural properties of bio-inorganic complexes and has been extended in recent years to supramolecular chemistry.

Main research interest:

- 1- Material structural studies and supramolecular chemistry.
- 2- Structural and solution studies of vitamin B<sub>12</sub> models.
- 3- Structural studies of metal complexes with nucleobases and/or dipeptides.
- 4- Structural studies of metal complexes having catalytic activity

Ennio Zangrando

Department of Chemical and Pharmaceutical Sciences

University of Trieste

via Giorgieri 1

34127 TRIESTE

email: ezangrando@units.it

mobile +39 338 1666979

### Some recent papers

1. P. Bhandari, R. Modak, S. Bhattacharyya, **E. Zangrando** & P.S. Mukherjee  
Self-Assembly of Octanuclear Pt<sup>II</sup>/Pd<sup>II</sup> Coordination Barrels and Uncommon Structural Isomerization of a Photochromic Guest in Molecular Space  
*JACS Au*, 1, 2242–2248, 2021 doi: 10.1021/jacsau.1c00361
2. S. Chakraborty, A. Patra, A. Mondal, S. Lohar, **E. Zangrando** & P. Chattopadhyay  
A new phenolato-bridged dinuclear manganese(II) complex as a *turn-on* fluorosensor for Zn<sup>2+</sup> ions via Mn<sup>2+</sup> ion replacement  
*Polyhedron*, 203 115226, 2021 doi: 10.1016/j.poly.2021.115226



ICCDL-2022@DHWU

## Crystallography in our daily lives

Ennio Zangrando

*Department of Chemical and Pharmaceutical Sciences, University of Trieste (Italy)*

This contribution aims to underline the importance of crystallography, being no basic enterprise in chemistry than the determination of the geometrical structure of a molecule.

In the talk some examples of structural determinations in the field of bioinorganic chemistry will be illustrated, following my academic research life. In detail, after the discovery of cisplatin, a large variety of Pt complexes were studied to account for the coordination modes of nucleobases. Then the story of a Ru complex, having antimetastatic properties and synthesised in my department, and finally the study of cobaloximes and related systems, the most studied complexes mimicking the vitamin B12 coenzyme.



## ICCDL-2022@DHWU



Dr. Dilip Kumar Maiti, *FRSC*

- ❖ **Ph. D. degree** in synthetic organic chemistry from *Indian Institute of Chemical Biology in 1998* (Jadavpur University).
- ❖ **Postdoctoral Studies** at the *School of Medicine, Wayne State University, USA (2002-2004)*.
- ❖ Scientist in the R & D of *Ciba India Pvt. Ltd. (Mumbai)* in **1998**
- ❖ Group Leader in the R & D of RPG Life Sciences Ltd., Navi Mumbai in **1999**
- ❖ Assistant Professor in Chemistry, Dumkal College Basantapur, Murshidabad in 2000
- ❖ Reader, Department of Chemistry, University of Calcutta in 2005
- ❖ Currently **Professor** (from 2011), Department of Chemistry, University of Calcutta
- ❖ **Fellow of Royal Society of Chemistry (FRSC)** by RSC, London
- ❖ **Editorial Board Member: Scientific Reports of Nature Publishing Group (NPG)**
- ❖ **Research Interest: Organic Synthesis, Nanoscience, Organic Electronics & Devices**
- ❖ **Research Scholar Guided (Total): 75; Ph. D. students: 42; Postdoc Fellows: 33**
- ❖ **Publication of papers: 150**
- ❖ **Book Chapters: 9**
- ❖ **Projects completed (DST, SERB, DST Nanomission, CSIR & UGC): 11**



## ICCDL-2022@DHWU

### Smart Organic Nanomaterials for AIE, Sensing, Inkless Writing and Devices

Dr. Dilip K. Maiti

*Professor, Department of Chemistry, University of Calcutta, 92 A. P. C. Road, Kolkata-700009*

*Email: dkmchem@caluniv.ac.in, web site: dkmaitiresearchgroup.org*

Design and synthesis of new organic compounds, fabrication of unidirectional nanomaterials are important for developing aggregation induced emission (AIE), sensing lethal gases, inkless writing and achieving high-tech devices of ultimate sensitivity.<sup>1</sup> We have fabricated highly ordered one-dimensional low molecular mass organic nanostructured materials of sugar-based chiral imidazoles and halogenated bithiophines which displayed AIE properties.<sup>1a,f</sup> The phenazine-based organic nanomaterials have used for fabrication of crossbar device to achieve organic resistive random access memory (RRAM) device and write-once-read-many-times (WORM) devices which have valuable application in non-editable database, archival memory, electronic voting, and radio frequency identification (RFID) application.<sup>1c,g</sup> A novel organic luminescent nanomaterial was fabricated for inkless writing and self-erasing application which is a remarkable solution to reduce paper waste, recycling cost in the printing industry. Utilizing this purely organic material, we demonstrated reversible inkless writing/printing employing photothermal effect of sunlight in which sunlight acts as an "inkless pen".<sup>1d</sup> Organic nanofibrils are designed for sensing lethal gas phosgene.<sup>1e</sup> Herein, penetration confers a fast chemical reaction, which is linear to the phosgene concentration and delivers a very low detection limit of 0.087 ppm. Importantly, LOD of gaseous phosgene in all type of solid-protocols used is far lower than the safety level phosgene concentration to human exposure.

**References:** 1. (a) S. Halder, P. Pandit, N. Chatterjee, D. De Joarder, N. Pramanik, A. Patra, P. K. Maiti, D. K. Maiti, *J. Org. Chem.*, 2009, **74**, 8086. (b) P. Pandit, K. S. Gayen, S. Khamarui, N. Chatterjee, D. K. Maiti, *Chem. Commun.*, 2011, **47**, 6933. (c) D. K. Maiti, S. Debnath, M. Nawaz, B. Dey, E. Dinda, D. Roy, S. Ray, A. Mallik, S. A. Hussain, *Sc. Rep.*, 2017, **7**, 13308. (d) T. Panda, M. K. Panda, D. K. Maiti, *ACS Appl. Mater. Interfaces*, 2018, **10**, 29100. (e) K. Maiti, D. Ghosh, R. Maiti, V. Vyas, P. Datta, D. Mandal, D. K. Maiti, *J. Mater. Chem. A*, 2019, **7**, 1756. (f) T. Ghosh, S. Mitra, S. K. Maity, D. K. Maiti, *ACS Appl. Nano Mater.*, 2020, **3**, 3951. (g) T. Ghosh, S. Mondal, R. Maiti, S. M. Nawaz, N. N Ghosh, E. Dinda, A. Biswas, S. K. Maity, A. Mallik, D. K Maiti, *Nanotechnology*, 2021, **32**, 025208.



# ICCDL-2022@DHWU

OP-01

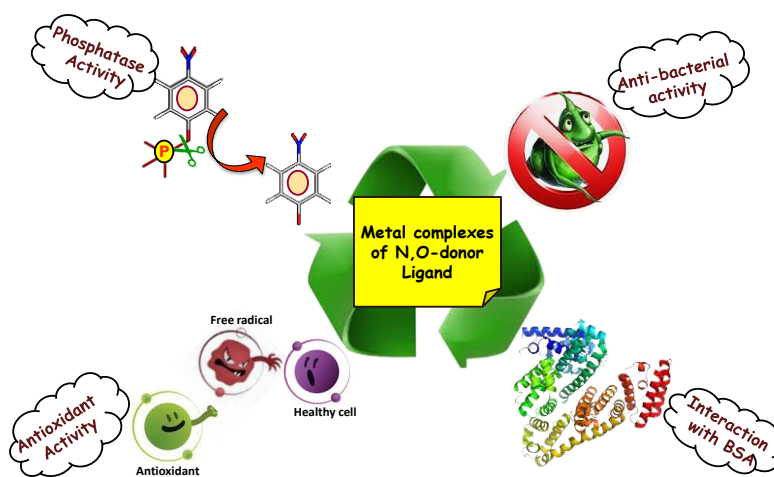
## Antioxidant and Anti-microbial drugs and Our Contribution to Chemistry

**Tania Chowdhury, Debasis Das\***

University of Calcutta, 92, APC Road, Kolkata- 700009, West Bengal, India.

e-mail: [dasdebasis2001@yahoo.com](mailto:dasdebasis2001@yahoo.com), [tania.chowdhury1994@gmail.com](mailto:tania.chowdhury1994@gmail.com)

“Why we look old with age??”—the answer is the Free radicals, which are produced by a number of endogenous processes in our bodies, and cause oxidative damage to healthy cells, leading to homeostatic imbalance. Here comes the need for an antioxidant which scavenges free radicals, and prevents or delays oxidative damage. There is much potency for the Zn(II) complexes to act as anti-oxidant. To search for a drug which can act as both anti-oxidant and anti-microbial has been a crucial job.



Hence six zinc(II) complexes have been manufactured by using two homologous Schiff base ligands for the purpose to perustrate their bio-relevant activities, their exploitation as potential drugs and to explicate the chemistry working behind the activities. Anti-oxidant property is tested on DPPH radical and anti-microbial activities are tested against the microbes *Listeria monocytogenes* ATCC<sup>®</sup>19111™, *Staphylococcus aureus* ATCC<sup>®</sup> 700699™, *Salmonella typhimurium* ATCC<sup>®</sup> 23564™ and *Escherichia coli* ATCC<sup>®</sup> 25922™. Finally the disposal of drugs though the coalescence with the serum protein has been another focus of this work.



## ICCDL-2022@DHWU

OP-02

### Synthesis of heterocycle-annulated pyridine derivatives *via* Povarov reaction

**Pamela Pal<sup>a</sup>**, Sayanti Show<sup>a</sup>, Sayantika Bhakta<sup>b</sup>, Sukanya Das<sup>a</sup>, Tapas Ghosh<sup>b,c\*</sup> and R. K. Nandi<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Diamond Harbour Women's University, Sarisha, West Bengal, India

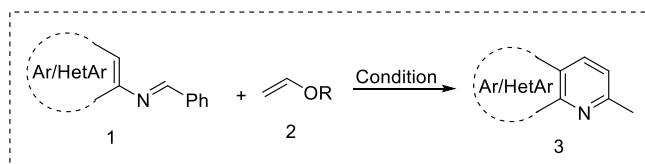
<sup>b</sup>Department of Applied Science, MAKAUT, Kalyani, Nadia

<sup>c</sup>Department of Chemistry, Jadavpur University, Jadavpur, West Bengal, India

e-mail : [palpamela1995@gmail.com](mailto:palpamela1995@gmail.com)

Among the nitrogen heterocycles, pyridine derivatives represent an important class of organic molecules due to their wide applications as pharmaceuticals and agrochemicals as well as useful synthetic blocks in the preparation of several alkaloids. Although many syntheses of pyridine derivatives are known, but the development of new synthetic approaches always remains an active research area<sup>1-3</sup>.

The Diels-Alder (DA) reaction has recognized as a powerful method in the synthetic strategies for small heterocycle based natural and unnatural cyclic compounds because of its synthetic diversity<sup>4</sup>. The Povarov reaction is a classic example of inverse-electron-demand DA reactions between an aromatic imine and an alkene<sup>5</sup>. Povarov discovered that imines derived from aromatic amines undergo Lewis acid catalyzed formal [4+2]-cycloaddition with electron rich alkenes to give quinolines<sup>6</sup>. Typically, the alkenes employed were electron rich, with enol ethers being the most widely studied substrates to date.



Recently we have demonstrated a new one step synthesis of heterocycle (bioactive heterocycles) annulated pyridine derivatives *via* Povarov reaction. The imine is a condensation product from an aromatic primary amine compound which reacts with an aldehyde or vinyl/enol ether type compounds under organic acidic condition.

#### References:

- 1) Katritzky, A. R.; Rachwal, S.; Rachwal, B. *Tetrahedron*, **1996**, *52*, 15031.
- 2) Kouznetsov, V.; Palma, A.; Ewert, C.; Varlamov, A. *J. Heterocycl. Chem.* **1998**, *35*, 761.
- 3) Kouznetsov, V.; Vargas Me´ndez, L. Y.; Mele´ndez Go´mez, C. M. *Curr. Org. Chem.* **2005**, *9*, 141.
- 4) Smith, M. B. *Organic Synthesis*, 2nd ed.; Mc Graw-Hill: New York, NY, **2002**, 844.
- 5) Povarov, L. S.; Mikhailov, B. M. *Izv. Akad. Nauk SSR, Ser. Khim.* **1963**, 953.
- 6) Povarov, L. S.; Grigos, V. I.; Mikhailov, B. M.; *Izv. Akad. Nauk SSR, Ser. Khim.* **1963**, 2039.



ICCDL-2022@DHWU

OP-03

## Simple Technique to Prepare Robust, Durable, Water-repellent Thin Coating on Textile Surface

Ananya Chaudhuri<sup>a</sup>, Jayanta Maity<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Sidho-Kanho-Birsha University, Ranchi Road, P.O.- Purulia, Pin-723104, West Bengal, India.

<sup>b</sup>Department of Chemistry, Diamond Harbour Women's University, Diamond Harbour Road, Sarisha, South 24 Parganas, Pin-743368, West Bengal, India.

\*Corresponding author e-mail- jayantajune@gmail.com

### **Abstract:**

Hydrophobic, robust, durable, self-cleaning coating was successfully fabricated on silk surface using surfactant-aided polymerization of fluoro-monomer. The study was inspired from naturally occurring superhydrophobic surfaces such as lotus leaf, water strider limbs, lizard legs etc. Initial hydrophobic character of the modified silk was studied by droplet stay time assessment and water contact angle studies. Microscale nano-structural roughness induced by the polymer coating was investigated by SEM images. The generated coating did not alter the aesthetic appearance of silk. The new bond formation onto the silk surface after the surface treatment was analyzed by FTIR study and compared with that of the unmodified silk surface. The best WCA of the polymer-coated silk was found to be 140.1°. The modified silk was studied to check the durability of the polymer coating. The hydrophobic surface showed enthralling durability against multiple washing cycles and abrasion cycles and showed efficient degree of oil/water separation ability.

Keywords: Abrasion resistance; Coating; Contact angle; Durable; Fluoro-monomer; Textile.





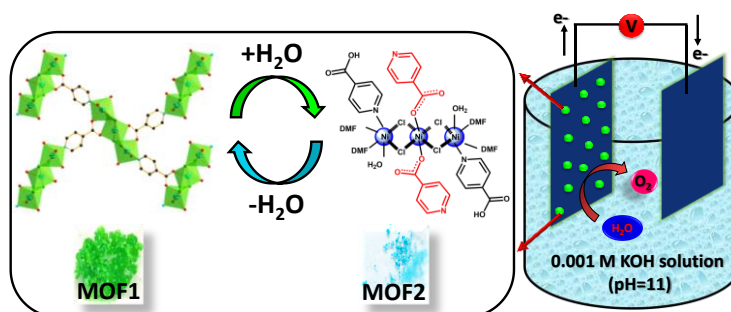
## Atmospheric Water Induced Reversible Structural Transformation of a Two-dimensional Ni(II) based Ferromagnetic MOF: A Highly Efficient Water Oxidation Electrocatalyst and Colorimetric Water Sensor

Suhana Karim,<sup>\*a</sup> Amit Adhikary,<sup>\*a</sup> Md Estak Ahmed,<sup>b</sup> Debabrata Samanta,<sup>c</sup> and Debasis Das<sup>\*a</sup>

University of Calcutta, 92' A. P. C Road, Kolkata- 700009

Email: [suhana.k13@gmail.com](mailto:suhana.k13@gmail.com)

A two-dimensional metal-organic framework, formulated as  $[\text{Ni}_3(\text{nic})_2(\mu\text{-Cl})_4(\text{DMF})_4]\cdot 2 \text{ DMF}$  (**MOF1**), was self-assembled from Nickel(II) ion and 4-pyridinecarboxylic acid. The **MOF1** has a 6c-connected uninoidal net topology and can absorb atmospheric moisture, ensuring the structural transformation of **MOF1** into **MOF2**. The transformation is reversible as **MOF2** can be returned quickly to its initial structure **MOF1** upon heating. The reversible conversion is associated with a color change between green (**MOF1**) and blue (**MOF2**), and it can be used as a colorimetric water sensor with a limit of detection (LOD) of 0.246  $\mu\text{M}$  (inorganic solvent) and 0.224  $\mu\text{M}$  (organic solvent). The water-capturing ability also leads to an electrocatalytic oxygen evolution reaction (OER). **MOF2** is the 1<sup>st</sup> Ni-containing OER electrocatalyst that needs only 180 mV overpotential in 0.001 M KOH to drive 10 mA  $\text{cm}^{-2}$  current density. The MOF shows an immense turnover number ( $\text{TON} = 3.8 \times 10^5$ ) and frequency ( $\text{TOF} = 10.6 \text{ S}^{-1}$ ), Faradaic efficiency (93.7%), and excellent robustness. The structural change ( $\text{MOF1} \leftrightarrow \text{MOF2}$ ) and OER process are additionally supported by a density functional theoretical (DFT) study. The structural transformation in the solid phase further changes the magnetic properties-both **MOF1** and **MOF2** showing ferromagnetic interactions. However, Neel temperature (TN) for **MOF1** < 5 K changes to  $\sim 16 \text{ K}$  for **MOF2**.



**Figure:** **MOF1** is capable of absorbing atmospheric water and reversibly transforming into **MOF2**. This structural transformation can be seen in the naked eye as color changes from green to blue. This modified material (**MOF2**) is beneficial for water oxidation reactions, and because of its low overpotential, it can be considered a real-life application.

### References:

- (1) Karim, S.; Chakraborty, A.; Samanta, D.; Zangrando, E.; Ghosh, T.; Das, D. A dinuclear iron complex as an efficient electrocatalyst for homogeneous water oxidation reaction. *Catal. Sci. Technol.* **2020**, *10*, 2830-2837.
- (2) Karim, S.; Chakraborty, A.; Das, S.; Banerjee, A.; Das, D. Devising SrFe<sub>2</sub>O<sub>4</sub> spinel nanoflowers as highly efficient catalyst for enhanced electrochemical water oxidation in different basic concentration. *J. Electroanal. Chem.* **2022**, 116465.
- (3) Nocera, D. G. Solar Fuels and Solar Chemicals Industry. *Acc. Chem. Res.* **2017**, *50*, 616-619.



## ICCDL-2022@DHWU

OP-05

### **An approach to nature resourced compound curcumin in radiochemical experiments.**

**Sayanti Show**, Puja Samanta, Susanta Lahiri\*, P. Banerjee\*, R. K. Nandi\*

*Diamond Harbour Women's University, Sarisha, West Bengal, India*

e-mail: sayantishow98@gmail.com

Isotope production followed by its application in nuclear medicine is now an advanced field of R&D. However, the basic condition remains the separation of NCA radioisotope from the irradiated target. In our recent studies, it has been observed that natural reagents (e.g., hesperidin, catechin) themselves could specifically bind to the produced radioisotope after irradiation, thereby separating it in its no-carrier-added form. Additionally, these natural products have free radical scavenging property that is significant while envisioning them as radioisotopic carriers.

As India is blessed with varied climate, it is no wonder each of the state of India produces some spices. Culinary spices have been used not only making food colour and taste but for health enhancing properties and a food preservative also. The medicinal importance of Indian spices and herbs are undeniable. The isolated organic compounds from various spices belong to many natural products like flavonoids (quercetin in onion), chalcogen (curcumin in turmeric), terpenoid ( $\alpha$ -pinene in cumin) families. Due to presence of many chelating functional groups like poly-phenol derivatives,  $\alpha$ -b unsaturated carbonyl groups etc. they are able to bind with many target probes. Probably this noncovalent interaction causes spices for curing of many diseases like diabetes, cardiovascular diseases, arthritis, cancer and AIDS. Recently our group is involved to use various natural resourced chemicals in developing radiochemical analysis. Herein we have extracted NRC curcumin from Indian spices turmeric using reported procedure. Characterization was done by IR and NMR (both  $^1\text{H}$  and  $^{13}\text{C}$ ) spectroscopy. Preliminary some DFT calculations have been carried out for investigation about interaction of this curcumin with different radioisotopes to get an idea for experimental of radiochemical separation.

#### *References:*

- (1) Tapsell, L.; Patch, C.; Fazio, V.; *MJA*. **2006**, 185, S1-S25
- (2) Lahiri, S.; Choudhury, D.; Sen, K.; *J. Radioanal. Nucl. Chem.* **2018**, 318, 3
- (3) Anderson, M, A.; Mitchell, S, M.; Mohan, S.; *J. Chem. Ed. Chem. Wisc. edu.* **2000**, 77, 3



ICCDL-2022@DHWU

OP-06

**Bond dissociation energies of  $\text{GeX}_2$  and  $\text{GeX}_2^\pm$  (X= F, Cl, Br, I)**

**S. Ghosh\***, T.K. Ghosh

*Department of Physics, Diamond Harbour Women's University, Sarisha, West Bengal, India.*

e-mail: sudeshna.dhwu.physics@gmail.com

Among the divalent  $\text{MX}_2$  and  $\text{MXY}$  compounds of the major Group 14 elements (M=C, Si, Ge, and Pb; X, Y=H and/or halogens) have been extensively and actively explored by both experimentalists and theoreticians due to their fundamental importance as intermediates in various chemical reactions for producing modern semiconductor devices. Ge-based perovskites are actually environment-friendly and stable at room temperature. In recent year a number of Ge-based halide perovskites were synthesized. Over the past 20 years, research into divalent germanium compounds has exploded, resulting in the exploration of numerous novel chemical species including monomeric and divalent silicon, germanium, tin, and lead compounds with small organic substituents using chelating ligands.

It is found that dihalides and other compounds with group-IV atoms (eg.  $\text{MCl}_2$ ,  $\text{MBr}_2$ ,  $\text{MI}_2$ ,  $\text{MHCl}$ ,  $\text{MHBBr}$ , and  $\text{MHI}$ ; M=Ge, Si, Pb etc.) and also their ionic systems are produced during the halogen-assisted etching of semiconductors. That's why a thorough understanding of molecular properties, BDE etc. are very much helpful to understand the chemistry involved in the processes of plasma-assisted chemical etching (PACE) and plasma-assisted chemical vapour deposition (PACVD), particularly occurred in the fabrication of microelectronic devices.

An extensive basis set is used to calculate the structure, vibration frequency, dissociation energy, and many spectroscopic parameters for the aforementioned halides. Geometries and frequencies have been obtained at the MP2 and QCISD(T) level of theories. The energy values are obtained at the QCISD(T)//MP2 and QCISD(T)//QCISD(T) level of theories. BDEs of neutral dihalides are calculated using BDEs of ionic dihalides and EA, IP of related molecules. Theoretical calculations of these systems are limited, because of the concerned heavy atoms. In this sense, our calculated data may serve as future references

*References:*

- (1) Benavides-Garcia, M.; Balasubramanian, K. *J. Chem. Phys.* **1992**, *97*, 7537-7544
- (2) Mok, D.; Chau, Foo-tim.; Lee, E.; Dyke, J. M. *ChemPhysChem.* **2005**, *6*, 719-731
- (3) Ng, CH.; Nishimura, K.; Ito, N.; Hamada, K.; Hirotoni, D.; Wang, Z.; Yang, F. *Nano Energy*, **2019**, *58*, 130-137



## ICCDL-2022@DHWU

### OP-07

## **Application of nanoparticles against parasites of fishes as a novel tool of diseases control**

**Riya Mondal** and Biplab Bhowmik\*

*Parasitology Laboratory, Department of Zoology, Diamond Harbour Women's University, Diamond Harbour – 743368, West Bengal, India*

*E mail: [panchakotbb@gmail.com](mailto:panchakotbb@gmail.com)*

At the bottom there is a plenty of room where interdisciplinary foot steps can accommodate very comfortably (Feynman, 1961). In recent decades different type of water soluble nanoparticles with extensive biochemical application like life cycle imaging of living laboratory animals, drug delivery , disease control were pursue (Tripathi and Sarkar, 2015). In the aquaculture, disease prevalence and the bioaccumulation of toxic chemical has emerged as essential challenges which can be deal with nanotechnology as innovative and novel tool. Apart from traditional top down and bottom up approach, green synthesis of nanoparticle using microorganism, enzyme, plant and plant extract is popularised as eco-friendly alternative (Daniel et al., 2021). This nanoparticle could penetrate all tissues of fish including brain through blood brain barrier. Nanoparticles can disrupt cell membrane and induce generation of reactive oxygen species causes cell death (Saleh et al.,2017). It shows inhibition of cell division and affect pathogenicity of parasites (Nasr-Eldahan et al.,2017) (Pimentel-Acosta et al.,2019). Here, we mainly focused on nanotechnology as a tool of controlling parasite to promote sustainable aquaculture with special reference of metal and biologically synthesized nanoparticles against disease causing pathogens.

### References:

1. Feynman, R.P., **1961**. There's plenty of room at the bottom: An invitation to enter a new field of physics. *Miniaturization, Reinhold*.
2. Tripathi, S. and Sarkar, S., **2015**. Influence of water soluble carbon dots on the growth of wheat plant. *Applied Nanoscience*, 5(5), pp.609-616.
3. Daniel, S.C.G.K., Kumar, R., Sathish, V., Sivakumar, M., Sunitha, S. and Sironmani, T.A., **2011**. Green synthesis (*Ocimum tenuiflorum*) of silver nanoparticles and toxicity studies in zebra fish (*Danio rerio*) model. *Int J NanoSci Nanotechnol*, 2, pp.103-117.
4. Saleh, M., Abdel-Baki, A.A., Dkhil, M.A., El-Matbouli, M. and Al-Quraishy, S., **2017**. Antiprotozoal effects of metal nanoparticles against *Ichthyophthirius multifiliis*. *Parasitology*, 144(13), pp.1802-1810.
5. Nasr-Eldahan, S., Nabil-Adam, A., Shreadah, M.A., Maher, A.M. and El-Sayed Ali, T., **2021**. A review article on nanotechnology in aquaculture sustainability as a novel tool in fish disease control. *Aquaculture International*, 29(4), pp.1459-1480.
6. Pimentel-Acosta, C.A., Morales-Serna, F.N., Chávez-Sánchez, M.C., Lara, H.H., Pestryakov, A., Bogdanchikova, N. and Fajer-Ávila, E.J., **2019**. Efficacy of silver nanoparticles against the adults and eggs of monogenean parasites of fish. *Parasitology research*, 118(6), pp.1741-1749.



ICCDL-2022@DHWU

OP-08

## Study of surface morphology with electrical and optical properties of GO and rGO

Aniruddha Mondal<sup>1,2</sup>, Hari Shankar Biswas \*

<sup>1\*</sup> Department of Chemistry, Surendranath College, Kolkata 700 009, India, <sup>2</sup>Harindanga High School, Falta, South 24 Parganas, Pin-743504

e-mail: aniruddha.chem007@gmail.com

### Abstract

Graphene oxide (GO) thin film possess a 2D sheet structure and were synthesized indigenously via the enhanced solvothermal Hummer method. Conventionally, the redox approach can be a characteristic technique to fabricate GO films on an expanded scale. AFM characterization shows GO film had a 2D lamellar layer structure and the thickness between 3 to 5 nm. Using heat treatment, the GO film is reduced to reduced graphene oxide (rGO). Atomic force microscopy (AFM), scanning electron microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) were employed to characterize the morphological, optical of the GO and rGO thin films. Electrical properties of the thin films were studied with current-voltage (I-V) properties. It is seen that the rGO thin film shows higher conductivity than GO and the value  $\approx 5.1 \times 10^{-4} S/cm$ , and also changes the morphology and optical properties. The change of the morphological and optical properties indicates the GO losses oxygen groups to form rGO.

### References:

- (1) Daniela C. Marcano ET AL.; *ACS Nano* **2010**, 4, 8, 4806-4814
- (2) Aliakbar Gholampour ET AL.; *ACS Appl. Mater. Interfaces* **2017**, 9, 49, 43275-43286
- (3) Raluca Tarcan ET AL.; *J. Mater. Chem. C* **2020**, 8, 1198-1224
- (4) Hari Shankar Biswas.; S. Bala.; A. K. Kundu.; I. Saha.; S. Poddar.; S. Sarkar.; P. Mandal.; *Inorganic chemistry communications* **2022**, 139, 109356



**ICCDL-2022@DHWU**

**PP-01**

**Conformations of linalool investigated through FTIR spectroscopy and electronic structure calculations**

**Puja Samanta and Pujarini Banerjee**

*Diamond Harbour Women's University*

e-mail: [spuja821@gmail.com](mailto:spuja821@gmail.com)

Volatile organic compounds (VOCs) emitted by plants constitute an important class of plant secondary metabolites. Although such VOCs have been identified in many floral and leaf extracts, there are limited reports of their structural and chemical attributes. Linalool, belonging to the class of terpenoids, is one such VOC which has been investigated in the present work, by combining FTIR spectroscopy with quantum chemical calculations. Linalool is predicted to be present in a large number of conformations, of which some involve intramolecular O-H... $\pi$  hydrogen bonds, while others involve free O-H groups. FTIR spectroscopy of linalool in CCl<sub>4</sub> solution in the  $\nu_{\text{O-H}}$  region suggests presence of both closed and open conformations of the molecule, with the former being the dominant type. Electronic structure calculations also predict an energetic preference for the closed conformation. In the presence of additional H-bond acceptors in the environment, there is likely to be a competition between intermolecular and intramolecular O-H... $\pi$  H-bonding. This possibility has also been explored in the present study.



## ICCDL-2022@DHWU

PP-02

### SYNTHESIS OF POTENTIALLY BIOACTIVE URACIL DERIVATIVES BY THE USE OF TRANSITION-METAL CATALYSED REACTIONS

Prasenjit Mistry<sup>a,b</sup> and Brindaban Roy<sup>a\*</sup>

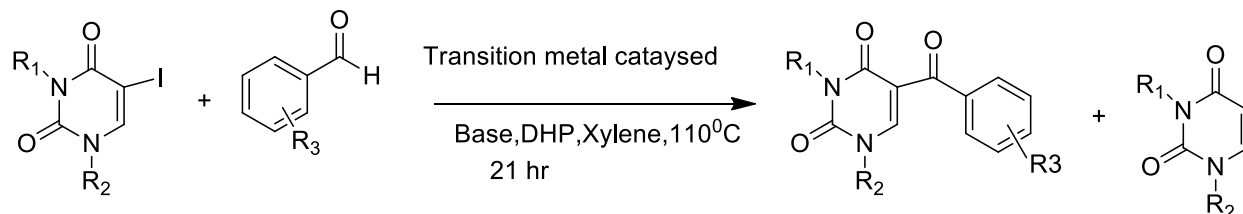
<sup>a</sup>Department of Chemistry, University of Kalyani, Kalyani-741235, India

<sup>b</sup>Department of Chemistry, Jangipur College, Jangipur-742225, India

e-mail: [broybsku@gmail.com](mailto:broybsku@gmail.com)

Different heterocyclic compounds play a central role as versatile building blocks for many drugs. These biologically active heterocyclic molecules draw huge attention for their unique potentiality. The uracil derivatives, the basic unit of RNA, are widely reported for their antiviral and anti-tumour activities.<sup>1-3</sup> It also exhibit herbicidal, insecticidal and bactericidal activities.<sup>4</sup> These bioactive properties associated with uracil derivatives have made the synthesis of these molecules more demanding. Uracils functionalized specifically at C-5 and C-6 positions are an important class of pyrimidine derivatives possessing a wide variety of biological activities. The functionalization at C5-position of pyrimidines are the choice of interest, because this site is not involved in Watson–Crick base pairing<sup>5</sup>.

Metal catalysed C-H activation of uracil derivatives are reported<sup>6,7</sup> but the synthesis carbonyl derivatives by using metal catalysed direct C-H carbonylation without the use of toxic carbonyl source is not reported yet. Uracil functionalization using transition metal is one of the key areas of modern research in organic chemistry. We have developed strategy for C-H functionalization via C-H activation by environmentally benign pathway.



References:

- 1) Megati, S.; Phadtare, S.; Zemlicka, J. *J. Org. Chem.* **1992**, 57, 2320.
- 2) Mitsuya, H.; Yarchoan, R.; Broder, S. *Science* **1990**, 249, 1533.
- 3) Haines ; D. R.; Tseng ; C. K. H.; Marquez, V. E.J. *Med.Chem.* **1987**, 30, 943.
- 4) Larsson, A.; Stenberg, K.; Ericson, A. C.; Haglund, U.; Yisak, W. A.; Johansson, N. G.; Öberg, B.; Datema, R. *Antimicrob. Agents Chemother.* **1986**, 30, 598
- 5) Yi-Yun Yu and Gunda I. Georg\* *Chem. Commun.*, **2013**, 49, 3694-36
- 6) Mondal, B; Hazra, S; Roy, B; *Tetrahedron Letters*. **2014**, 55, 1077, (<http://dx.doi.org/10.1016/j.tetlet.2013.12.092>)
- 7) Mondal, B; Hazra, S; Panda, T. K; Roy, B; *Beilstein J. Org. Chem.* **2015**, 11, 1360, ([doi:10.3762/bjoc.11.146](https://doi.org/10.3762/bjoc.11.146))



ICCDL-2022@DHWU

PP-03

## **A comprehensive study of ROS mediated filaricidal and mosquitocidal activities of silver nanoparticles**

Priya Roy<sup>1\*</sup>, Monalisa Pramanik<sup>1</sup>

<sup>1</sup>Department of Zoology, Diamond Harbour Women's University, Sarisha-743368, India

Email: [royprya12@gmail.com](mailto:royprya12@gmail.com)

### **Abstract**

The silver nanoparticles (AgNPs) are designed and synthesized through ultrasound assisted green process using unique combination of a biomolecule (tyrosine) and a natural polymer, starch. A comprehensive mechanistic study on the reactive oxygen species (ROS) mediated filaricidal (against *Setaria cervi*) and mosquitocidal (against second and fourth instar larvae of *Culex quinquefasciatus*) activities of AgNPs has been made for the first time for controlling filariasis by taking care of both filariid and its vector. The mechanism may help in formulating antifilarial drug based on bio-polymer inspired AgNPs. The role of natural polymer in inspiring bioactivity of AgNPs has been investigated and its activities have been compared with the commercially available AgNPs. Cytotoxicity of AgNPs on macrophages of Wistar rat has been evaluated to ensure its selectivity towards filariid and larvae.

**Keywords:** carbohydrate polymer, silver nanoparticle, filaricidal, mosquitocidal, ROS, apoptosis





ICCDL-2022@DHWU

PP-04

## Experimental and Theoretical Investigation of the Catalytic Performance of Reduced Schiff Base and Schiff Base Iron Complex: Transformation to Magnetically Retrievable Catalyst

**Rimpa Mondal<sup>1</sup>, Aratrika Chakraborty,<sup>2\*</sup> Tanmay Chattopadhyay<sup>\*1</sup>**

<sup>1</sup>Diamond Harbour Women's University, Sarisha, West Bengal, India.

<sup>2</sup>Lady Brabourne College, P-1/2 Suhrawardy Avenue, Kolkata-700017

e-mail: rimpamondal956@gmail.com

Catalytic efficiencies for the oxidation of alcohols of a mononuclear Schiff base Iron complex (**FeL**) and an analogous reduced Schiff base one (**FeRL**) have been assessed experimentally and theoretically. The structure of **FeL** had been previously reported by our group. Here, we have synthesized the reduced Schiff base complex **FeRL** where RL=2,2'-(2,2-dimethyl-1,3-propanediyl)bis(iminomethylene)]bis[2,4-dichlorophenol]. The Single Crystal X-Ray analyses of the new complex reflected its mononuclear nature and an umbrella like framework. Homogeneous catalytic experiments revealed the superiority of **FeRL** over **FeL**, which could be rationalized by comparing the stability of the corresponding  $\text{Fe}^{\text{V}}=\text{O}$  species characterized through Density Functional Theory calculations. Based on its excellence, **FeRL** was chosen for surface modification of magnetite nanoparticles coated with dopamine to generate magnetically recoverable  $\text{Fe}_3\text{O}_4@\text{Dopa}@\text{FeRL}$  (**FDFeRL**). **FDFeRL** was characterized with the aid of Field Emission Scanning Electron Microscopy, Transmission Electron Microscopy, powder X-ray diffraction and Fourier-transform infrared spectroscopy and efficiently used in the oxidation of a variety of alcohols. Our synthesis of the supported catalyst can be deemed as a simple, economical and sustainable one. Catalyst recovery could be easily achieved by simple application of a magnet. **FDFeRL** could be reused several times without compromise in its catalytic efficiency.

### References:

- (1) Mondal, R. **Chakraborty**, A, Ghanta, R, Menéndez, M.I, Chattopadhyay, T. *Appl. Organomet. Chem.* **2021**, 35, 9, e6332
- (2) Chakraborty, A, Chowdhury, T, Menedez, M.I, Chattopadhyay, T. *ACS Appl. Mater. Interfaces* **2020**, 12, 34, 38530–38545.



## ICCDL-2022@DHWU

PP-05

**Triton X-100 functionalized Cu(II) dihydrazone based complex immobilized on Fe<sub>3</sub>O<sub>4</sub>@dopa: A highly efficient catalyst for oxidation of alcohols, alkanes, and sulfides and epoxidation of alkenes**

**Rinku Ghanta, Tanmay Chattopadhyay\***

*Diamond Harbour Women's University, Sarisha, West Bengal, India.*

e-mail: rinkughanta96@gmail.com

Here, we have presented a protocol for green synthesis, characterization, and catalytic application of TX100/Fe<sub>3</sub>O<sub>4</sub>@dopa@CuL (FDCTX) magnetically separable nanoparticles. Fe<sub>3</sub>O<sub>4</sub>@dopa@CuL (FDC) was synthesized using a fourstep procedure: (i) synthesis of a dihydrazone derivative, (ii) reaction of the dihydrazone derivative with copper perchlorate salt to generate a copper complex of the dihydrazone derivative, (iii) immobilization of the complex onto Fe<sub>3</sub>O<sub>4</sub>@dopa to generate FDC, and (iv) coating of FDC with surfactant Triton X-100. The as-synthesized homogeneous complex was well characterized using UV–Vis., Fourier-transform infrared (FT-IR), electrospray ionization–mass spectrometry, and single-crystal X-ray techniques. Single-crystal X-ray analysis revealed the tetranuclear framework of the complex. The heterogeneous nanoparticles (FDCTX) were characterized using FT-IR, powder X-ray diffraction, scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray spectroscopy, magnetic hysteresis, and dynamic light scattering techniques. Finally, both the homogeneous and heterogeneous catalysts were utilized for efficient oxidation of alcohols, alkanes, and sulfides and epoxidation of alkenes.

*References:*

- (4) Chakraborty, T, Mondal, R, Ghanta, R, Chakraborty, A, Chattopadhyay, T. *Appl Organomet Chem.* **2020**;e5695
- (5) Mondal, R, Chakraborty, A, Ghanta, R, Menendez, M.I, Chattopadhyay, T. *Appl Organomet Chem* **2021**,e6332.



## ICCDL-2022@DHWU

### PP-06

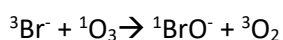
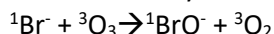
#### Ab initio calculation of ozone depleting reactions



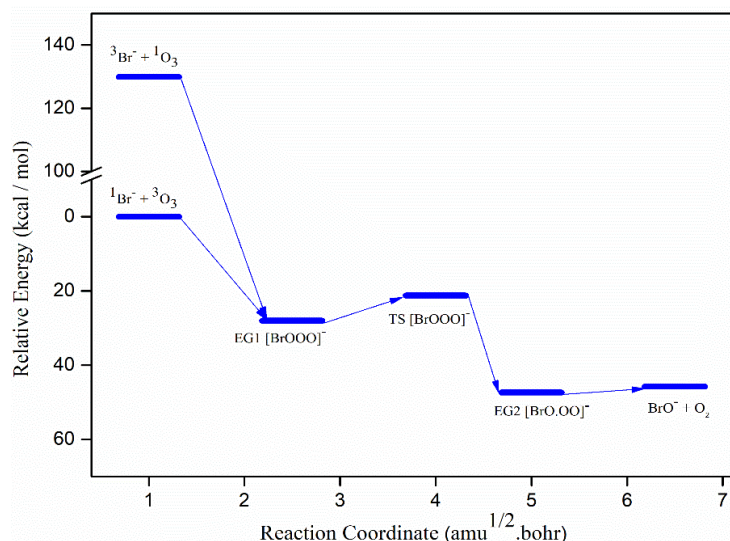
Gargi Nandi\*, T.K.Ghosh

Department of Physics, Diamond Harbour Women's University  
Sarisha, DH Road, South 24-Pgs, West Bengal-743368, India  
e-mail: garginandiindia@gmail.com

In few years, scientific and public interest is grown up about the changing nature on the earth. The halogen (Br) ions play most important role in catalytic ozone destruction in the stratosphere via the reactions:



It has been observed that, during spring season in the polar regions, unique photochemistry converts inert halide salt ions into reactive halogen species that deplete ozone in the boundary layer. However, some experimental investigations are available for these systems, many key processes remain poorly understood and in particular, theoretical investigations along these systems are limited in literature.



Ab initio calculations have been done to investigate various minimum energy geometries and transition state geometries of these ozone depleting reactions for the triplet potential energy surfaces using correlation consistent basis sets including polarization functions and effective core potential. Geometries and frequencies have been identified at the MP2 level of theory. The energetics are obtained at the CCSD(T) and QCISD(T) levels. Possible reaction pathways are discussed on the basis of IRC calculation. New features have been identified in the present work.

References: (1) Gladich, I., Francisco, J. S., Buszek, R. J., Vazdar, M., Carignano, M. A., & Shepson, P. B., *J. Phys. Chem A* **2015**, *119*(19), 4482–4488.

(2) W.L. Chameides, D.D. Davis, *J. of Geo. Res.: Oceans* **1980**, *85*, 7383–7398.



# ICCDL-2022@DHWU

PP-07

## Ab initio study for the reaction mechanism of ozone with bromine ion

**Soma Naskar\***, Tapas Kumar Ghosh

*Diamond Harbour Women's University, Sarisha, West Bengal, India.*

e-mail: [somanaskar1993@gmail.com](mailto:somanaskar1993@gmail.com)

Ab initio calculations have been performed to investigate the reaction mechanism of the ozone depleting reaction  ${}^1\text{Br}^-({}^1\text{S}) + {}^1\text{O}_3({}^1\text{A}_1) \rightarrow {}^1\text{BrO}^-({}^1\Sigma\text{g}) + {}^1\text{O}_2({}^1\Sigma\text{g}^-)$ . Ozone depletion by halogen ions has been found to occur in winter and spring in the Arctic boundary layer air and snow pack at Alert, Canada (82°N, 62°W). Experimental investigations are performed mainly for the reaction rate constant and efficiency of ozone depletion. To get the information about the intermediate isomers and reaction paths, one must perform theoretical investigations.

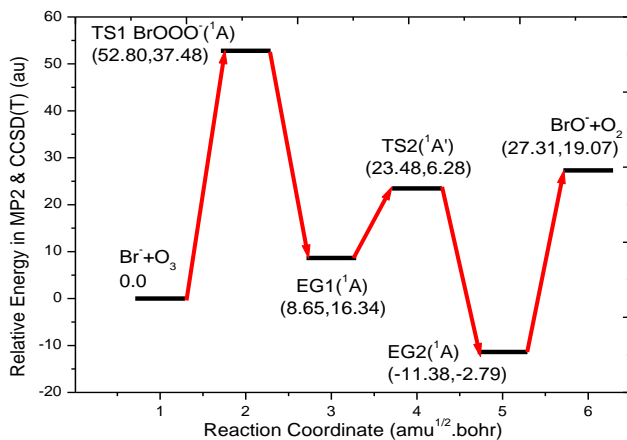


Fig : Relative energy diagram for Br+O<sub>3</sub> reaction

The structure of various minimum energy geometries, transition state geometries and their frequency related to the above ozone depleting reaction are obtained at the Moller-Plasset Perturbation method MP2 level using correlation consistent basis sets. The energy values are obtained using Couple Cluster single- double including triples terms CCSD(T) method. IRC results have been performed at the MP2 level to find out the reaction pathways. New features have been obtained on the reaction pathways from our investigation in comparison to previously reported works.

*References:*(1) Bejianian, y.; Bras, G. L.; Poulet, G.; J. Phys. Chem., **1998**, A012-10501.

(2) Gladich, I.; Francisco, S. J.; Buszek, J. R.; Vazdar, M.; Carignano, A. M.; Shepson, B. P.; J. Phys. Chem., **2015**, 119, 19, 4482–4488.

(3) Solomon, S.; Garcia, R.R.; Ravishankara, A.R.; J. Geophys., **1994**, 99, 20491.

(4) Bottenheim, J. W.; Fuentes, J. D.; Tarasick, K. G.; Atoms. Environ. **2002**, 2535–2544.

(5) Simpson, W. R.; Glasow, R. von.; Riedel, K.; J. Phys. Chem., **2007**, 7, 4375-4418.



# ICCDL-2022@DHWU

PP-08

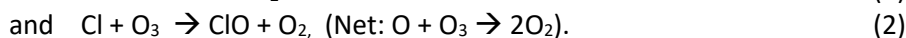
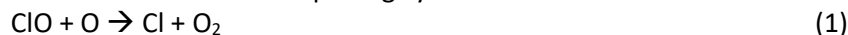
## A comparative study of the mechanism of the reaction $\text{ClO} + \text{O} \rightarrow \text{Cl} + \text{O}_2$

T. K. Ghosh\*

Department of Physics, Diamond Harbour Women's University,, Sarisha, West bengal, India

\*e-mail: tapaskrg@yahoo.com

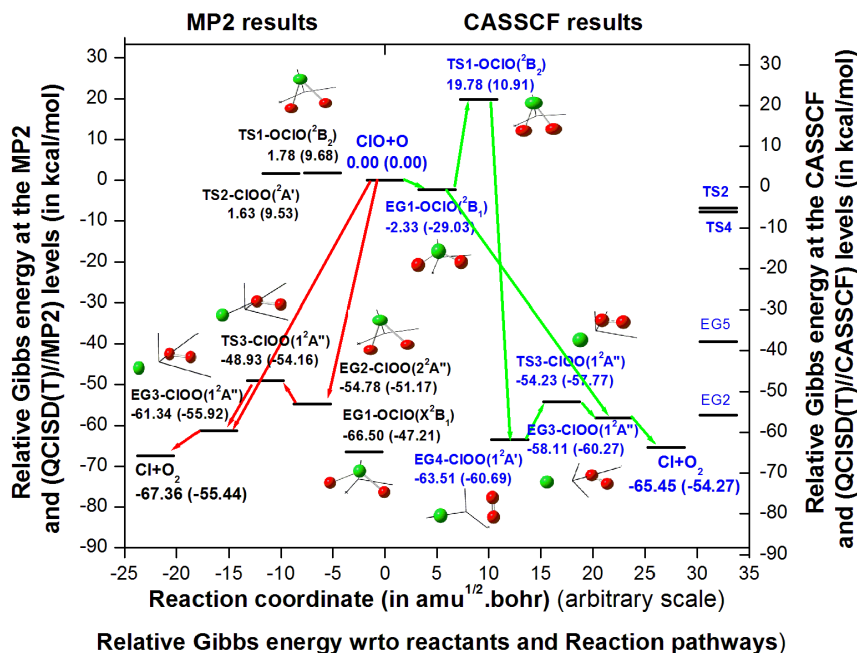
In recent years, a worldwide concern has been grown up about the environmental threat on the earth due to depletion of ozone layer in the lower stratosphere. Halogen atoms and their oxides play a key role in atmospheric ozone destruction. One of such ozone depleting cycles for  $\text{Cl}^1$  is:



The reaction (1) is crucial for determining the rate and efficiency of ozone depletion. The only ab initio study on the reaction (1) was reported by Zhu and Lin<sup>2</sup> usin

256g PW91/6-311G(3df) method and reported product formation directly via the equilibrium geometry as  $\text{ClO} + \text{O} \rightarrow \text{ClOO} \rightarrow \text{Cl} + \text{O}_2$ . From MCSDCI study, Peterson & Werner<sup>3</sup> suggested qualitatively that  $\text{OClO}$  may predissociate to  $\text{ClO} + \text{O}_2$  via its excited state  $\text{OClO}(^2A_2)$  and possibility of direct dissociation as  $\text{ClOO}(X^2A'') \rightarrow \text{ClO} + \text{O}_2$ .

In this context, a comparative study has been reported for the geometries and reaction pathways at the MP2/cc-pVTZ(sp-diff) and CASSCF(7,6)/6-31G\*\* levels. At the multi-configuration level some new isomers are identified. Some interesting features for the reaction pathways, obtained from IRC calculations, are found, which are new to be reported. The energetics are obtained at the QCISD(T)//MP2 and QCISD(T)//CASSCF level of theories.



References:(1) Molina, M. J.; Rowland, F. S. *Nature* **1974**, 249, 810-812.(2) Zhu, R. S.; Lin, M. C. *J. Chem. Phys.* **2003**, 119, 2075-2082. (3) Peterson, K. A.; Werner, H. J. *J. Chem. Phys.* **1992**, 96, 8948-8961.



## ICCDL-2022@DHWU

PP-09

### **Development of an efficient magnetically separable nanocatalyst : application for various organic Transformations**

**Tanmay Chattopadhyay**

*Diamond Harbour Women's University, Sarisha, West Bengal, India*

e-mail: tanmayc2003@gmail.com

Schiff base metal complexes have been extensively used as homogeneous catalysts for oxidation of various organic substrate. They show high efficiency since the active site is easily accessible, but their separation from the reaction mixture is really a difficult task. For this various difficult methods are applied which causes unnecessary time consumption and sometimes hazardous chemicals are also employed which causes the environment pollutant. But Heterogeneous catalysts appear to avoid this problems. In heterogeneous catalytic systems, the active catalytic sites and the reactants are in the different phases, so isolation and separation can be readily accomplished. Hetero-genization is commonly achieved by entrapment or grafting of the active molecules of surfaces or inside the pores of a solid support, such as silica, alumina, organic nanotube etc. However, the active sites in heterogeneous catalysts are not as accessible as in a homogeneous system, and thus the activity of such catalysts become lowered. So, a catalytic system showing high activity and selectivity (like a homogeneous system) and ease separation and recovery (like a heterogeneous system) would be highly desirable. This goal can be achieved using magnetic nanoparticles (MNPs), which are able to bridge the gap between homogeneous and heterogeneous catalysis, preserving the desirable attributes of both systems. The development and growth of nanotechnology has caused a continuous shift in every aspect of modern science. So far, it has changed the perspective of the scientific community towards catalysis and brought remarkable transformations in the synthetic chemical processes. MNPs nowadays have attracted immense scientific and technological interest due to their unique physical and chemical properties which make them an ultimate choice in the field of catalysis. The preparation and the use of MNPs in organic synthesis has become a subject of intense investigation as they offer advantages in clean and sustainable chemistry.

#### *References:*

- (1) Mondal, R , Chakraborty,A,Ghanta, R,Menendez, M.I, Chattopadhyay, T.Appi.Organomet. Chem. 2021, 35, 9,e6332.
- (2) Chakraborty,T, Mondal, R, Ghanta, R, Chakraborty, A, Chattopadhyay,T,Appl Organomet Chem.2020;e5695.



# ICCDL-2022@DHWU

PP-10

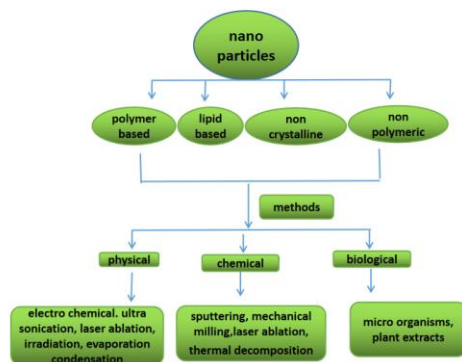
## Synthesis of Nano Materials and Challenges: A Brief Review

Dr.Kazi Sabnam Banu

Netaji Nagar Day College, Kolkata , West Bengal, India

e-mail: [kazisabanam80@gmail.com](mailto:kazisabanam80@gmail.com)

Nano materials are the chemical compounds having exceptionally high surface area with external dimensions in billionths of a meter<sup>1</sup>. The contributions of nano materials in research areas including nano technology, nano engineering and nano science are enormous<sup>2</sup>. The application of nano materials are huge in various fields like medicine, industry, agriculture, aviation sector, energy sector, as catalysts, in the environment, in food and dye technology and many more<sup>3</sup>. Nanomaterials have huge control on the discipline like physics, chemistry, microbiology, material science, bio technology, biochemistry, micro electronics in scientific fields. So it is the need of the hour to manufacture more and more nano materials of variable properties like magnetic, electrical, optical, mechanical, and catalytic to get maximum benefits from these. This review explains the synthesis of nano materials of varying size, different surface characteristics, varying functional behaviour from the diverse range of materials like ceramic, semiconductors, metals, metal oxides , polymers for the production of polymer based, lipid based, non polymeric and non crystalline nanoparticles. Various techniques such as from assembling the atoms together to disassemble (bottom up to bottom down approaches) i.e bio assisted method, by applying different physical and chemical methods for the synthesis of nanomaterials have been discussed briefly<sup>4</sup>. The application of nano materials in various field have also been discussed.



### References:

[1] Khan, I.; Saeed, K.; Khan, I. *Arabian Journal of Chemistry*.**2019**, *12*, 908-931

[2] C. Roco, Mihail. *Journal of Nanoparticle Research*.**2011**, *13*,427–445

[3] Anu Mary Ealia,S; Saravanakumar, M P.; *IOP Conf. Ser.: Mater. Sci. Eng.* **2017**, *263*, 032019

[4] Dhand,C.; Dwivedi,N.; Jun Loh, X.; Ng Jie Ying,A.; Verma,N.K., W. Beuerman,R.; Lakshminarayanan, R.;Ramakrishna, S. *RSC Adv.*, **2015**, *5*, 105003



## ICCDL-2022@DHWU

### PP-11

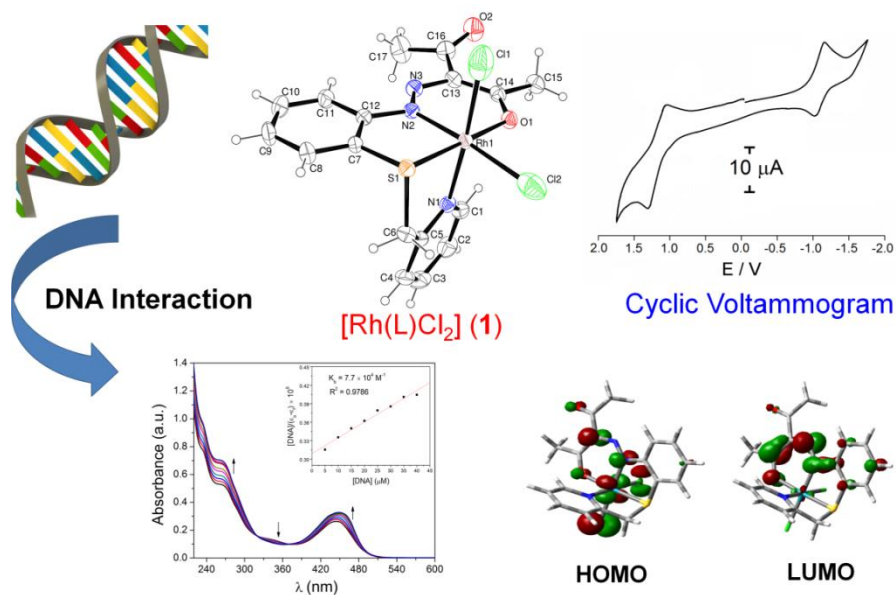
#### New Rh(III) chloro complex of a tetradentate S-picoyl azo ligand of acetyl acetone: Synthesis, X-ray structure, spectral characterization, electrochemistry, DFT computation and interaction with DNA

**Dr. Puspendu Roy**

Netaji Nagar Day College Kolkata-700092, West Bengal, India.

e-mail: [royuspendu1991@gmail.com](mailto:royuspendu1991@gmail.com)

New rhodium(III) complex with thioether containing NSNO donor azo-ligand (HL) is synthesized and characterized. The distorted octahedral geometry of the complex is confirmed by single crystal X-ray diffraction method. Cyclic voltammogram exhibits quasi-reversible Rh(III)/Rh(IV) oxidation along with ligand based reduction in acetonitrile. Electronic structure, electrochemical and absorption properties of the complex are interpreted by DFT and TDDFT calculations.



The ability of the complex to bind with CT DNA is investigated by UV-vis method and the binding constant is found to be  $7.70 \times 10^4 \text{ M}^{-1}$ . Competitive binding study with ethidium bromide (EB) by fluorescence method suggests that the Rh (III) chloro complex efficiently displaces EB from EB-DNA. The Calculated Stern-Volmer dynamic quenching constant,  $K_{SV}$  is  $2.07 \times 10^4 \text{ M}^{-1}$ .

#### References:

- (6) Jana, S.; Jana, M.S.; Biswas, S.; Sinha, C.; Mondal, T.K. J. Mol. Struct. **2014**, 1065-1066, 52-60.
- (7) Zhang, Z.; Qian, X.H. Int. J. Biol. Macromol. **2006**, 38, 59-64.
- (8) Pradhan, A. B.; Haque, L. S.; Bhuiya, A. Ganguly, S.; Das, J. Phys. Chem. **2015**, B 119, 6916-6929.
- (9) Anjomshoa, M. H.; Hadadzadeh, M.; Torkzadeh-Mahani, S.J.; Fatemi, M. Adeli-Sardou, H.A.; Rudbari, V.M. Eur. J. Med. Chem. **2015**, 96, 66-82.





ICCDL-2022@DHWU

PP-12

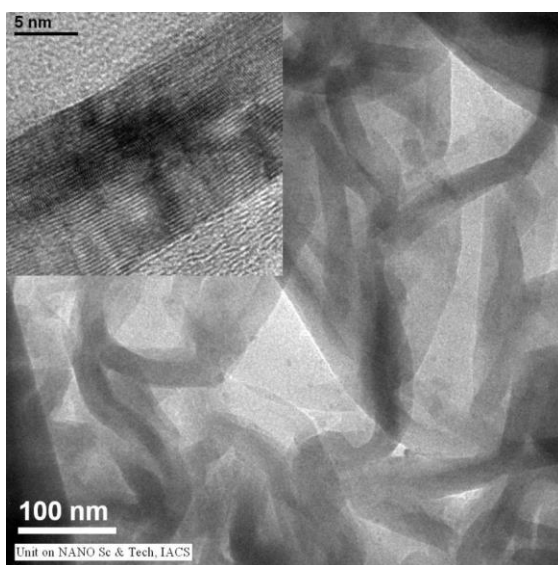
## Study of antibacterial activity of multiwalled carbon nanotubes synthesized by Spray pyrolysis method

Uday Das\*

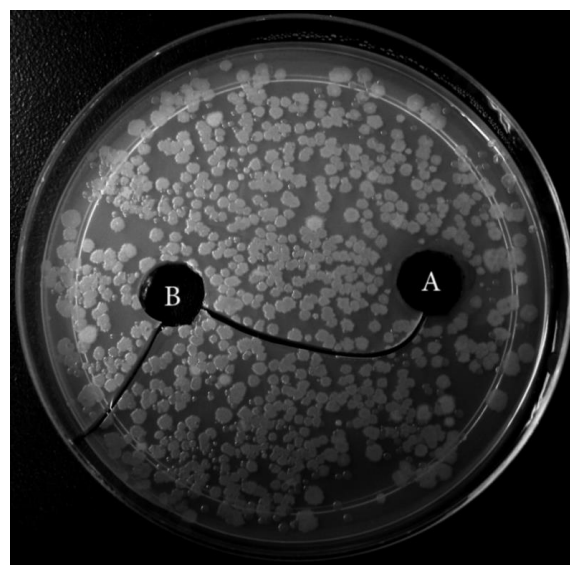
*Department of Physics, Hooghly Mohsin College, Chinsurah, Hooghly-712110 West Bengal, India*

e-mail: udaydas\_ju@yahoo.co.in

Multiwalled carbon nanotubes (MWCNTs) were synthesized by spray pyrolysis technique at an optimum temperature of 700°C using turpentine oil as the carbon source. Ar is used as the carrier gas to generate the turpentine mist, and Ag-Cu nanoparticles are used as the catalyst. The morphological structures of the MWCNTs are investigated by Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), X-ray diffraction pattern. The mixture of Ag and Cu nanocatalysts increases the yield of MWCNTs compared to a pure Ag nanocatalyst. Antibacterial activity of the synthesized MWCNTs has been evaluated against *Escherichia coli* using the cup-plate method<sup>1</sup>.



TEM micrograph of MWCNTs, the inset shows the HRTEM micrograph



Antibacterial activity of CNTs synthesized using a mixture of Ag and Cu nano catalyst. Cup A and Cup B contain CNTs and distilled water respectively

### *References:*

- (1) British Pharmacopoeia 1993; Pharmacopoeia of India 1985



ICCDL-2022@DHWU

PP-13

## Design and synthesis of biopolymer inspired gold nanoparticle as an efficient antifilarial agent

Swadhin Kumar Saha<sup>1\*</sup> and Priya Roy<sup>2</sup>

<sup>1</sup>Department of Chemistry, Kazi Nazrul University, Asansol-713340, India

<sup>2</sup>Department of Zoology, Diamond Harbour Women's University, Sarisha-743368, India

Email: [swadhin.chem@gmail.com](mailto:swadhin.chem@gmail.com)

### ABSTRACT

The gold nanoparticles (AuNPs) have been synthesized biogenically by using black pepper (*Piper nigrum*) extract according to the principles of green chemistry in presence and absence of a biopolymer, chitosan. The synthesized nanomaterials have been characterized by UV-Vis spectroscopy, TEM imaging, EDX elemental analysis, DLS and Zeta potential measurements. A comprehensive study (up to cellular level) on the antifilarial (against *Setaria cervi*) activity of AuNPs has been made for the first time with a view to use it clinically. The bioactivity of biopolymer capped biogenic AuNP increases significantly compared to simple biogenic AuNP. The biopolymer plays an important role in inspiring AuNP through its inherent positive charges and hydrophobicity. The developed nanomaterial boosts the production of ROS (reactive oxygen species) and misbalances the antioxidant parameters of parasites such as GSH, GST, GPx, SOD and catalase. The produced ROS ultimately induces oxidative stress, which leads to apoptotic cell death in filarial worms. In addition, the designed biopolymer capped gold nanomaterials exhibit negligible toxicity towards human PBMCs. Thus, the present study may serve as a fruitful platform to explore biopolymer capped gold nanoparticles as efficient antifilarial agents. The mechanism may increase the therapeutic prospects of AuNPs to control lymphatic filariasis in near future.

**Keywords:** Gold nanoparticle, Antifilarial activity, Biogenic, Chitosan, ROS, Antioxidant



ICCDL-2022@DHWU

PP-14

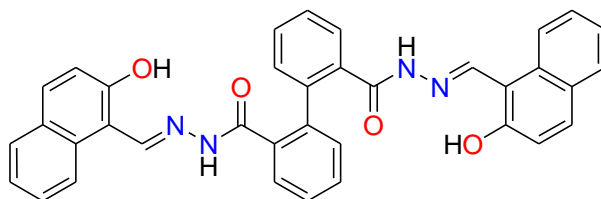
**Hydroxy-naphthaldehyde and Biphenyl-containing amido Schiff base  
derivative as a turn-on fluorescent chemosensor for Al<sup>3+</sup> ion**

**Anamika Hoque, Md. Akhtarul Alam\***

*Aliah University, Action area IIA/27, New Town, Kolkata-700160*

*e-mail: anamikahoque35@gmail.com*

A hydrazine-derived bis(2-hydroxy-naphthalidene)-[1,10-biphenyl]-2,20 dicarbohydrazide (sensor **1**) has been synthesized and its sensing properties toward different metal ions have been demonstrated using simple UV-visible spectroscopy, fluorometry and visible colour change techniques. The sensor **1** showed high fluorescence selectivity and sensitivity toward Al<sup>3+</sup> ion in aqueous DMF media. The fluorescence intensity of **1** is increased in the presence of Al<sup>3+</sup> at 485 nm and 458 nm respectively. Visual color change under 350 nm UV light exhibits a greenish-yellow fluorescence light in the presence of Al<sup>3+</sup> ion. Job's plot analysis show that sensor **1** and metal ions formed a 1 : 2 coordination complex. Furthermore, "Test Kits" coated with sensor **1** showed the successful selective detection of Al<sup>3+</sup> ion under UV light.



Sensor **1**

*References:*

- (1) Hoque, A, Islam, S, Khan, M.A., Ghosh, S., Sekh, A., Hussain, S., Alam, A., *New J. Chem.*, **2022**, 46, 16025.
- (2) Liu, Y., Zhang, L., Chen, L., Liu, Z., Liu, C., Che, G., *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 20, 1386-1425.



## ICCDL-2022@DHWU

PP-15

### Theoretical Exploration of Multi-Diels-Alder reaction on neutral & Li<sup>+</sup>-encapsulated C<sub>60</sub> fullerenes

**Soumadip Banerjee**, Abhijit Kr. Das\*

School of Mathematical & Computational Sciences  
Indian Association for the Cultivation of Science; Jadavpur Kolkata-32  
email:banerjee.soumadip@gmail.com

Over the last few decades, the chemical functionalization of fullerene systems has drawn greater scientific attention<sup>1,2</sup>. These functionalized materials have fascinating properties to be used for wide-scale applications such as biomedical field, electron transport layers, and organo-inorganic hybrid halide perovskite solar cells (PSCs) etc<sup>3</sup>. In this regard, covalent functionalization and endohedral modification are emerged to be suitable for modifying fullerene's physical and chemical properties. Diels-Alder (DA) reaction is one of the chemical tools for fullerene functionalization, producing unique derivatives<sup>4</sup> for potential applications. Nevertheless, experimental limitations hinder the utilization of corresponding oligo-products which are expected to have significant utilizations.

In this aspect, the sequential Diels-Alder reactions, i.e., Multi-Diels-Alder (MDA) of neutral and Li<sup>+</sup>-encapsulated C<sub>60</sub> with 1,3-butadiene have been investigated in the light of Density Functional Theory.

The aim is to investigate the kinetic and thermodynamic feasibility of the maximum number of butadiene attachments on the fullerene surface. The impact of Li<sup>+</sup>-encapsulation on the reaction sequences has also been monitored, based on the earlier reports<sup>5</sup> on the effect of Li<sup>+</sup>-confinement in mono-DA<sup>6</sup>.

The MDA reaction commences with the 1:1 encounter complex between the mono-functionalized fullerene product and the second butadiene molecule. Thereafter, two approaches, namely 'Direct' and 'Alternative', have been considered for second butadiene attachment to check whether the first functionalization makes the rest double bonds non-equivalent towards the second butadiene inclusion or not. Ultimately, each step following these two approaches forms the same tetra-functionalized final product with a high degree of exothermicity. The outcome of Li<sup>+</sup>-confinement is the diminished barrier heights and more negative exothermicity, compared to pristine one in each step of the MDA. The regioselectivity, just like the mono- and bis-functionalization reported earlier, is also retained. In short, this present study<sup>7</sup> will be instrumental in the field of fullerene chemistry for subsequent developments.



#### References:

- (1)Castro, E.; Garcia, A. H.; Zavala, G.; Echegoyen, L. *J. Mater. Chem. B* **2017**, *5*, 6523-6535. (2) Lin, H. -S.; Matsuo, Y.; *Chem. Commun.* **2018**, *54*, 11244-11259. (3) Jia, L., Chen, M.; Yang, S. *Mater. Chem. Front.* **2020**, *4*, 2256-2282(4) Ueno, A H.; Kawakami, H.; Nakagawa, K.; Okada, H.; Ikuma, N.; Aoyagi, S.; Kokubo, K.; Matsuo, Y.; Oshima, T. *J. Am. Chem. Soc.* **2014**, *136*, 11162-11167 (5) Ueno, H.; Nishihara, T.; Segawa, Y.; Itami, K. *Angew. Chem. Int. Ed.* **2015**, *54*, 3707-3711.(6) Debnath, T.; Ash, T.; Saha, J. K.; Das, A. K. *Chemistry Select.* **2017**, *2*, 4039-4053. (7) Ash, T.; Banerjee, S.; Debnath, T.; Das, A. K. *Int. J. Quantum Chem.* **2022**, *122*(2), e26824.

## Mononuclear cobalt(III) halide complexes with tetradentate Schiff base: Syntheses, structures and properties

Sumitava Khan

Department of Chemistry, Burdwan Raj College, Burdwan 713 104, West Bengal

e-mail: mynamesumitavakhan@gmail.com

Two hexacoordinated mononuclear Co(III) compounds of the type  $cis-[Co(L)(N_3)_2]X$  [**1**, X = ClO<sub>4</sub>; **2**, X = PF<sub>6</sub>; L = N,N'-(bis(pyridine-2-yl)benzylidene)-1,4-butanediamine] have been synthesized and characterized by physico-chemical and spectroscopic methods. The crystal structures of complexes **1** and **2** both have distorted octahedral geometry with two terminal azides in mutual cis orientations. In the crystalline state, two mononuclear units of **1** are associated by weak C-H... $\pi$  interactions to produce a dimeric unit, which packs through C-H...O hydrogen bonds and  $\pi$ ... $\pi$  interactions leading to a 2D continuum. The mononuclear units in **2** are engaged in weak cooperative intermolecular C-H... $\pi$  interactions and multiple C-H...F hydrogen bonds giving rise to a 3D network structure. These diamagnetic compounds are redox-active and show luminescence in DMF solutions.

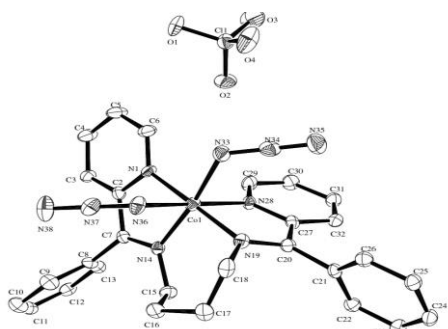


Fig.1. ORTEP of **1**

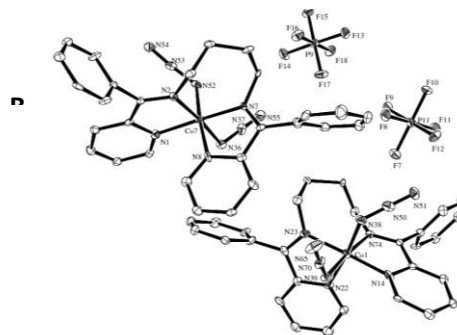


Fig.2. ORTEP of **2**

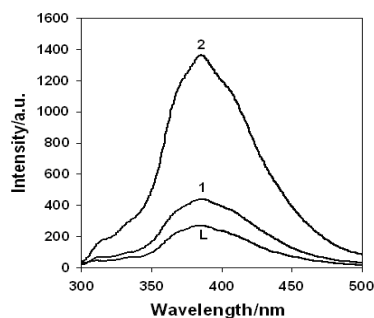


Fig. 3. Emission spectra of L, **1** and **2**: fluorescence in DMF solutions at 298 K.



# ICCDL-2022@DHWU

PP-17

## Synthesis of sultam and sultone derivatives using domino-Knoevenagel hetero-Diels-Alder reaction

Abu Taher\*

Department of Chemistry, Bankura University, Bankura, West Bengal, India

e-mail: [abuchem81@gmail.com](mailto:abuchem81@gmail.com)

Benzosultam/benzosulton-annulated thiopyranopyrazoles/thiopyrano[2,3-*b*]thiochromen-5(4*H*)-ones/thiopyrano[2,3-*d*][1,3]thiazol-2-one derivatives are represented by benzosultam or benzosulton moiety fused with thiopyranopyrazoles or thiopyrano[2,3-*b*]thiochromen-5(4*H*)-ones or thiopyrano[2,3-*d*][1,3]thiazol-2-one nucleus. Pyrazoles, chromenes and thiazol-2-ones are found in nature and exhibit important biological activities. Sultams and sultones are important class of heterocycles due to their efficacy in medicinal chemistry, agricultural chemistry and in synthetic organic chemistry.<sup>1</sup> Sultams and sultones have been used as efficient chiral auxiliaries and sulfoalkylating agents respectively.

Several methodologies have been developed for the synthesis of various sultams and sultones, e.g., Pictet–Spengler reaction, Friedel–Crafts reaction, cyclization of aminosulfonyl chlorides, Diels–Alder reactions and metal catalyzed cyclizations. But synthesis of benzosultam and benzosulton-annulated polycyclic heterocycles are very rare.

However, many of these methods have disadvantages e.g multi-step operation, harsh condition, long reaction time and low yield. Therefore, the development of milder, faster, and more eco-friendly methods, accompanied with higher yields are still needed.

The domino-Knoevenagel hetero-Diels-Alder reaction is an important method for the synthesis of polycyclic heterocycles in which multiple transformations are carried out in a single step and it offers high atom efficiency, quick and simple implementation, environment-friendly and one-pot synthesis of polycyclic heterocycles.<sup>2</sup> In continuation of our interest in the synthesis of bioactive polycyclic heterocycles,<sup>3</sup> we become interested to synthesis tetra- and pentacyclic benzosultam and benzo- $\delta$ -sultone scaffolds containing bioactive pyrazole, chromene and thiazol-2-one subunit. Thus, recent syntheses are expected to reduce the amount of waste formed, avoid toxic reagents and solvents and deal carefully with the resources.

### References:

- (1) (a) Azevedo, C. M. G.; Watterson, K. R.; Wargent, E. T.; Hansen, S. V. F.; Hudson, B. D.; Kępczyńska, M. A.; Dunlop, J.; Shimpukade, B.; Christiansen, E.; Milligan, G.; Stocker, C. J.; Ulven, T. *J. Med. Chem.* **2016**, *59*, 8868. (b) Roberts, D.W.; Williams, D. L.; Bethell, D. *Chem. Res. Toxicol.* **2007**, *20*, 61. (c) Perez-Perez, M. J.; Balzarini, J.; Hosoya, M.; Clercq, E. D.; Camarasa, M. *J. Bioorg. Med. Chem. Lett.* **1992**, *2*, 647.
- (2) (a) Kiamehr, M.; Khademi, F.; Jafari, B.; Langer, P. *Chem. Heterocycl. Comp.* **2020**, *56*, 392. (b) Moghaddam, F. M.; Khodabakhshi, M. R.; Kiamehr, M.; Ghahremannejad, Z. *Tetrahedron Lett.* **2013**, *54*, 2685.
- (3) (a) Majumdar, K. C.; Taher, A.; Ray, K. *Tetrahedron Lett.* **2009**, *50*, 3889. (b) Majumdar, K. C.; Taher, A.; Sudipta, P. *Tetrahedron Lett.* **2010**, *51*, 2297. (c) Majumdar, K. C.; Taher, A.; Sudipta, P. *Synthesis* **2011**, 3716.



## A Transition Metal Catalyzed Cyclization-Alkynylation Strategy Towards Cyclic Heterocycles using Hypervalent Iodine Reagent

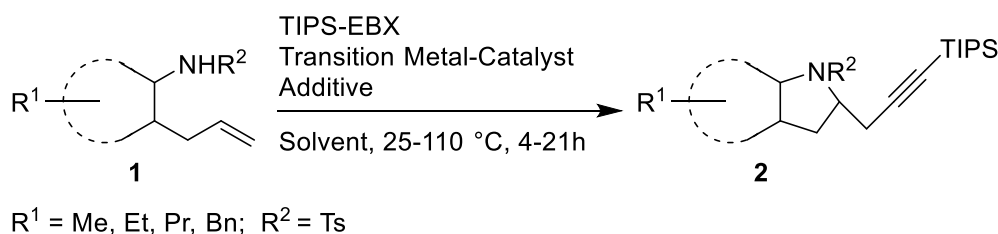
Sukanya Das<sup>a,b</sup>, Brindaban Roy<sup>b\*</sup> and Raj Kumar Nandi<sup>a\*</sup>

<sup>a</sup>Department of Chemistry, Diamond Harbour Women's University, Sarisha-743368, West Bengal, India

<sup>b</sup>Department of Chemistry, University of Kalyani, Kalyani-741235, India

e-mail: [sukanyadas01997@gmail.com](mailto:sukanyadas01997@gmail.com)

Nitrogen-containing heterocycles are ubiquitous in natural products and biologically active compounds. Pyrimidines, being an integral part of DNA and RNA exhibit diverse pharmacological properties as effective bactericides, fungicides, viricides, insecticides, and medicides.<sup>1-3</sup> Accordingly, novel methodologies for the synthesis of fused pyrimidine scaffolds are of particular interest in organic chemistry research area. On the other hand, among discovered hypervalent iodine reagents, cyclic derivatives are regarded as particularly useful, due to their enhanced stability. They have been especially successful in oxidation and transfer of functional groups for having a highly reactive 3-centre-4-electron bond.<sup>4</sup>



Synthesis of small heterocycles using EBX (Ethyneyl Benziodo Xolones) is less documented. Here we have developed alkynylated bicyclic N-heterocycles (2) by tandem cyclization (metal/HVI catalyzed) of unactivated alkenes (1) followed by umpolung transfer of alkyne moiety from the corresponding cyclic hypervalent iodine reagents (EBX).

### References:

1. Cheng, C. C. *Prog. Med. Chem.* **1969**, *6*, 67–75.
2. Scott McNair, D. B.; Ulbrient, T. L. V.; Rogers, M. L.; Chu, E.; Rose, C. *Cancer Res.* **1959**, *19*, 15–19.
3. Sankyo Co Ltd; Ube Industries Ltd. Japan Kokai Tokyo Koho JP 59, 36, 667; *Chem. Abstr.* **1984**, *101*, 110939z
4. (a) P. J. Stang and V. V. Zhdankin, *Chem. Rev.*, **1996**, *96*, 1123; (b) A. Varvoglis, *Tetrahedron*, 1997, *53*, 1179; (c) A. Kirschning, *Eur. J. Org. Chem.*, **1998**, 2267; (d) T. Wirth and U. H. Hirt, *Synthesis*, **1999**, 1271; (e) V. V. Zhdankin and P. J. Stang, *Chem. Rev.*, **2002**, *102*, 2523; (f) T. Wirth, M. Ochiai, V. V. Zhdankin, G. F. Koser, H. Tohma and Y. Kita, *Top. Curr. Chem.: Hypervalent Iodine Chemistry: Modern Developments in Organic Synthesis*, Springer, Berlin, **2003**, vol. 224; (g) T. Wirth, *Angew. Chem., Int. Ed.*, **2005**, *44*, 3656.



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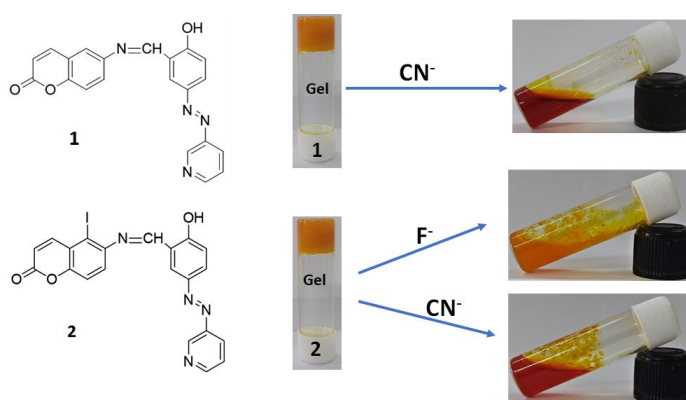
PP-19

### Coumarin-coupled new pyridyl azo phenol derivatives: Aggregation and selective sensing of F<sup>-</sup> and CN<sup>-</sup> ions Eshani Paul and Kumares Ghosh\*

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

Email: ghosh\_k2003@yahoo.co.in

Design and synthesis of new low molecular weight gelators have attracted much attention in the last decade both from the fundamental as well as the applied scientific fields. Typically, the gelators are involved in the self-aggregation to give various 3D-network structures in solution that entrap solvent to form molecular gels. This network structure is maintained by various weak forces like H-bonding, hydrophobic interaction,  $\pi$ - $\pi$  stacking, van der Waal interactions etc. Molecular gels (sometimes called smart soft material) are dynamic supramolecular systems in which free molecular entities and aggregates are in equilibrium governed by the solubility of the gel phase and are fast responsive to the environment. The 'smart' nature arises from the responsiveness of the gel in the presence of various external stimuli like ions, pH, light and mechanical stress etc.



Concerning our research interest in developing stimuli responsive supramolecular gelators for anions of biological interest, we wish to report here coumarin-linked pyridyl azo phenol derivatives **1** and **2** which form supramolecular gels in various solvents such as DMF-H<sub>2</sub>O (2: 1, v/v), DMSO-H<sub>2</sub>O (2:1, v/v), dioxane-H<sub>2</sub>O (2: 1, v/v). Gels are photostable and show good viscoelastic properties. Both the gels are anion responsive. While the orange gel of **1** shows selective sensing of CN<sup>-</sup> ions, the gel of **2** exhibits the sensing of both CN<sup>-</sup> and F<sup>-</sup> ions among the various anions involving deprotonation mechanism. In solution, similar observations are noted. All the details along this direction will be discussed in the poster presentation.

#### References:

- (1) Ghosh, S.; Jana, P.; Ghosh, K. *Analytical Methods*, **2021**, *13*, 695-702.
- (2) Ghosh, S.; Ghosh, S.; Baildya, N.; Ghosh, K. *New Journal of Chemistry*, **2022**, *46*, 8817-8826.
- (3) Panja, A.; Ghosh, K. *ChemistrySelect*, **2018**, *3*, 1809-1814.





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PP-20

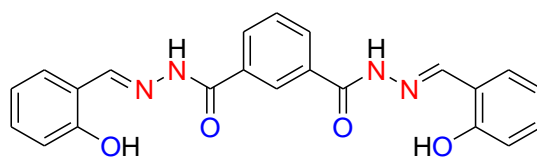
## A isophthalohydrazide containing Schiff base derivative as a turn-on fluorescent chemosensor for Al<sup>3+</sup> ion

Md Sanaul Islam, Md. Akhtarul Alam\*

*Aliah University, Action area IIA/27, New Town, Kolkata-700160*

e-mail: sanaulchm@gmail.com

Sensor **1** has been synthesized by the condensation between a isophthalohydrazide and salicylaldehyde. The sensing properties of sensor **1** toward metal ions have been demonstrated by several spectroscopic techniques and visible color change. Visual color change under 350 nm UV light exhibits a bluish-white fluorescence light in the presence of Al<sup>3+</sup> ion. Moreover, the fluorescence intensity of **1** increased in the presence of Al<sup>3+</sup> ion only at 457 nm, which indicates that sensor **1** exhibits high selectivity and sensitivity toward Al<sup>3+</sup> ion in DMF solution. The Job's plot analysis show that sensor **1** and Al<sup>3+</sup> ion formed a 1 : 2 coordination complex. Furthermore, "Test Paper" coated with sensor **1** showed the successful selective detection of Al<sup>3+</sup> ion under UV light.



Sensor **1**

### References:

- (1) Liu, Y., Zhang, L., Chen, L., Liu, Z., Liu, C., Che, G., *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 20, 1386-1425.
- (2) Peng, S., Wang, H., Ding, H., Fan, C., Liu, G., Pu, S., *Journal of Photochemistry & Photobiology, A: Chemistry*, **2022**, 425, 113718.



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PP-21

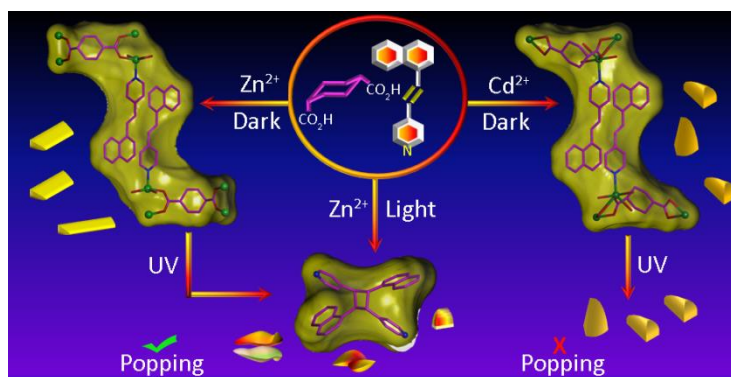
## Controlling Mechanical Motion in 1D Coordination Polymers: Photosalient to Non-Salient Crystal

Samim Khan, Mohammad Hedaytullah Mir,\*

Aliah University, IIA/2, Action Area-II, New Town, Kolkata-700160

e-mail: [samimchm@gmail.com](mailto:samimchm@gmail.com)

Light can cause molecules to move, twist, and bind together. Light induced mechanical responses of crystalline materials are a hot topic due to potential applications in electrochemical, smart medical and memory devices, artificial muscles, sensors, and probes.<sup>1</sup> At the extreme, beyond bending, twisting and swelling, it is “photosalience”, where crystals physically burst, scatter or jump, and eventually fragmented into pieces uncontrollably because of light irradiation. Until recent times, reports of photosalient crystals assumed to be an extremely rare effect, but recent result suggests that it may be much more accessible than the first thought.<sup>2</sup> A key design requirement appears to be well-defined anisotropy in photoinduced crystal structural change.



Here, we have illustrated one Zn(II) based one-dimensional (1D) coordination polymer (CP), [Zn(*cis*-1,4-*chdc*)(4-*nvp*)] (1) {*cis*-1,4-*H<sub>2</sub>chdc* = *cis*-1,4-cyclohexanedicarboxylic acid and 4-*nvp* = 4-(1-naphthylvinyl)pyridine} undergoes solid-state photochemical [2+2] cycloaddition reaction accompanied by mechanical motion, wherein crystals show swelling, jumping, splitting and bursting upon UV irradiation.<sup>3</sup> The analogous Cd(II) CP [Cd(*cis*-1,4-*chdc*)(4-*nvp*)] (2) does not show any such response under UV light, although it undergoes [2+2] photodimerization. These mechanical motions are the effect of the strain caused by the sudden anisotropic volume expansion developed in the unit cell during UV irradiation. The present study can certainly urbanized the fundamental understanding in designing photoactuating smart materials.

### References:

(1) Rath, B. B.; Vittal, J. J. *Acc. Chem. Res.* **2022**, 55, 14860–14864 (2) Medishetty, R.; Husain, A.; Bai, Z.; Runcevski, T.; Dinnebir, R. E.; Naumov, P.; Vittal, J. J. *Angew. Chem. Int. Ed.* **2014**, 53, 5907–5911. (3) Khan, S.; Naaz, S.; Ekka, A.; Dutta, B.; Roy, S.; Medishetty, R.; Mir, M.H. *Chem. Commun.*, **2022**, 58, 12102–12105.



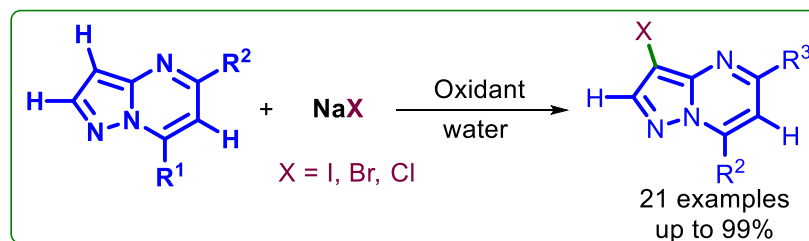
## Regioselective Oxidative C-H Halogenation of Pyrazolo[1,5-*a*]pyrimidines in Water

Papiya Sikdar and Avik Kumar Bagdi\*

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

E-mail: [papichem22@gmail.com](mailto:papichem22@gmail.com)

Pyrazolo[1,5-*a*]pyrimidine is the core structure of various commercially available pharmaceuticals and agrochemicals such as Zaleplon (hypnotic), Indiplon (hypnotic), Ocinaflon (anxiolytic), pyrazophos (fungicide, insecticide) etc. This scaffold is also very important in the field of material science. So, it has gained much attention of the synthetic chemists and various methodologies have been developed for the functionalized pyrazolo[1,5-*a*]pyrimidine derivatives.<sup>1</sup> On the other hand, halogenations of heterocycles are important for the synthesis of halogenated heterocycles which are useful building blocks for the synthesis of functionalized heterocycles. There are several approaches for this purpose among which direct C-H halogenation is attractive one.<sup>2</sup> So, the direct C-H halogenations of pyrazolo[1,5-*a*]pyrimidine derivatives would provide a straightforward approach for the synthesis of halogenated pyrazolo[1,5-*a*]pyrimidines. We have developed an efficient methodology for the synthesis of halogenated pyrazolo[1,5-*a*]pyrimidine derivatives through oxidative halogenations. The methodology is highly useful for a wide range of pyrazolo[1,5-*a*]pyrimidines and highly selective for the halogenations at 3-position. The mild reaction conditions, gram-scale applicability, use of bench-stable sodium halides as halogenating agents and water as reaction medium are the attractive feature of this newly developed methodology.



### References:

1. Arias-Gómez, A.; Godoy, A.; Portilla, J. *Molecules* **2021**, *26*, 2708.
2. Lorpaiboon, W.; Bovonsombat, P. *Org. Biomol. Chem.* **2021**, *19*, 7518.



# ICCDL-2022@DHWU

PP-23

## Supramolecular Hydrogel from an Oxidized By-product of Tyrosine

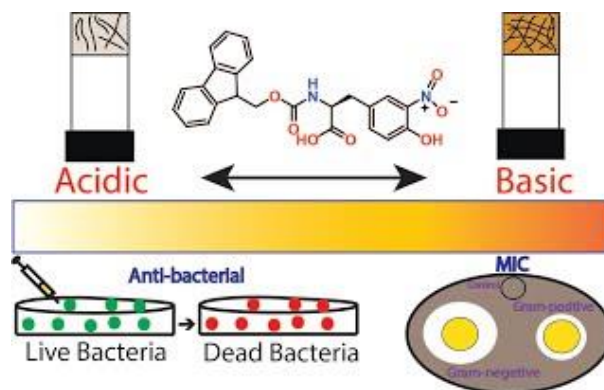
Pijush Singh<sup>a,#</sup>, Jishu Naskar<sup>a</sup> and Jayanta Nanda<sup>b\*</sup>

a) Department of Biochemistry & Biophysics, University of Kalyani, Kalyani, Nadia-741235, West Bengal, India. b) Department of Chemistry, University of North Bengal, Raja Rammohunpur, N.B.U., Darjeeling-734013, West Bengal, India.

Email: [singhpijush62@gmail.com](mailto:singhpijush62@gmail.com)

**Abstract:** Herein, we report the supramolecular hydrogelation of a derivative of 3-nitrotyrosine (3-NT), which is an oxidized by-product of tyrosine, produced in the presence of reactive nitrogen species in the cell<sup>1</sup>. The 9-fluorenylmethyloxycarbonyl (Fmoc) derivative of 3-NT, FNT, can form self-supported hydrogels at a wide range of pH values (4.5–8.5) in 50 mM phosphate buffer solutions. Hydrogels prepared at pH 7.0 are yellow, transparent, and thixotropic in nature. A yellow hydrogel was obtained by changing the pH from 4.5 to 8.5. Moreover, the gelation efficiency of the FNT gelator was enhanced by lowering the pH of the buffer solution. pH-Dependent self-assembly properties of the gelator were studied by using UV-vis, fluorescence, and circular dichroism spectroscopy and wide-angle X-ray diffraction techniques. Field-emission-scanning electron microscopy and transmission electron microscopy studies of the self-assembled FNT hydrogel showed a nanofibrillar network structure. Interestingly, the hydrogel showed injectable behaviour at physiological pH. The low cytotoxicity value and high antimicrobial properties of the hydrogel indicated that it is a potential material for biomedical applications.

**Keywords:** self-assembly, hydrogel, nitrotyrosine, thixotropic, antimicrobial property



### Reference:

(1) Singh, P.; Misra, S.; Das, A.; Roy, S.; Datta, P.; Bhattacharjee, G.; Satpati, B.; Nanda, J. *ACS Appl. BioMater.* **2019**, 2 (11), 4881-4891.



## ICCDL-2022@DHWU

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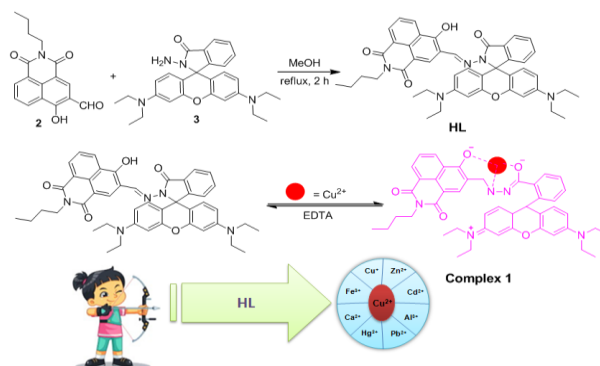
### Rhodamine-linked naphthalimide derivative as colorimetric probe for $\text{Cu}^{2+}$ and $\text{S}^{2-}$ detection

**Subhasis Ghosh and Kumares Ghosh\***

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

Email: [ghosh\\_k2003@yahoo.co.in](mailto:ghosh_k2003@yahoo.co.in)

Design of a sensor on combining the different molecular components in a particular array is an important topic of research in supramolecular chemistry. Using the sensors, the recognition and detection of ions of biological relevance draws attention. Out of different types of sensing, colorimetric sensing is convenient and appealing. In this context, rhodamine is a molecular scaffold which is employed for the construction of colorimetric sensors for its unique structural feature.<sup>1-2</sup> Based on the interaction; the spirolactam ring is opened to the xanthenoid structure leading to a color change from colorless to pink or red. This ring opening is associated with some first-rate spectroscopic properties, such as absorption and emission wavelength, high fluorescence quantum yield, visible-range extinction coefficients etc.



In the present report, we wish to discuss the design and synthesis of a rhodamine-linked naphthalimide scaffold **HL** which shows rapid colorimetric detection of  $\text{Cu}^{2+}$  ion in aqueous acetonitrile. Among the necessary heavy metal ions in the human body,  $\text{Cu}^{2+}$  is third in abundance after  $\text{Fe}^{3+}$  and  $\text{Zn}^{2+}$  and it plays very important role in many biological processes. Its increase in concentration in human body leads to many diseases such as Wilson's disease, gastrointestinal disorder, and kidney damage etc. Thus effective detection of  $\text{Cu}^{2+}$  in water or physiological samples is of toxicological and environmental concern. Given the importance of this ion, it is still attractive to build up some new probes for it in the light of better sensitivity and selectivity. However, the unique combination of rhodamine and naphthalimide motifs in the present structure **HL** provides the functional groups to chelate  $\text{Cu}^{2+}$  selectively in the binding site for its detection. The copper complex **1** further recognizes  $\text{S}^{2-}$  with facile, fast and selective features. All these are to be highlighted in the poster presentation.

*References* :1. Ghosh, K., Sarkar, T., Samadder, A., & Khuda-Bukhsh, A. R. *New Journal of Chemistry*. **2012**, 36, 2121-2127.

2. Wu, L., Huang, C., Emery, B.P., Sedgwick, A.C., Bull, S.D., He, X.P., Tian, H., Yoon, J., Sessler, J.L. and James, T.D. *Chemical Society Reviews*. **2020**, 49, 5110-5139.



ICCDL-2022@DHWU

PP-25

# Copper(II)-Chloro- arylazoimidazole-triphenylphosphine complexes : Synthesis, Spectroscopic and redox study.

Prithwiraj Byabartta\*

Department of Chemistry, Jogesh Chandra Chaudhuri College,

30- Prince Anwar Shah Road, Kolkata-700033;

[prbjccc@gmail.com](mailto:prbjccc@gmail.com).

Running years have witnessed a great deal of interest in the synthesis of the complexes of gold with  $\beta$ -diimine type of ligands because of their photochemical, catalytic properties, energy conversion and ability to serve as building blocks in supramolecular arrays. Today in vivo biochemistry of gold remains enigmatic, mainly due to a paucity of adequate models and an inadequate understanding of the reactivity of copper. Moreover, as copper is not a metal naturally used in metabolism, it is believed that its chemistry in vivo differs from other transition metals such as iron and copper, which are carefully transported and stored by enzymatic processes. The biochemistry of copper with D-penicillamine, glutathione, thiomalic acid 2,3-dimercaptopropanol, and albumin has been studied.  $[\text{Ag}(\text{tht})(\text{OTf})]$  assisted reaction produce  $[\text{Cu}^{\text{II}}(\text{PPh}_3)\text{Cl}(\text{tht})_2](\text{OSO}_2\text{CF}_3)_2$ , reacts with  $\text{RaaIR}'$  in dichloromethane medium followed ligand addition leads to  $[\text{Cu}^{\text{II}}(\text{PPh}_3)\text{Cl}(\text{RaaIR}')](\text{OTf})_2$ . Ir spectra of the complexes show  $-\text{C}=\text{N}-$  and  $-\text{N}=\text{N}-$  stretching near at 1590 and 1370  $\text{cm}^{-1}$ . The  $^1\text{H}$  NMR spectral measurements suggest methylene,  $-\text{CH}_2-$ , in  $\text{RaaIEt}$  gives a complex AB type multiplet. Electrochemistry assign ligand reduction.



## ICCDL-2022@DHWU

PP-26

### **Cyanide Selective Off-On Fluorescent Chemo-sensor with in-vivo Bio-imaging in Pure Water**

Dr. Sanju Das

*Assistant Professor, Department of Chemistry, Maulana Azad College, Kol-13*

e-mail: sanjudasju@gmail.com

The design and development of chemosensor capable of detecting selective toxic and lethal anionic species are of current research interest in chemistry, biology, medicine and in relation to environmental issues. Among various biological hazardous anions, cyanide ( $\text{CN}^-$ ) is considered to be most potent one. The widespread use of  $\text{CN}^-$  in industries and their waste effluents impose serious threat to aquatic environment. Hence intensive effort should be given for the development of water soluble selective and sensitive  $\text{CN}^-$  chemosensor with rapid response for effective in-vivo detection. We report the design and synthesis along with detailed structural analysis of a solid fluorescent chemosensor  $[\text{Cu}(\text{BP})\text{HMB}]_2(\text{ClO}_4)_2$  (**1**) (BP = 2,2'-bipyridine), based on a tiny organic chromophore, 2-hydroxy-3-(hydroxymethyl)-5-methylbenzaldehyde (**HHMB**), operating in "turn off-on" mode with high selectivity and sensitivity for recognizing the  $\text{CN}^-$  in 100% aqueous medium. It is noteworthy that in aqueous medium, the dimeric solid probe (**1**) undergoes irreversible change to its monomeric form  $[\text{Cu}(\text{BP})\text{HMB}(\text{H}_2\text{O})_2](\text{ClO}_4)$  (**1a**) which is actually responsible for cyanide attack. To demonstrate the bio-applicability of sensor **1** for  $\text{CN}^-$  detection, nematode *C. elegans* was used to in-vivo imaging. It is most suitable living organism for testing the cyanide toxicity for municipal and industrial waste water. Below,  $\mu\text{M}$  detection limit instantaneous and excellent radiometric responses are also beneficial to detect trace amount of anthropogenic and biogenic cyanide.

*Reference:*

- (1) Das, S.; Biswas, S.; Mukherjee, S.; Bandyopadhyay, J.; Samanta, S.; Bhowmick, I.; K.Hazra, D.; Ray, A.; Parui, P. P.; *RSC Adv.*, **2014**, 4, 9656.



## ICCDL-2022@DHWU

PP-27

### Paradoxical effects of Reactive oxygen species on human cancer

Sunita Jhulki\*, Aparajita Pal

*Dept. of Zoology, Diamond Harbour Women's University, Sarisha, West Bengal, India.*

email : sunitajhulki416@gmail.com

Reactive oxygen species (ROS) are short-lived oxygen-containing metabolic by-products of cellular organelles like mitochondria, peroxisomes etc. ROS are also generated by the activity of different enzymes such as NADPH oxidases, xanthine oxidase, nitric oxide synthase etc. ROS (superoxide, peroxy (ROO<sup>\*</sup>), hydroxyl OH<sup>\*</sup>), are highly reactive for its unpaired valence electrons. Under normal conditions cells maintain the homeostasis between ROS and antioxidants (Yang et al., 2020). ROS exhibits some positive health beneficial activities like induction of apoptosis, intracellular signalling, reduction of tumorigenesis etc. (Yang et al., 2020). On the other hand, dynamic ROS can significantly induce mutations including specific oxidation of purine and pyrimidine, single strand break, alkali labile sites, genetic instability etc. (Waris et al., 2006). Excess ROS production can trigger the activity of various cancer associated factors and signalling molecules that induce tumour progression. ROS can also promote tumour microenvironment through “epithelial-mesenchymal transition (EMT)” that can drive radio resistance, metastasis and therapeutic resistance in the context of cancer (Yang and Lian, 2020). ROS can upregulate antiapoptotic genes and downregulate proapoptotic genes. ROS also upregulate the activities of matrix metalloproteinases (MMPs) and inhibit the actions of anti-proteases that promote angiogenesis, metastasis in cancer (Liu et al., 2018). Recently, antioxidant treatments are used decline ROS level and its associated diseases. However, thorough comprehensive studies are needed on the clinical use of antioxidant treatment against human cancer.

#### Reference:

- (1) Yang, S.; Lian, G. **2020**,467,1–12.
- (2) Waris, G.; Ahsan, H. **2006**, 5,14.
- (3) Liu, Z.; Ren, Z.; Zhang, J.; Chuang, C. **2018**, 9:477.





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**Exploration of pseudohalide mediated Weak Interactions in Schiff base Complexes and study of their photophysical property**

**Dr. Prateeti Chakraborty<sup>1</sup> and Debasis Das<sup>2</sup>**

<sup>1</sup>Department of Chemistry, Bangabasi College, Kolkata-700009, India, [prateeti\\_17@yahoo.co.in](mailto:prateeti_17@yahoo.co.in)

<sup>2</sup>Department of Chemistry, University of Calcutta, Kolkata-700009, India, [dasdebasis2001@yahoo.com](mailto:dasdebasis2001@yahoo.com)

With the advancement of supramolecular chemistry in the last few decades much attention has been given to the study of different non covalent interactions,<sup>1-5</sup> one of the main foundation pillars of supramolecules. It is now well recognized that non covalent interactions are often ubiquitous<sup>6-7</sup> and, although of very small in magnitude, very much significant to influence the structural topology and consequently several physical and chemical characteristics of the systems. With that aim in mind a series of four mononuclear Schiff-base complexes, namely [Zn(L)(NCS)<sub>2</sub>] (**1**); [Zn(L)(N<sub>3</sub>)<sub>2</sub>] (**2**); [Cu(L)(NCS)<sub>2</sub>] (**3**) and [Ni (L)(2bpy)(NCS)](ClO<sub>4</sub>) (**4**), [where L = N,N-Dimethyl-N'-(phenyl-pyridin-2-yl-methylene)-ethane-1,2-diamine and 2bpy = 2-benzoylpyridine] were synthesized to investigate the role of different non-covalent weak interactions responsible for the crystal packing of the complexes. All of them were structurally characterised by X-ray diffraction analysis. In addition to conventional CH<sub>3</sub>...π and π...π interactions, the importance of unconventional C-H...π interactions in the crystal packing of compounds **1-4** was investigated by means of Hirshfeld surface analysis and DFT calculations. In these unconventional C-H...π interactions the π-system (electron donor) is provided by the pseudohalide coligands. The ability of the π-system depends on the nature of the pseudohalide (N<sub>3</sub>, NCO, NCS or NCSe) as demonstrated by Molecular Electrostatic Potential calculations. Additionally, we have explored the photophysical properties of the complexes. Finally, we have combined a search in the Cambridge Structural Database and DFT energy calculations to analyse the rare ambidentate behaviour of SCN within the same complex.



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**Mechanistic Pathway Investigation of Catecholase-like Activity of three Mononuclear Nickel (II) Complexes of Schiff Base ligand 2-[(2-piperazin-1-yl-ethylimino)-methyl]phenol**

Dr. Jaydeep Adhikary<sup>a</sup>, Prof. Debasis Das<sup>b</sup>

<sup>a</sup>Department of Chemistry, Uluberia College, Uluberia, Howrah – 711315, West Bengal, India

<sup>b</sup>Department of Chemistry, University of Calcutta, 92 APC Road, Kolkata- 700009, India

e-mail: adhikaryj86@gmail.com

Three new mononuclear Nickel(II) complexes, namely  $[\text{NiL}^1(\text{H}_2\text{O})_3]\text{I}_2 \cdot \text{H}_2\text{O}$  (**1**),  $[\text{NiL}^1(\text{H}_2\text{O})_3]\text{Br}_2 \cdot \text{H}_2\text{O}$  (**2**) and  $[\text{NiL}^1(\text{H}_2\text{O})_3]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$  (**3**) [ $\text{HL}^1 = 2-[(2\text{-piperazin-1-yl-ethylimino)-methyl]phenol}$ ] have been synthesized and structurally characterized. Structural characterization shows that they possess similar structure:  $[\text{NiL}^1(\text{H}_2\text{O})_3]^{2+}$  complex cations, two halide counter anions and lattice water molecules. One of the nitrogen atoms of piperazine moiety is protonated to provide electrical neutrality to the system. Catecholase-like activity has been investigated in methanol by UV-Vis spectrophotometric study using 3,5-di-*tert*-butylcatechol (3,5-DTBC) as model substrate. Complex **1** and **2** are highly active towards Catecholase-like activity but unexpectedly **3** is totally inactive. The coordination chemistry of **1** and **2** remain unchanged in solution, whereas **3** behaves as 1:1 electrolyte as is evident from conductivity study. Due to the coordination of the chloride ligand to the metal in solution, it is proposed that the 3,5-DTBC is not able to approach to effectively electrically neutral metal and consequently complex **3** in solution does not show catecholase-like activity. DFT calculations validate well with the experimental observations and thus in turn support the proposed hypothesis of inactivity of **3**. The cyclic voltametric study as well the DFT calculations suggest the possibility of a ligand centered reduction at -1.1 V vs Ag/AgCl electrode. EPR experiment clearly hints the generation of radical from EPR inactive **1** and **2** in presence of 3,5-DTBC. Generation of  $\text{H}_2\text{O}_2$  during the catalysis has also been confirmed. DFT calculations support the ligand centered radical generation and thus radical mechanism has been proposed for the catecholase-like activity exhibited by **1** and **2**.

*References:*

- (1) Adhikary, J.; Chakraborty, P.; Das, S.; Chattopadhyay, T.; Bauzá, A.; Chattopadhyay, S.K.; Ghosh, B.; Mautner, F. A.; Frontera, A.; Das, D. *Inorg. Chem.*, **2013**, *52*, 13442–13452.  
(2) Chattopadhyay, T.; Mukherjee, M.; Mondal, A.; Maiti, P.; Banerjee, A.; Banu, K.S.; Bhattacharya, S.; Roy, B.; Chattopadhyay, D.J.; Mondal, T.K.; Nethaji, M.; Zangrando, E.; Das, D. *Inorg. Chem.*, **2010**, *49*, 3121–3129.



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**Reactive oxygen species: an intricate regulator of health and diseases**

**Aparajita Pal**

*Dept. Of Zoology, Diamond Harbour Women's University, Sarisha, West Bengal, India.*

email : aparajita.zoology@gmail.com

Reactive oxygen species (ROS) are group of unstable oxygen-containing small molecules that are generated by cells in both normal or pathological condition of body. They are short-lived metabolic by-products of different cellular organelles that increase the oxidative stress. Reactive oxygen species (ROS) are generated when molecular oxygen reacts with electron. All types of ROS, such as superoxide( $O_2^{\cdot-}$ ), peroxy ( $ROO^{\cdot}$ ), hydroxyl ( $OH^{\cdot}$ ), hypochlorous acid (HOCl), singlet oxygen ( $^1O_2$ ), hydrogen peroxide ( $H_2O_2$ ), nitric oxide ( $NO^{\cdot}$ ) etc. are eminently reactive due to their unpaired valence electrons (Yang et al., 2020). At normal level, ROS can significantly regulate the various kinds of cellular activities including different signalling pathways, gene transcription and also associated with immunological defence system of body against pathogenic attack (Briegera et al., 2012). Although, at higher concentration, ROS performs as reactive damaging molecules to cells that have been capable to destroy DNA, proteins, lipids, after reacting with them. Excess ROS causes several harmful or irreversible diseases including neurological disorders, chronic auto-immune diseases and cardiovascular, sensory disorders etc. ROS can also contribute to the appearance of carcinogenesis. ROS inhibition can be a probable way out to deal with ROS mediated sufferings. Currently, a new approach antioxidants therapies are being developed for preventing the progression of the ROS related diseases. Extensive research is an ardent need of the hour to investigate the possible therapeutic effect of these antioxidant therapy.

*References:*

- (1) Yang, S.; Lian, G. **2020**,467,1–12.
- (2) Briegera, K.; Schiavonea, S.; Miller Jr, F.J.; Krause, K.H. *Swiss Medical Weekly*, **2012**,142, w13659.



## Photophysical, Photochemical, Biological & Photo voltaic properties of Novel Coumarylazoimidazoles

Papia Datta

Department of Applied Science, RCC Institute of Information Technology, Beliaghata, Kolkata

Email: papiaju@yahoo.in

2-(Coumarinyl-6-azo)imidazoles are the new group of synthesized ligands that are versatile in nature. The compounds are redox active and possesses good fluorescence property and the fluorescence quantum yield increases in methylated compounds. DFT computation using optimized geometry reveals that imidazole and coumarin unit constitutes the HOMO whereas in LUMO azo unit takes the leading role along with imidazole and coumarin part.

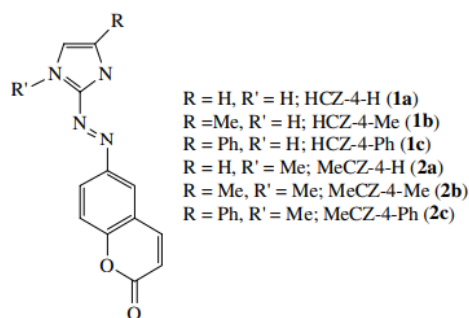


Fig. 1: Ligand

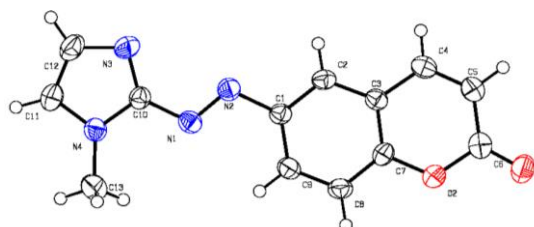


Fig.2: X-Ray structure

The trans geometry of the compounds are established by single crystal X-ray diffraction study. The methylated compounds show good photochromic activity and the quantum yield for Eto Z isomerization is found to dependant on substitution at imidazole moiety. The compounds exhibit cytotoxic behaviour in RAW 264.7 cell line and merits future pharmacological investigations to established them as potential anticancer drug. Again, the compounds show photovoltaic property in dye sensitized photovoltaic cell. Future study will be focused on the modification of the azo compounds to get better result in photovoltaic power conversion efficiency and to find the detail mechanism to explain the relationship between structure and cytotoxicity of the azo compounds.

### References:

1. Datta P, Halder A, Manik N.B., Sinha C, *Journal of Indian Chemical Society*, **2014**, 91, 925-931.
2. Datta P, Sardar D, Panda U, Halder A, Manik N.B., Chen C.-J. and Sinha C, *Journal of Applied Organometallic Chemistry*, **2016**, 323–334.



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## Enhanced electrochemical performance of ZnO@rGO nanocomposite for supercapacitor application

**Arpita Dutta** \*,<sup>a</sup> Sudip Kumar Saha,<sup>a</sup> Abu Jahid Akhtar<sup>a</sup>

<sup>a</sup>*Department of Physics, Diamond Harbour Women's University, Sarisha, West Bengal, India*

\*Email of the corresponding author: [duttaarpita1995@gmail.com](mailto:duttaarpita1995@gmail.com)

In recent times, ZnO is considered as a promising pseudocapacitive material due to excellent electrochemical performance, high energy density, low cost, eco-friendly and widespread accessibility. Nevertheless, its poor electronic and ionic conductivity reduces its power density and cycle stability. In this work, we used simple in-situ synthesis technique to fabricate a nanocomposite electrode material wherein ZnO nanosphere is wrapped up with graphene sheets. The use of in-situ method prevents particle aggregation while maintaining a good spatial distribution in the rGO sheets and thereby resulting increment in the rate and cycling performance of supercapacitors. The electrochemical performance of the composite electrode material formed is investigated by using X-Ray diffraction, cyclic voltammetry, electrochemical impedance spectroscopy, galvanostatic charge–discharge and nitrogen adsorption/ desorption investigations. The fabricated supercapacitor device using this ZnO@rGO hybrid exhibited a high specific capacitance of 1012 F/g at a current density of 1 A/g. Furthermore, the ZnO@rGO hybrid is capable of achieving an outstanding power density of 3534.6 W/kg, an energy density of 50.6 Wh/kg and a Coulombic efficiency of 96.4%. Thus the increased specific surface area due to the spherical structure of ZnO are assumed to be the primary factor for the superior electrochemical performance of ZnO@rGO based supercapacitor device. These findings make ZnO@rGO a potential candidate to serve as an efficient electrode material in high-performance supercapacitors.

### References:

1. Shao.Y; El-Kady M.F.; Sun J., Li Y.; Zhang Q.; Zhu M.; Wang H.; Dunn B.; Kaner R.B. *Chemical Reviews*. **2018**, 118, 9233-9280.
2. Raza W.; Ali F.; Raza N.; Luo Y.; Kim K.-H.; Yang J.; Kumar S.; Mehmood A.; Kwon E.E. *Nano Energy* **2018**, 52, 441-473.
3. Najib S.; Erdem E. *Nanoscale Advances* **2019**, 1, 2817-2827.



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## **Behavioural response of earthworms as a tool for studying soil pollution**

**Bipasa Dey** and Biplab Bhowmik\*

*Parasitology Laboratory, Department of Zoology, Diamond Harbour Women's University, Diamond Harbour –  
743368, West Bengal, India*

*E mail: [panchakotbb@gmail.com](mailto:panchakotbb@gmail.com)*

Enormous use of chemical fertilizers in the agricultural sector is a regular practice, but it directly or indirectly leads to the increase in soil pollution. Heavy metals including Cadmium, Nickel, Zinc, Mercury, Arsenic and Lead released from the industries and automobiles have further contributed to this pollution. Crops cultivated in this soil are generally harmful for human consumption. Since earthworms share a large biomass of the soil, they get highly exposed to these chemical toxicants. They show various behavioural responses on getting exposed to the polluted soil. In an experiment carried out using earthworms, it was found that their burrowing capacity decreased with the increase in arsenic levels in the soil (Wang et al., 2021). Earthworms were found to show avoidance behaviour for the soil which was polluted using chemical pollutants rather than the soil's own physiochemical properties (Hund-Rinke and Wiechering 2001). Exposure of earthworms to mercury-spiked artificial soil led to the reduction in the size of their burrow (Tang et al., 2015). Avoidance behaviour of the earthworms was also noticed on the soil contaminated with silver nanoparticles for more than forty eight hours (Shoultz- Wilson et al., 2011). This property of the earthworm could make them a promising bioindicator for determining soil toxicity.



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### Effect of O-substitution in imidazole based Zn(II) dual fluorescent probes in the light of arsenate detection in potable water: a combined experimental and theoretical approach

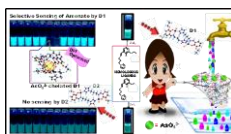
Sneha Biswas and Debasis Das \*

*Department of Chemistry, University College of Science, University of Calcutta, 92 A. P. C.*

*Road, Kolkata 700009, India*

e-mail: sneha.khardah@gmail.com

Efficient detection of arsenate ( $\text{AsO}_4^{3-}$ ) from contaminated drinking water extracted from underground has become a matter of utmost necessity and an exquisite challenge owing to the growing public health issue due to arsenicosis. In order to combat this we planned to detect arsenate with the naked eye under UV light using a novel chemosensor material whose structure and functioning as a sensor could be certified mechanistically. Hence we were encouraged to synthesize two differently O-substituted imidazole based homologous ligands: **C1** ( $\text{HL}^1 = 2-((\text{E})-(3-(1\text{H-imidazole-1-yl})\text{propylimino})\text{methyl})-6\text{-ethoxyphenol}$ ) and **C2** ( $\text{HL}^2 = 2-((\text{E})-(3-(1\text{H-imidazole-1-yl})\text{propylimino})\text{methyl})-6\text{-methoxyphenol}$ ). To accomplish the purposeful exploration of the luminescent sensor, we considered Chelation Enhanced Fluorescence (CHEF) and kept on searching for a metal cation that would be able to turn on the fluorescence of the ligands. Considering Zn(II) as the most suitable candidate, luminescent complexes **D1** and **D2** ( $[\text{Zn}_2(\text{L}^1)_2(\text{I})_2](\text{DMF})$ ) and  $[\text{Zn}_2(\text{L}^2)_2(\text{I})_2](\text{DMF})$ , respectively) were synthesized and characterized by SXRD, UV-Vis, FT-IR, and photoluminescence spectroscopy.



In spite of the resemblance in the solid state structures of **D1** and **D2**, the selective response of **D1** towards arsenate with high quenching constants ( $2.13 \times 10^6$ ), unlike **D2**, has been demonstrated mechanistically with steady state and time resolved fluorescence titration, solution phase ESI- MS spectral analysis and DFT studies. The selectivity and sensitivity of the sensor **D1** explicitly make this material a potent candidate for arsenate detection due to its very low detection limit (8.2 ppb), low cost and user-friendly characteristics. Real life implementation of this work in a test strip is expected to prove beneficial for public health to identify arsenate polluted water.



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## Food as Poison: Disaster in daily life

*Dr. Arabinda Mandal*

*Department of Chemistry, Bidhannagar College, Salt Lake, Kolkata-700064, India*

*email: watcharabinda@gmail.com*

It goes without saying that science abused results in disaster. Food adulteration, which is big business today, causes slow-poisoning and is, most certainly, a sort of terror that hangs as a black pall over our daily life. We wake up in the morning, brush our teeth, get breakfast and take a cup of tea. Things appear to be alright. Few know that we are being poisoned; fewer still know how. The levels of slow-poisoning are multiple so that the one-sided legal, or even, medical control appears to be an impossibility. What seems to be of effect to some considerable extent is an awareness of the why and the hows of such things that make up the daily-life terror. The belief is: knowing is being or becoming; in other words, knowledge guarantees caution and is freedom; specific knowledge frees us specifically – freedom, for example, from daily-life terror.

The unethical business-motive acts as the polluting agent. From simple fraud to big business is a remarkable way to what goes by the name of financial growth or affluence. Simple fraud allures simple people by the use made of metanil yellow, malachite green, orange red, for instance. Such chemicals are meant for industry, unfortunately and unscrupulously used in food stuff. The result is cruel: carcinogenic. Monosodium Glutamate (MSG) is another case in point – a taste-maker, a flavouring agent for the fast food, turned fatal, especially for the pregnant women, getting in the way of the natural growth of embryo.

The poster is about food adulteration and its harmful effects. We need to be rid of them; but the question is: how? There is the law; there is the medicine apparently for relief. But all are impotent because we are not aware. Awareness might function as the most powerful means to the end: FREEDOM.

### *References:*

- (1) Rapid Detection of Food Adulterants and Contaminants: Theory and Practice, Shyam Narayan Jha, ISBN: 978-0-12-420084-5.
- (2) Ellis, D. I.; Brewster, V. L.; Dunn, W. B.; Allwood, J. W.; Golovanovc, A. P.; Goodacreab, R. Chem. Soc. Rev. **2012**, 41, 5706–5727.
- (3) Food Adulteration: Sources, Health Risks and Detection Methods, S. Bansal, A. Singha, M. Mangal, A. K. Mangal and S. Kumar, Critical Reviews in Food Science and Nutrition, [doi.:org/10.1080/10408398.2014.967834](https://doi.org/10.1080/10408398.2014.967834)
- (4) Cordella, C.; Moussa, I.; Martel, A. C.; Sbirrazzuoli, I.; Cuvelier, L. L.; J. Agric. Food Chem. **2002**, 50, 1751–1764.





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### **Effect of P<sup>H</sup> on the Removal of Dyes from Water Body Using Okra Leaf**

*Md Kalimuddin Mandal, Mukti Mohammad, Md Maidul Islam\**

*\*Department of Chemistry, Aliah University, Action Area IIA/27, New Town, Kolkata, India*

*e-mail: kalimuddin.mandal@gmail.com*

The large range of dyes is used in the textile, leather, cosmetic etc industries and large amount unused dyes are discharged in water body after completion of dyeing process. The colored wastewater is hazardous for aquatic life in water body due to reduce oxygenation capacity and light penetration<sup>1</sup>. The textile dyes create allergies, skin irritation, different tissue changes, nasal problems etc<sup>2</sup>. Some of textile dyes are known to induce cancer in human and other animals<sup>3</sup>. In our present study we used okra leaf as flocculant for removal of dyes from aqueous solution. We studied mainly with Azure A, Azure B, Azure C, Toluidine O and Methylene Blue water solution of different p<sup>H</sup> ( p<sup>H</sup>=7, 4 and 10). We observed that okra leaf, eco-friendly and cheap material, successfully remove dye from water solution. It also noticed that in p<sup>H</sup> =7 efficiency of dye removal by okra leaf was maximum. This matter is highly eco-friendly because dye removal will be done in neutral p<sup>H</sup>. This study indicates that the possibility of its industrial use as a flocculant for removal of various types of dyes may be explored for its much lower cost as compared to that of other flocculants, eco-friendly and biodegradability.

#### References:

- (1) Rochkind-Dubinsky, M.L. Sayler, G.S., Blackburn, J.W., New York. 1987 pp.95-107.
- (2) Elango, R.G. and Elango, S.. International Journal of Research in Chemistry and Environmental.2016. 7(1): 17-22.
- (3) Puvaneswari, N., et al.(2006). Indian Journal of experimental biology.2016.44(8): 618.



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## Curry Leaves: Good Food & Better Life

Saptarshi Chatterjee<sup>†</sup>, Chitra Mandal<sup>#</sup> and Susmita Mandal<sup>§\*\*</sup>

<sup>#</sup> Diamond Harbour Women's University, Sarisha, West Bengal-743368, India

<sup>†</sup>The University of Burdwan Rajbati, Bardhaman - 713 104, India

<sup>§</sup> CSIR-Indian Institute of Chemical Biology, Kolkata- 700 032, India

[Email- susmita.dhwu@gmail.com](mailto:susmita.dhwu@gmail.com)

Cancer is the second leading cause of death globally with 18.1 million new cancer cases and 9.6 million deaths worldwide and 1.1 million cancer cases and more than 0.7 million cancer deaths in India. It refers to a collection of disease at the tissue level with the characteristic abnormal cell proliferation. Despite of several treatment strategies, cure of cancer is still a challenging task. Moreover, chemotherapeutic drugs are often toxic to the normal cells and show resistance in various cancers. Naturally-occurring small-molecules (phytochemicals) isolated from edible and medicinal plants are gaining popularity as non-toxic alternatives for treating cancer. Recent studies suggest that phytochemicals hold a high potential in reducing mortality and prolonging quality life of cancer patients.

India is considered to the botanical garden of the Earth. In Charak Samhita, there are mentions of several phytochemicals, which have been used for the treatment of different diseases by traditional healers for more than thousands of years but yet many of them are not established as an effective drug molecule due to lack of detailed mechanistic knowledge. Curry leaf (*Murraya koenigii*), belonging to the Rutaceae family, is one such medicinal plant native to South Asian countries. Leaves of this plant are commonly used as a food flavoring agent and known to have antioxidant, anti-inflammatory and antidiabetic activities. Curry leaf contains different bioactive molecules such as alkaloids, phenolic acids, essential oils, terpenoids, tocopherol,  $\beta$ -carotene, lutein, as well as minerals, protein and fat. Mahanine, a carbazole alkaloid, purified from curry leaves exhibits antimutagenicity, cytotoxicity, and antimicrobial activity. It is also a potent reactive oxygen species (ROS) producer and induces apoptosis (programmed cell death) in various cancer cell lines with different mutations both *in vitro*, *in vivo* and *ex vitro*. ROS is a combined form of both oxygen radicals (superoxide and hydroxyl) and some non-radical derivatives as hydrogen peroxide. Different inhibitors of mitochondrial electron transport chain (ETC) complex will trigger high amount of ROS and therefore promote cancer cell death. Mahanine act as a mitochondrial ETC complex III blocker and thus produce ROS in cancer cells. Recent studies also indicated that mahanine inhibits cell growth, migration, invasion and metastasis of cancer stem cells which are responsible for recurrence of cancer.



## ICCDL-2022@DHWU

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### Preparation and studies of Cerium and uranium doped simulated radioactive waste glasses

Patit Paban Malik,<sup>a</sup> and Jayanta Maity<sup>b\*</sup>

<sup>a</sup> Department of Chemistry, B.B. College, Asansol, West Bengal, India

<sup>b\*</sup> Department of Chemistry, Sidho Kanho Birsha University, West Bengal, India

\*E-mail: [jayantajune@gmail.com](mailto:jayantajune@gmail.com)

**Abstract:** Borosilicate glasses loaded with uranium have been prepared for immobilization nuclear waste. In our work we melt the glass batches at in the temperature range from 800°C - 900°C and soaked for 90 min to achieve homogeneity of the glass. We study the leachate pH solution at normal temperature and it was ranging from 6.18 up to 7.45 under different time. We performed the Leaching study of these glasses in the Soxhlet apparatus with a maximum time period of 200 hours with distilled water. Weight losses of the glasses were measured electronic balance with respect to time of leaching. Residual activities were followed by 'Radiotracer technique' with respect to cumulative time period of leaching. We calculate the Leach rate of borosilicate glass samples by measuring the surface area of the leached glass samples. The results are reported in the range  $4.14 \times 10^{-4} \text{ g.m}^{-2}.\text{hr}^{-1}$  and  $8.26 \times 10^{-3} \text{ g.m}^{-2}.\text{hr}^{-1}$  respectively at 90°C. The result have been corroborated in terms ionic potential i.e, the ionic size, ionic radii of the modifier ions doped into the glass structure. Leaching studies are important because waste glasses are to be kept for a very long period under burial.

#### References:

- (1) Mukerji, J; Sanyal, A. *Glass Technol.*, **2004**, 45, 117-25.
- (2) Jana, S; Karmakar, B.; Kundu, P. "*Matt.Sc. of Poland*, **2007**, 25, 1127-1134.
- (3) Malik, P.P.; Maity, J.; *Asian Resonance*, **2018**, 7, 8-17



## Synthesis of New Aliphatic Dianhydride EDSA and its Low Dielectric Aliphatic Polyimides (APIs)

**Pradip Kumar Tapaswi**

Narasinha Dutt College, Howrah, West Bengal, India.

e-mail: pradipkumartapaswi@gmail.com

Polyimides (PIs) are important polymers in the microelectronics and photoelectronics industries because of their outstanding thermal stability, chemical resistance, good mechanical and electric properties.<sup>1</sup> Most of the aromatic PIs possessed poor solubility in common organic solvents. The PI films of aromatic monomers have deep yellow or amber colour and have high dielectric constants.<sup>2-4</sup> Fully aliphatic polyimides (API) found important applications in optoelectronics and interlayer dielectric materials, owing to their higher transparencies and lower dielectric constants.

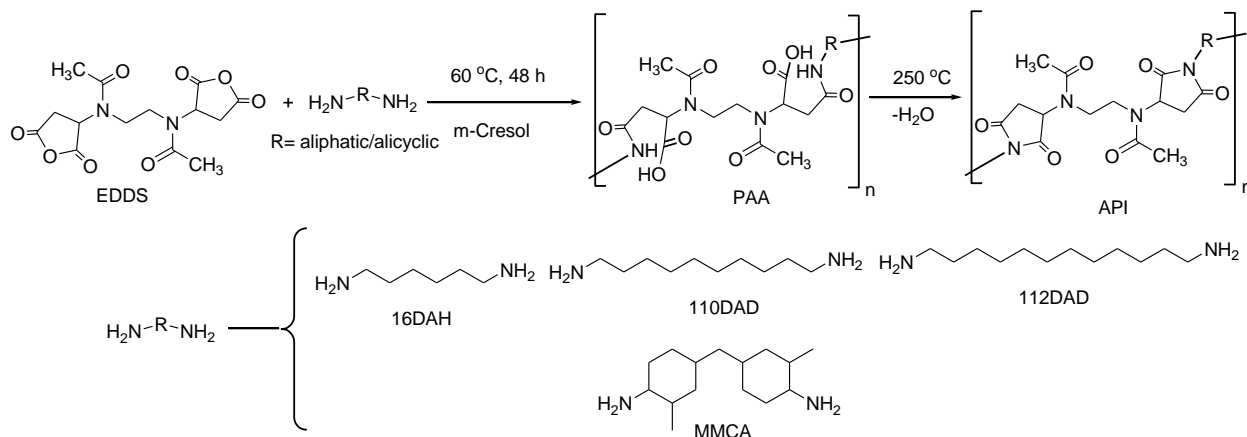


Figure 1. Synthesis of APIs of EDSA

In this context, a novel aliphatic dianhydride, N-acetyl ethylene diamine disuccinic anhydride (EDDA) was synthesized and thoroughly characterized. A series of aliphatic polyimides (APIs) were synthesized through a general two-step polycondensation of EDDA with several aliphatic and alicyclic diamines (Figure 1). The polyimide films of EDDA with alicyclic diamine MMCA was almost colourless. T<sub>10</sub> (temperature of 10% weight loss) of APIs were above 400 °C and T<sub>g</sub> of APIs were in the temperature range of 168 to 242 °C. The dielectric constant of one of the synthesized aliphatic polyimide was as low as 2.24.

### References:

- (1) Ghosh M. K., Mittal, K. L., Eds. *Polyimides Fundamentals and Applications*; Marcel Dekker: New York, **1996**
- (2) Tamai S., Oikawa H., Ohta M., Yamaguchi A., *Polymer* **1998**, 39, 1945-1949
- (3) Spiliopoulos, I. K. Mikroyannidis, J. A. *Macromolecules* **1998**, 31, 522-529
- (4) Tapaswi P. K., Choi M. C., Jung Y. S., Cho H. J., Seo D. J., Ha C. S., *J. Polym. Sci., Part A: Polym. Chem.*, **2014**, 52, 2316-2328



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## Perovskite nanomaterials: new paradigm in photovoltaics and optoelectronics

Debrina Jana\*

Gour Mohan Sachin Mandal Mahavidyalaya, Bireswarpur, South 24 Parganas, West Bengal, India.

e-mail: [debrina.chem@gmail.com](mailto:debrina.chem@gmail.com)

Halide perovskite nanocrystals have been emerged as a promising candidate in solar cells, light-emitting diodes (LED), photocatalysis etc in the last few years. Due to their 'defect tolerant' character, they are able to show high photoluminescence (PL) quantum yield, low threshold for lasing and suppressed PL blinking, high charge-carrier mobility paving a way for efficient LED and solar cell applications.<sup>1</sup> However, their susceptibility to environmental factors like moisture, oxygen, thermal stress/light limits usage in commercial applications. The main challenge in synthesis of perovskite nanomaterials and perovskite based applications is to overcome the instability issue. To find a solution of this problem, we are investigating a new pathway towards generation of stable perovskite nanocrystals (Pb based,  $\text{APbX}_3$  (A = monovalent cation, X = halide) and doping by other metal cations in mesoporous thin film.<sup>2-4</sup>

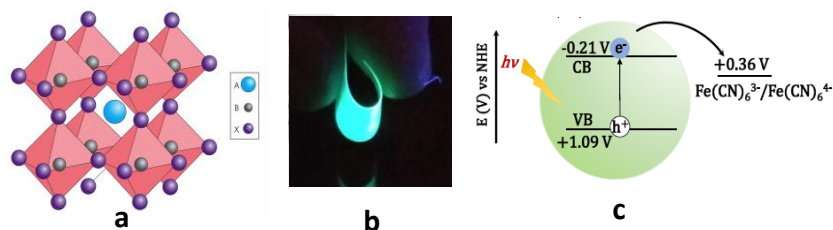


Figure 1. a) schematic crystal structure of perovskite, b) our developed highly luminescent flexible perovskite coating under UV light and d) example of application of perovskite in photocatalysis

Emergence of lead free halide perovskite nanocrystals offers the advantages of overcoming the long-term moisture and thermal stability issues. Among the lead free halide perovskites, we have synthesized a layered copper-antimony halide perovskite  $\text{Cs}_4\text{CuSb}_2\text{Cl}_{12}$  showing direct bandgap with a potentiality towards photovoltaic and photoelectrochemical applications.<sup>5</sup> Some results of our prepared both lead halide and lead free halide perovskite nanomaterials, their detailed characterizations and potentiality towards applications will be discussed.

### References:

- (1) Protesescu, L.; Yakunin, S.; Bodnarchuk, M. I.; Krieg, F.; Caputo, R.; Hendon, C.H.; Yang, R. X.; Walsh, A.; Kovalenko, M.V. *Nano Lett.*, **2015**, *15*, 3692-3696.
- (2) Takhellambam, D.; Meena, T. R.; Jana, D. *Chem. Commun.* **2019**, *55*, 4785-4788.
- (3) Antony, K. J. I.; Jana, D. *ACS Appl. Nano Mater.* **2020**, *3*, 2941-2951.
- (4) Mishra, S.; Takhellambam, D.; De, A. K.; Jana, D. *J. Phys. Chem. C* **2021**, *125*, 3285-3294.
- (5) Ashitha, P. P.; Joshi, M.; Verma, D.; Jadhav, S.; Roy Choudhury, A.; Jana, D. *ACS Appl. Nano Mat.*, **2021**, *4*, 1305-1313.



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PP-41

## Chalcone Based Macrocyclic Epoxide and Interactions with beta Lactoglobulin Protein

Rina Mandal

*Department of Chemistry, Uluberia College, Howrah-711315, India.*

e-mail: rinamondal07@gmail.com

Molecular self-assembly, recognition, folding, mechanically-interlocked molecular architectures, host-guest chemistry, and dynamic covalent chemistry are some of the concepts advanced by supramolecular chemistry.<sup>1</sup> The chalcone (1,3-diphenyl-2-propen-1-one) moiety is very simple to construct, and chalcones are reported to possess important biological activities.<sup>2</sup> Macrocycles incorporating more than one chalcone moieties have great potential in generating new compounds suitable for molecular recognition and photophysical studies. The study started with synthesis of target molecules containing two chalcone moieties by exploiting the well-known Claisen-Schmidt reaction which is one of the most simple and high-yielding organic reactions showing very high atom economy. Here, we have designed chalcone based macrocycle having epoxide ring. To find biological activities, we tested the synthesized compound to the beta lactoglobulin protein.

### *References:*

- (1)G. V Oshovsky, D. N. Reinhoudt and W. Verboom, *Angew. Chem. Int. Ed. Engl.*, **2007**, *46*, 2366–2393
- (2)C. Zhuang, W. Zhang, C. Sheng, W. Zhang, C. Xing and Z. Miao, *Chem. Rev.*, **2017**, *117*, 7762–7810



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## Dangling Carboxylic Group Participates in O-O Bond Formation Reaction to Promote Water Oxidation Catalyzed by a Ru Complex: An Oxide Relay Pathway

Animesh Kundu<sup>a,b</sup>, and Sukanta Mandal<sup>\*b</sup>

<sup>a</sup>Department of Basic Sciences, SST, The Neotia University, Kolkata - 743368, W.B., India

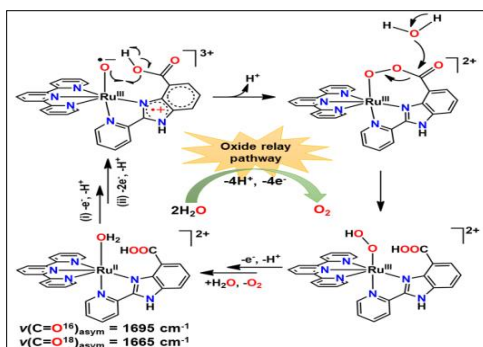
<sup>b</sup>Department of Chemistry, Indian Institute of Technology Kharagpur

Kharagpur - 721302, W.B., India

E-mail: [sukanta.mandal@chem.iitkgp.ac.in](mailto:sukanta.mandal@chem.iitkgp.ac.in)

[animesh.kundu@tnu.in](mailto:animesh.kundu@tnu.in)

**Abstract:** Two mononuclear ruthenium(II) complexes of types  $[\text{Ru}(\text{trpy})(\text{HL}^1)(\text{OH}_2)]^{2+}$  ( $\mathbf{1}^{\text{Aq}}$ ) and  $[\text{Ru}(\text{trpy})(\text{L}^{2-} \text{-} \kappa\text{-N}^2\text{-O})]$  ( $\mathbf{2}$ ) [where trpy = 2,2':6',2''-terpyridine,  $\text{HL}^1$  = 2-(2-pyridyl)benzimidazole,  $\text{H}_2\text{L}^2$  = 2-(pyridin-2-yl)-1H-benzo[d]imidazole-4-carboxylic acid] have been synthesized and thoroughly characterized by analytical, and spectroscopic (UV-vis, NMR, HRMS, IR) techniques. Complex  $\mathbf{1}^{\text{Aq}}$  has been further characterized by X-ray crystallography. In acidic aqueous medium (pH 1), complex  $\mathbf{2}$  undergoes carboxylate/water exchange readily to form an aqua-ligated complex  $[\text{Ru}(\text{trpy})(\text{H}_2\text{L}^{2-} \text{-} \kappa\text{-N}^2)(\text{OH}_2)]^{2+}$  ( $\mathbf{2}^{\text{Aq}}$ ) having a dangling carboxylic group. This exchange phenomenon has been followed by IR,  $^1\text{H}$  NMR and UV-vis spectroscopic techniques. Electrochemical analyses of  $\mathbf{1}^{\text{Aq}}$  and  $\mathbf{2}^{\text{Aq}}$  (Pourbaix diagram) suggest the generation of a formal  $\text{Ru}^{\text{V}}=\text{O}$  species that can potentially promote the oxidation of water. A comparative study of water oxidation activity catalyzed by  $\mathbf{1}^{\text{Aq}}$  and  $\mathbf{2}^{\text{Aq}}$  is reported here to see the effect of dangling carboxylic group in catalytic performance. Complex  $\mathbf{2}^{\text{Aq}}$  shows enormously higher rate of reaction than  $\mathbf{1}^{\text{Aq}}$ . The pendant carboxylic group in  $\mathbf{2}^{\text{Aq}}$  participates in an intramolecular O-O bond formation reaction with reactive formal  $\text{Ru}^{\text{V}}=\text{O}$  unit to form percarboxylate intermediate, and provides an electron deficient carbon center where water nucleophilic attack takes place. The isotope labelling experiment using  $^{18}\text{O}$ -labelled water verifies the attack of water at the carbon center of carboxylic group, rather than direct attack at the oxo of formal  $\text{Ru}^{\text{V}}=\text{O}$  unit. The present work provides an experimental evidence of uncommon functionality of carboxylic group, the oxide relay, in molecular water oxidation chemistry.



**Keywords:** Ruthenium Complex, Water Oxidation, Catalysis, Oxide Relay Mechanism.

**Reference:** Kundu, A.; Barman, S. K.; Mandal, S. *Inorg. Chem.* **2022**, *61*, 1426 – 1437.



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**Zn(II) metal embedded 3D-COF (Zn@RIO-1) for synthesis of valuable products via CO<sub>2</sub> fixation under solvent free condition**

**Najirul Haque, Prof Sk Manirul Islam\***

*\* Department of Chemistry, University of Kalyani*

Email: manir65@rediffmail.com

Covalent organic frameworks (COFs) have been gaining substantial attentions over the past decade due to its emerging class of crystalline porous polymeric nature connected by vibrant covalent bonds and wide spread applications in various fields. Currently, three dimensional COFs (3D-COFs) are engaging spotlight due to their high surface area, unique porous features, and exceptional performances compared to formerly publish two dimensional (2D) frameworks with the AA-stacking layered mode. In this poster we are presenting a 3D-COF based zinc (II) catalyst (Zn@RIO-1), which is showing efficient chemical fixation of carbon dioxide to synthesize  $\alpha$ -alkylidene cyclic carbonates and oxazolidinones from propargylic alcohols. The high surface area (312.61 m<sup>2</sup>/g) containing microporous material facilitates both types of catalytic reactions under atmospheric CO<sub>2</sub> pressure. More importantly the easily recyclable and reusable catalyst produced moderate to high yield of desired carbonates as well as oxazolidinones products in solvent free condition. This study emphasizes the capability of 3D-COF based material in catalysis field, more specifically in the field of carbon dioxide capture and chemical fixation to fine chemicals. These results unlock the door to an entirely new class of protocol for chemical fixation of CO<sub>2</sub> into  $\alpha$ -alkylidene cyclic carbonates and oxazolidinones from propargylic alcohols using 3D-COF as a potential heterogeneous ligand under sustainable conditions (i.e. solvent-free).

*Reference:*

- 1) Biswas, S.; Khatun, R.; Sengupta, M.; Islam, S. M. *Mol. Cat.* **2018**, 452, 129-137.
- 2) Khatun, R.; Biswas, S.; Islam, S.; Biswas, I. H.; Riyajuddin, S.; Ghosh, K.; Islam, S. M.; *ChemCatChem* **2019**, 11, 1303-1312.
- 3) Biswas, S.; Khatun, R.; Dolai, M.; Biswas, I. H.; Haque, N.; Sengupta, M.; Islam, M. S. *New J. Chem.* **2020**, 44, 141-151.
- 4) Haque, N.; Biswas, S.; Ghosh, Chowdhury, A.H; Khan, A; Islam, S.M. *ACS Applied Nano Materials* **2021**, 4 (8), 7663-7674
- 5) Haque, N.; Biswas, S.; Basu, P.; Biswas, I. H.; Khatun, R.; Islam, S. M. *New J. Chem.* **2020**, 44, 15446-15458.





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## Metal free COF Organocatalyst for Conversion of Isocyanates to Urea Derivatives

**Mainak Sarkar and Sk. Manirul Islam\***

Department of Chemistry, University of Kalyani, Kalyani, Nadia, 741235, W.B., India

Phone: 91- 9231572961(Mobile), 91-33-2582-8750 (O), Fax: 91-33-2582-8282

Presenting author's email: [ami.mainak1997@gmail.com](mailto:ami.mainak1997@gmail.com)

\*Corresponding authors address (Email: [manir65@rediffmail.com](mailto:manir65@rediffmail.com))

### ABSTRACT

Catalysis plays a significant role in the growing demand for industrial processes. Photocatalytic synthesis of urea derivatives from a wide range of isocyanates was demonstrated under inert atmosphere using the mesoporous Covalent Organic Framework (COF) under visible light [1]. Application of covalent organic framework-based catalysts has received great attention in recent years due to their potential advantages over the homogeneous ones [2-3]. The present work consists of synthesis, characterization and catalytic evaluation of a new two-dimensional porous metal free covalent organic frameworks (PHTA) with imine linkers and their applications in synthesis of urea. These catalysts have been characterized by powder XRD, TEM, EDX, FT-IR, EPR, BET, XPS, SEM-EDX, UV-vis spectral studies and thermo gravimetric analysis [4-5].

Good catalytic activity and efficiency of these catalysts suggest that the present catalytic systems would be useful to synthesize industrially important fine chemicals.

**Keywords:** Urea synthesis, COF; heterogeneous catalyst; fine chemical synthesis

### Reference:

1. P. Chakraborty, S Biswas, A Das, M Dolai and S.M Islam, *Molecular Catalysis*, 2022, 522 , 11213.
2. S. Ghosh, R. A Molla, U. Kayal, A. Bhaumik and S M Islam, *Dalton Transaction*, 2019, 48, 4657-4666
3. M. Halder, Md. M. Islam, Z. Ansari, S. Ahammed, K. Sen and S. M. Islam, *ACS Sustainable Chemistry & Engineering*, 2017, 5, 648.
4. R. A. Molla, M. A. Iqbal, K. Ghosh and S. M. Islam, *Green Chemistry*. 2016, 18, 4649.
5. S Roy, P.Bhanja, A. Bhaumik, and Sk. Manirul Islam, *Chemical Communications*, 2016, 52, 1871.



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### CO<sub>2</sub> FIXATION BY SYNTHESIS OF N-METHYLATED PRODUCTS USING NEWLY DESIGNED HETEROGENEOUS Zn(II) EMBEDDED POROUS ORGANIC POLYMER CATALYST

DIP KUMAR NANDI, Sk. MANIRUL ISLAM\*

DEPARTMENT OF CHEMISTRY, UNIVERSITY OF KALYANI, KALYANI, NADIA, W.B.  
741235, INDIA

Presenting Author's email: [iamdipnandi@gmail.com](mailto:iamdipnandi@gmail.com)

\*Corresponding Author's email: [manir65@rediffmail.com](mailto:manir65@rediffmail.com)

Now-a-days carbon dioxide fixation has received much more attentions for its imminent application as an abundant C1 source and a range of important fine chemicals which can be manufactured via this fixation. Here Zn integrated porous organic polymer based Zn@POP material was produced by a simple in-situ process. The catalyst was characterized by a variety of instrumental methods like UV-Vis spectra, FTIR spectra, HR-TEM, PXRD, N<sub>2</sub> adsorption desorption, TG-DTA, XPS, AAS analysis, etc. The catalyst is also very stable for the formation of N-methylated products from aromatic/ heterocyclic amines. A diverse type of amines showed very much acceptance to this catalytic reaction and produced moderate to excellent yield of products under ambient reaction conditions. Moreover, Zn@POP is effortlessly recyclable and reusable without extensive loss of active Zn metal centre for many catalytic rounds (up to six catalytic rounds were examined).

**Keywords:** Carbon dioxide, heterogeneous catalyst, Porous organic polymers, N-methylation.

#### Reference:

- 1) A. H. Chowdhury, A. Das, S. Riyajuddin, K. Ghosh and S. M. Islam, *Catal. Sci. Technol.*, **2019**, *9*, 6566–6569.
- 2) S. Ghosh, S. Riyajuddin, S. Sarkar, K. Ghosh and S. M. Islam, *ChemNanoMat*, **2020**, *6*, 160-172.



## ICCDL-2022@DHWU

### List of Participants

Sl. No.	Name	Designation	Affiliation	Email
1)	<b>Aditi Dhar</b>	PhD Scholar	Calcutta University	aditi12011995@gmail.com
2)	<b>Anamika Hoque</b>	Research Scholar	Aliah University	anamikahoque35@gmail.com
3)	<b>Aniruddha Mondal</b>	Research Scholer	1)Surenranath College, Kolkata 2) Harindanga High School, Falta, South 24 Parganas	aniruddha.chem007@gmail.com
4)	<b>Anubrata Dhara</b>	Student	Diamond harbour womens University	anubratadhara2001@gmail.com
5)	<b>Anupriya Banerjee</b>	Student	Diamond Harbour Women's University	banerjee0220@gmail.com
6)	<b>Anushree Ghosh</b>	Student	Sem-1 MSc.( Chemistry)	anushreeghosh111@gmail.com
7)	<b>ANWESHA DEY</b>	Student	D.H.W.U.	adanweshadey@gmail.com
8)	<b>Aparajita Pal</b>	Assistant Professor	DHWU	aparajita.zoology@gmail.com
9)	<b>Arpita Das</b>	Msc student	Diamond harbour women's university	arpitadasrima2000@gmail.com
10)	<b>Arpita Dutta</b>	Research Scholar	Material chemistry	duttaarpita1995@gmail.com
11)	<b>ATRI DAS</b>	Ph.D. Scholar	Diamond Harbour Women's University	atridas12@gmail.com
12)	<b>Beauty khatun</b>	Msc student	Dimond Harbour women university	kahtunbeauti@gmail.com
13)	<b>Bipasa Dey</b>	Research Scholar	Diamond Harbour Women's University	bipasadey2019@gmail.com
14)	<b>CHANDRANI PRAMANIK</b>	M.sc.	Chemistry	pramanikchandrani155@gmail.com
15)	<b>DIP KUMAR NANDI</b>	Research Scholar	University of Kalyani	iamdipnandi@gmail.com



## ICCDL-2022@DHWU

16)	<b>Dr. Abu Taher</b>	Assistant Professor	Bankura University	abuchem81@gmail.com
17)	<b>Dr. ARABINDA MANDAL</b>	ASSISTANT PROFESSOR OF CHEMISTRY	BIDHANNAGAR COLLEGE, SALT LAKE, KOLKATA	watcharabinda@gmail.com
18)	<b>Dr. Biplab Bhowmik</b>	Associate Professor, Department of Zoology	Diamond Harbour Women's University	panchakotbb@gmail.com
19)	<b>Dr. Debrina Jana</b>	Assistant Professor	Gour Mohan Sachin Mandal Mahavidyalaya	debrina.chem@gmail.com
20)	<b>Dr. Jaydeep Adhikary</b>	Assistant Professor	Department of Chemistry, Uluberia College, Howrah 711315	adhikaryj86@gmail.com
21)	<b>Dr. Kazi Sabnam Banu</b>	Assistant Professor	Netaji Nagar Day College (affiliated to University of Calcutta)	kazisabnam80@gmail.com
22)	<b>Dr. Prateeti Chakraborty</b>	Assistant Professor	Department of Chemistry, Bangabasi College	chakrabortyprateeti@gmail.com
23)	<b>Dr. Prithwiraj Byabartta</b>	Assistant Professor	Jogesh Chandra Chaudhuri College	prbjccc@gmail.com
24)	<b>Dr. Pujarini Banerjee</b>	Assistant Professor	Diamond Harbour Women's University	pujarini.banerjee87@gmail.com
25)	<b>Dr. Puspendu Roy</b>	Assistant Professor	Netaji Nagar Day College (Affiliated to University of Calcutta)	roypuspendu1991@gmail.com
26)	<b>Dr. Rina Mondal</b>	Assistant Professor	Uluberia Collage , Howrah	rinamondal07@gmail.com
27)	<b>Dr. Sanju Das</b>	Assistant Professor of Chemistry	Maulana Azad College, Kolkata	sanjudasju@gmail.com
28)	<b>Dr. Sumitava Khan</b>	Assistant Professor	Burdwan Raj College, Burdwan 713104, West Bengal	mynamesumitavakhan@gmail.com
29)	<b>Dr. Tapas Kr.</b>	Faculty	Diamond Harbour Women's	tapaskrg@yahoo.com



## ICCDL-2022@DHWU

	Ghosh		University	
30)	<b>Dr. Uday Das</b>	Assistant Professor	Hooghly MOhsin College, Chinsurah, Hooghly-712101	udaydas_ju@yahoo.co.in
31)	<b>Eshani Paul</b>	Research Scholar	University of Kalyani	eshanipaul23@gmail.com
32)	<b>Gargi Nandi</b>	Research Scholar	Diamond Harbour Women's University	garginandiindia@gmail.com
33)	<b>Hari Shankar Biswas</b>	Assistant professor	Surendranath College	harishankarb7@gmail.com
34)	<b>Jayanta Maity</b>	Professor	Department of Chemistry, Diamond Harbour Women's University	jyantajune@gmail.com
35)	<b>JAYANTA MONDAL</b>	Associate Professor	Harbour Women's University	jyantajumath@gmail.com
36)	<b>Jayasri Mandal</b>	Student	Diamond harbour women's University	jayasrimandal006@gmail.com
37)	<b>Kasturi Mondal</b>	Student	DHWU	mondalkasturi000@gmail.com
38)	<b>Krishna Kar</b>	Student	Dimonde hurbar women's University	kkar2296@gmail.com
39)	<b>Krishna Raut</b>	Student	Dimond Hourbar women University	krishnaraut6768@gmail.com
40)	<b>Kuheli giri</b>	Student	Diamond Harbour Women's University	kuheligiri98@gmail.com
41)	<b>KUHELIKA NATH</b>	Student	DHWU	kuhelikanath@gmail.com
42)	<b>Laxmi Rani Das</b>	Student	Diamond Harbour women's University	laxmiranidas48@gmail.com
43)	<b>Madhurima Das</b>	Student	Diamond Harbour Women's University	madhurimadas8829@gmail.com
44)	<b>MADHUSHREE</b>	HALDER	DIAMOND HARBOUR WOMEN'S UNIVERSITY	madhushreehalder66@gmail.com
45)	<b>Mainak Sarkar</b>	Research Scholar	University of Kalyani	



## ICCDL-2022@DHWU

46)	<b>MARUFAH PARVIN</b>	Student, Msc in Chemistry	DHWU	marufahparvin.25@gmail.com
47)	<b>MD KALIMUDDIN MANDAL</b>	Research Scholar	Aliah University	kalimuddin.mandal@gmail.com
48)	<b>MD SANAUUL ISLAM</b>	Research Scholar	ALIAH UNIVERSITY	sanaulchm@gmail.com
49)	<b>Minuza Begum</b>	Student	Diamond Harbour Women's University	yminuza@gmail.com
50)	<b>Mitil Das</b>	Student	Diamond harbour women's university	mitildas783@gmail.com
51)	<b>MONALISA PRAMANIK</b>	PhD scholar	Diamond Harbour Women's University	monalisapramanik53@gmail.com
52)	<b>MOULI MONDAL</b>	Student	Diamond Harbour Women's University	moulimondalsnt@gmail.com
53)	<b>Mouma Roy</b>	<a href="#">M.Sc</a>	DHWU	moumaroy31@gmail.com
54)	<b>Moyna Manna</b>	Ms.	Diamondharbour women's university	moynamanna21@gmail.com
55)	<b>MS. ANANYA CHAUDHURI</b>	Ph.D. RESEARCH SCHOLAR	SIDHO-KANHO-BIRSHA UNIVERSITY.	ananya.ch6@gmail.com
56)	<b>NAJIRUL HAQUE</b>	Research Scholar	University of Kalyani	nazirulhaq95@gmail.com
57)	<b>PAMELA PAL</b>	Research Scholar	Diamond harbour women's University	palpamela1995@gmail.com
58)	<b>Papia Datta</b>	Head & Assistant Professor	Department of Applied Science, RCC Institute of Information Technology	papiaju@yahoo.in
59)	<b>Papiya Sikdar</b>	Research Scholar	University of Kalyani	papichem22@gmail.com
60)	<b>Patit Paban Malik</b>	Associate professor	B. B. College, Asansol, West Bengal	patitbu99@rediffmail.com
61)	<b>Pijush Singh</b>	JRF	University of Kalyani	singhpijush62@gmail.com
62)	<b>PIU SAMUI</b>	Research	Department of Mathematics, Diamond Harbour Women's	piusamui18@gmail.com



## ICCDL-2022@DHWU

		Scholar	University	
63)	<b>Piyali Maity</b>	Student	Diamond Harbour Women's University	iampiyali173@gmail.com
64)	<b>Pradip Kumar Tapaswi</b>	Assistant Professor	Narasinha Dutt College, Howrah, West Bengal, India	pradipkumartapaswi@gmail.com
65)	<b>Prasenjit Mistry</b>	Assistant professor	Jangipur College, Murshidabad	prasenjit.mistry@gmail.com
66)	<b>Pritilata Kundu</b>	M.sc.	Diamond Harbour Women's University	kundu.priti007@gmail.com
67)	<b>PRIYA ROY</b>	ASSISTANT PROFESSOR	DEPARTMENT OF ZOOLOGY, DIAMOND HARBOUR WOMEN'S UNIVERSITY	royprya12@gmail.com
68)	<b>Priyanka sen</b>	Msc	Diamond harbour women's university	senpriyanka161616@gmail.com
69)	<b>Puja Samanta</b>	Research Scholar	Diamond Harbour Women's University	spuja821@gmail.com
70)	<b>Raj Kumar Nandi</b>	Assistant Professor	Department of Chemistry, Diamond Harbour Women's University	Rajnandi007@yahoo.com
71)	<b>Reshmi Khatoon</b>	Student	Diamond harbour women's university	reshmikhatoon200@gmail.com
72)	<b>Ria Sanyal</b>	Assistant Professor	Department of Chemistry, Diamond Harbour Women's University	sanyalria2021@gmail.com
73)	<b>Riddhi Chakraborty</b>	MSc Chemistry SEM 3	DHWU	ridz.2598@gmail.com
74)	<b>Rifat Parveen</b>	Student	Diamond Harbour Women's University	rifatp438@gmail.com
75)	<b>Rimpa Mondal</b>	Research scholar	Diamond harbour women's University	rimpamondal956@gmail.com
76)	<b>Rinku Ghanta</b>	Research Scholar	Diamond Harbour Women's University	rinkughanta96@gmail.com
77)	<b>RITUSHREE</b>	STUDENT	DIAMOND HARBOUR	rituliza2512@gmail.com



## ICCDL-2022@DHWU

	JANA		WOMEN'S UNIVERSITY	
78)	<b>RIYA MONDAL</b>	Research Scholar	Diamond Harbour Women's University	riyabio05@gmail.com
79)	<b>Riya Samanta</b>	Student	Diamond Harbour Women's University	samanta.r2018@gmail.com
80)	<b>Sabari Panda</b>	<u>M. Sc</u>	Diamond Harbour Women's University	riya.panda2017@gmail.com
81)	<b>Sajeda saheli Mazumder</b>	Student	Diamond Harbour Women's University	mazumdersaheli64@gmail.com
82)	<b>Samim Khan</b>	CSIR RA	Aliah University	samimchm@gmail.com
83)	<b>Sangita Giri</b>	Student	Diamond Harbour Women's University	sangitagiri769@gmail.com
84)	<b>Sangita saha</b>	Student	Diamond Harbour Women's University	sangitasaha2209@gmail.com
85)	<b>Satan Sarinda</b>	M.Sc	Diamond Harbour Women's University	satansarinda@gmail.com
86)	<b>SAYANTI SHOW</b>	RESEARCH SCHOLAR	DIAMOND HARBOUR WOMEN'S UNIVERSITY	Sayantishow98@gmail.com
87)	<b>Shabnam Sultana</b>	Student	MSc chemistry	sultanashabnam2018@gmail.com
88)	<b>Shantabha Das</b>	Assistant Professor	Department of Chemistry, Diamond Harbour Women's University	shantanabha2008@gmail.com
89)	<b>Sharmistha Maji</b>	Student	DHWU	sharmistha.toton1999@gmail.com
90)	<b>Shatabdi Ghosh</b>	M.Sc.(Pursuing)	Student	shatabdighosh4100@gmail.com
91)	<b>Shreejita Halder</b>	Student	Diamond Harbour Women's University	shreejitahalder02@gmail.com
92)	<b>Sibani Mal</b>	Student	Diamond harbour women's University	isibani1305@gmail.com
93)	<b>Sneha Biswas</b>	Senior Research Fellow	Calcutta University	sneha.khardah@gmail.com





## ICCDL-2022@DHWU

94)	<b>Sneha Mondal</b>	Student	Diamond Harbour Women's University	snehamondal472@gmail.com
95)	<b>SOMA NASKAR</b>	RESEARCH SCHOLAR	DIAMOND HARBOUR WOMEN'S UNIVERSITY	somanaskar1993@gmail.com
96)	<b>SOUMADIP BANERJEE</b>	SENIOR RESEARCH FELLOW	INDIAN ASSOCIATION FOR THE CULTIVATION OF SCIENCE	banerjee.soumadip@gmail.com
97)	<b>Sreejani Jana</b>	Student	International seminar	sreejanijana98@gmail.com
98)	<b>SRIYANKA BHANDARI</b>	STUDENT (M.SC)	DHWU	sbhandari1732000@gmail.com
99)	<b>SUBHASIS GHOSH</b>	Research Scholar	University of Kalyani	subhasis.ghosh95@gmail.com
100)	<b>Sudeshna Ghosh</b>	Research Scholar	Diamond Harbour Women's University	sudeshna.dhwu.physics@gmail.com
101)	<b>SUHANA KARIM</b>	PhD	Research Scholar	suhana.k13@gmail.com
102)	<b>SUKANYA DAS</b>	Research Scholar	DIAMOND HARBOUR WOMEN'S UNIVERSITY	sukanyadas01997@gmail.com
103)	<b>Sukanya Kundu</b>	M.Sc student	Vidyasagar University	sukanyakundu23@gmail.com
104)	<b>SUMANA SHEE</b>	Student	DIAMOND HARBOUR WOMENS' UNIVERSITY	sumanashee1@gmail.com
105)	<b>Sunita Jhulki</b>	PhD scholar	Diamond Harbour Women's University	sunitajhulki416@gmail.com
106)	<b>Suprita Hati</b>	Student	Learning	supritakhuku@gmail.com
107)	<b>Supriti Maity</b>	M.Sc	Diamond Harbour Women's University	supriti.maity7501@gmail.com
108)	<b>Sushmita Nandy</b>	Student	Yes	sushmitanandy532@gmail.com
109)	<b>Susmita Chakraborty</b>	Student -M.Sc 3rd Semester ( Inorganic Special)	Diamond Harbour Women's University	susmitachakraborty294@gmail.com
110)	<b>Susmita Ghosh</b>	Student	Sem-1	gsusmita8701@gmail.com
111)	<b>Susmita Mondal</b>	Assistant	Diamond Harbour Women's	susmita.dhwu@gmail.com



## ICCDL-2022@DHWU

		Professor	University	
112)	<b>Sutapa Samanta</b>	M.Sc	Diamond harbour women's University	sutapasamanta761@gmail.com
113)	<b>SWADHIN KUMAR SAHA</b>	ASSISTANT PROFESSOR	DEPARTMENT OF CHEMISTRY, KAZI NAZRUL UNIVERSITY	swadhin.chem@gmail.com
114)	<b>Swarnali Khan</b>	Research Scholar	Diamond Harbour Women's University	swarnalikhan807@gmail.com
115)	<b>Tania Chowdhury</b>	Research Scholar	University of Calcutta	tania.chowdhury1994@gmail.com
116)	<b>Taniya Banerjee</b>	M. Sc. Student	Diamond harbour women's university	banerjeetaniya89@gmail.com
117)	<b>Tanmay Chattopadhyay</b>	Assistant Professor	Department of Chemistry, Diamond Harbour Women's University	tanmayc2003@gmail.com
118)	<b>Urmila Mandal</b>	<u>M.Sc</u>	DHWU	urmilamandal2001@gmail.com

					B 5 10.81 Boron 	C 12.01 Carbon 
					Al 13 26.98 Aluminum 	Si 28.09 Silicon 
Co 27 58.93 Cobalt 	Ni 28 58.69 Nickel 	Cu 29 63.55 Copper 	Zn 30 65.38 Zinc 	Ga 31 69.72 Gallium 	Ge 72.64 Germanium 	
Rh 45 102.91 Rhodium 	Pd 46 106.42 Palladium 	Ag 47 107.87 Silver 	Cd 48 112.41 Cadmium 	In 49 114.82 Indium 	Sn 118.71 Tin 	
Ir 77 192.22 Iridium 	Pt 78 195.08 Platinum 	Au 79 196.97 Gold 	Hg 80 200.59 Mercury 	Tl 81 204.38 Thallium 	Pb 207.2 Lead 	
Mt 109 288 Mendelevium 	Ds 110 285 Darmstadtium 	Rg 111 272 Roentgenium 	Uub 112 285 Ununbium 	Uut 113 288 Ununtrium 	Uuq 114 289 Ununquadium 	
Eu 63 151.96 Europium 	Gd 64 157.25 Gadolinium 	Tb 65 158.93 Terbium 	Dy 66 162.5 Dysprosium 	Ho 67 164.93 Holmium 	Er 167.26 Erbium 	
Am 95 243 Americium 	Cm 96 247 Curium 	Bk 97 247 Berkelium 	Cf 98 251 Californium 	Es 99 252 Einsteinium 	Fm 257 Fermium 	