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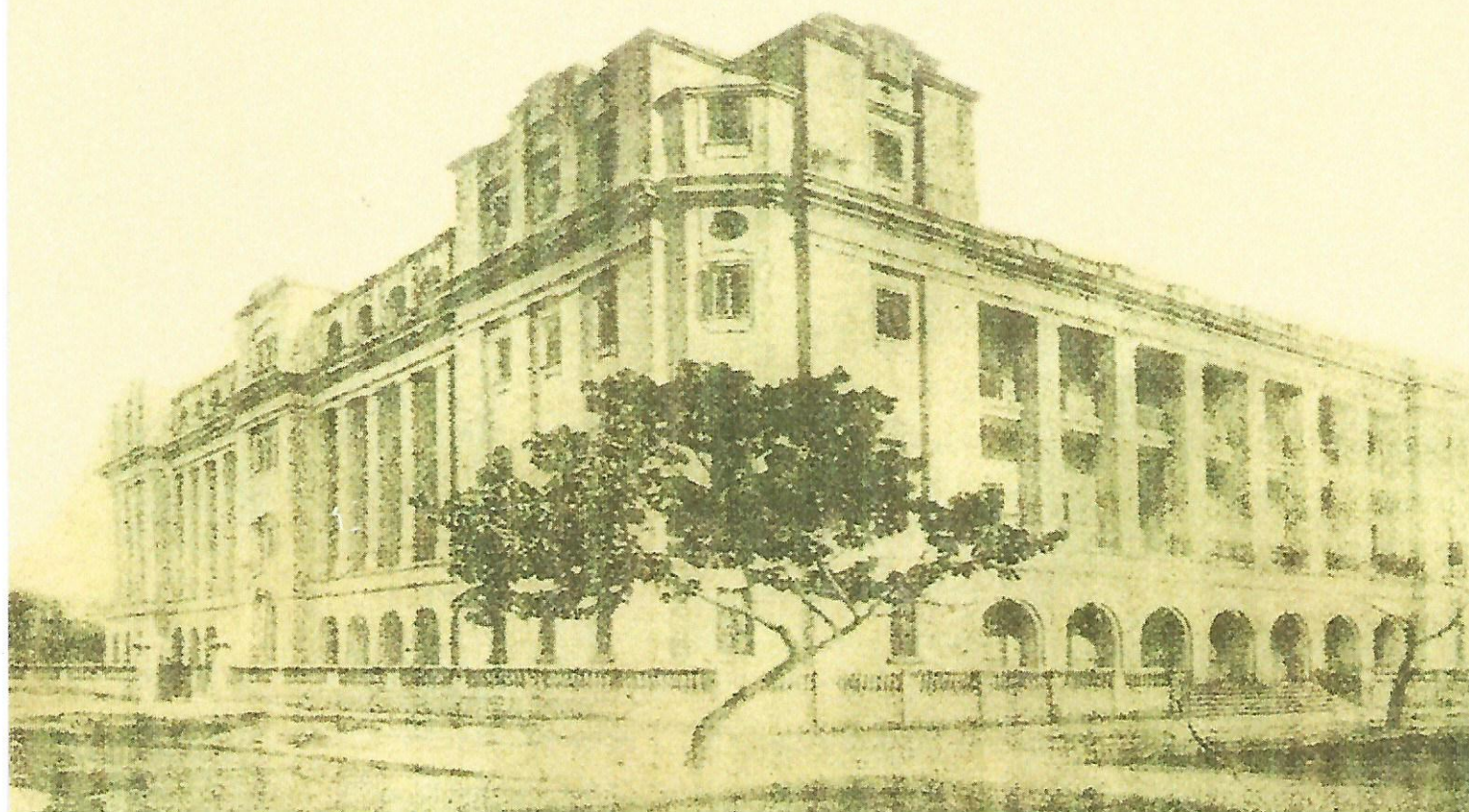


"RECENT TRENDS IN MACROMOLECULAR CHEMISTRY" [RTMC - 2018]

10th January 2018

Organized by
City College
Department of Chemistry
(102/1, Raja Rammohan Sarani, West Bengal, India)
Kolkata - 700009

In association with
Indian Chemical Society, Kolkata





City College – A Glorious Journey and Beyond

It was the time of the beginning of renaissance in Bengal. Ananda Mohan Bose, Shibnath Shastri and Surendranath Banerjea, three extremely talented and devoted fiery young leaders of Bengal founded the City school in 1879 which was elevated to a college in 1881 an effort which was patronised by top ranked officials of the then British Govt. In 1883, law classes were started (where Sir Ashutosh Mukherjee was a student). Even M.A classes were held in the college for some years.

The reputation of City College as a first grade degree college spread throughout India not only because every year it's students fared better than Govt. and missionary run higher educational institutions in University examination but it did so without any financial aid from the Govt. No other private college of India can boast of so many elevated educationist in Teacher's roll as in City college including Surendranath Banerjee, Ananda Mohan Bose, Umesh Chandra Dutta, Heramba Chandra Maitra, Acharya P. C. Roy, Dr. Rajendra Prasad, Acharya Suniti Kumar Chattopadhyay, Harendra Kumar Mukherjee, Prasanta Mahalanobis, Poet Jibanananda Das, Narayan Ganguli and many other luminaries. In those days, students and teachers were frequently involved in various social works and later in many ways with the Freedom movement.

Overcoming stiff resistance from the society the then leaders of the Brahma Samaj succeeded in introducing degree classes for girl students in the college and a women's department was operational in 1943. Chemistry teaching was introduced as early as in 1884. Since then, countless students from chemistry department have excelled in their fields both in India and abroad making the college proud for their achievements. Such endeavours are persisting even today and would obviously scale greater heights in future.

A Few Words about the Department of Chemistry, City College

In 1881, City College came into existence. Within a few years City College became the embodiment of the concept of modern education in india embracing Mathematics, Natural Philosophy, Chemistry and Anatomy with other useful sciences. Since its inception in 1884, the Department of Chemistry along with other science streams gradually assimilated the available modern knowledge from the western countries and in turn trained the young minds accordingly.

This trend continues even today. Through different era, so many distinguished teachers have made the department proud with their teaching prowess and countless students with their scientific excellence in the post college life. A short list of a few of them are given below:-

1. Prof. Haridas Bhanja (Teacher and Head of the Department)
2. Dr. Suresh Sengupta (Teacher)
3. Prof. Sukumar Aditya (Teacher)
4. Prof. Purushottam Banerjee (Teacher)
5. Prof. Jyotindranath Ray (Teacher)
6. Prof. Saroj Kumar Bose (Teacher and Head of the department)
7. Prof. Dwipendra Kumar Bose (Teacher)
8. Prof. Bijan Sen (Ex-student and Teacher)
9. Prof. Parimal Kumar Sen (Ex-student and Teacher)
10. Prof. Sundar Gopal Ghosh (Ex-student) (Professor, I.I.T Chennai)
11. Prof. Swadhin Chandra Jana (Ex-student) (Professor, Lisbon University, USA)
12. Prof. Pradyut Ghosh (Ex-student) (Professor, I.A.C.S & Bhatnagar Awardee)

At present many of the students of the Departments are studying in different IITs and IISER pursuing post graduate studies and research activities. We take pride in stating that a National seminar entitled “Scarcity of Portable Water: Health, Management and Future” was held in the department on 13.3.2004 under sponsorship of UGC.

In recent years, the teachers of the department regularly participate in seminars held at different institutions throughout the years. A few young teachers of the department are already engaged in research activities in the department.



CITY COLLEGE

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Kolkata – 700009**

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Date: 04.01.2018

Message from the Principal

I am very happy to know that the Department of Chemistry, City College is organising an International Seminar on **Recent Trends In Macromolecular Chemistry 2018 (RTMC-2018)** at City College, 102/1, Raja Rammohan Sarani, Kolkata – 700009 (Ground Floor, Room no. 6) in association with Indian Chemical Society, Kolkata.

Macromolecules are the building blocks of almost all the living and non-living systems on earth and they have widespread applications in Chemistry, Physics and Biology.

This Seminar will provide a platform to the Young Scientists, Researchers, Faculties and Students to refresh their enthusiasm and create an interest to contribute more to the advancements of the society through their innovative research.

I convey my very best wishes for an effective, successful and productive seminar

Sital Prasad Chattopadhyay
Dr. Sital Prasad Chattopadhyay

Principal, City College

Date: December 19, 2017



Message

I am extremely happy to learn that the City College, Kolkata in association with the Indian Chemical Society is organizing an International Seminar entitled "Recent Trends in Macromolecular Chemistry" at the Department of Chemistry, City College, Kolkata on January 10, 2018. The Organising Committee deserves appreciation for undertaking such a commendable task.

It is a matter of great delight that distinguished researchers in the field of Macromolecular Chemistry from West Bengal would meet and deliberate on the fundamental and applied aspects of the subject. The seminar would provide an appropriate forum for interaction with the experts in the field and the budding scientists would be inspired to take up new challenges for carrying out research in the fascinating area of Chemistry and also to strive for advancement and propagation of scientific knowledge.

I wish the seminar a grand success.

A handwritten signature in black ink, appearing to read "D. C. Mukherjee". The signature is fluid and cursive.

Dulal C. Mukherjee

Professor of Chemistry (Retd.), University of Calcutta and
President, Indian Chemical Society



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Ref. No: ICS/Hony. Sec./17

Date: December 08, 2017

To
Dr. S S Bhattacharjee
Head, Department of Chemistry
City College
Kolkata – 700 009

Dear Dr. Bhattacharya,

Thank you very much for your letter dated December 07, 2017 requesting for collaboration of the Indian Chemical Society in the International Seminar to be held on January 10, 2018. We will be extremely happy to be associated with the proposed seminar without any financial commitment.

I wish a grand success of the Seminar.

With regards

Yours sincerely

Rahul Bhattacharya

for Professor Chittaranjan Sinha
Honorary Secretary
Indian Chemical Society

Date: 02.01.2018

Message from Conveners

It gives us immense pleasure to welcome all attendees to the International Seminar on **Recent Trends In Macromolecular Chemistry [RTMC - 2018]** on 10th January, 2018 in association with Indian Chemical Society. At the outset let us express our sincerest thanks to the authority of City College for allowing us to organize this seminar. We are also thankful to Indian Chemical Society for their association.

We are honored to have Prof. D. C. Mukherjee (Retd., Professor, University of Calcutta and President, Indian Chemical Society and Prof. Ashutosh Ghosh (Ex Vice-Chancellor, University of Calcutta) as the Guest-in-Chief, Prof. Tien-Yau Luh, Distinguished Chair Professor, Department of Chemistry, National Taiwan University, Taipei, Taiwan and Prof. Pradyut Ghosh (S. S. Bhatnagar awardee), Senior Professor, Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, Kolkata-700032 and an students of our department as the Key Note Speakers in this occasion.

The main goal of organizing this seminar is to share and enhance the knowledge of each and every individual in various fields of Chemistry and Chemical Technology.

We believe that the seminar will provide exposure to the students on modern day researches on diverse fields of chemical science and technology and encourage them to be a part of these endeavors. The response to the poster presentation within this short time from all over the country has been very encouraging.

We sincerely thank all the participants, advisers and volunteers for extending their kind cooperation and welcome you all to our college to have a great time.

Dr. Biswajit Panda

Dr. Pampa Guha

PROGRAMME SCHEDULE

12:30 PM – 1:00 PM	Registration
1:00 PM – 1:30 PM Inaugural Session	Introduction: Dr. Pampa Guha, Convener, Seminar Organising Committee Inauguration: Dr. Sital Prasad Chattopadhyay, Principal, City College, Kolkata Welcome Address: Dr. S. S. Bhattacharjee, Head, Dept. of Chemistry, City College Vote of Thanks: Dr. Biswajit Panda, Convener, Seminar Organising Committee
1:30 PM - 2:15 PM Lecture - I	Fundamentals to Applications of Anion Recognition Prof. Pradyut Ghosh (S. S. Bhatnagar Awardee) Indian Association for the Cultivation of Science, Kolkata
2:15 PM – 3:00 PM	Tea Break and Poster Session
3:00 PM – 3:45 PM Lecture – II	Discovery of DNA-Like Polymeric Ladderphanes -A Personal Account Prof. T.-Y. Luh (Distinguished Chair Professor) National Taiwan University, Taipei, Taiwan
3:45 PM – 4:00 PM	Concluding Session

Invited Lecture - I

Fundamentals to Applications of Anion Recognition

Pradyut Ghosh

*Department of Inorganic Chemistry, Indian Association for the Cultivation of Science, 2A
& 2B Raja S. C. Mullick Road, Jadavpur, Kolkata 700032, INDIA.*

The fundamental chemistry of selective recognition, sensing and extraction of various anions are considered to be very important to develop technologies in water purification process, industrial and nuclear waste reprocessing. Thus, developing receptors that selectively bind environmental and health related important anions is one of the major goals in anion chemistry. In recent times, recognition, sensing and extraction of anion/ion-pair by synthetic hosts have received enormous research attention with promising analytical, industrial and environmental applications. A wide variety of receptors containing ammonium, amide, urea groups as anion recognition elements with increasing complexities from tripodal, macrobicycle, molecular capsule to hexapodal have been synthesized by our group which will be discussed briefly. Further, selective liquid–liquid extraction of KF/KCl from aqueous solution using dual-host approach along with the discussion on sulfate extraction using carbonate encapsulated molecular capsules; quantitative capturing of aerial CO₂ in the form of CO₃²⁻ capsules and trapping of cyanide (for industrial waste water treatment) by molecular capsules etc. will be presented.

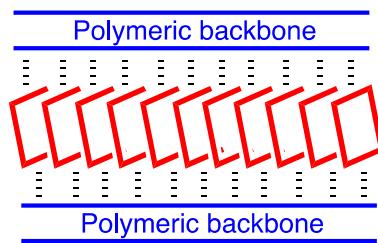
Invited Lecture - II

Discovery of DNA-Like Polymeric Ladderphanes-A Personal Account

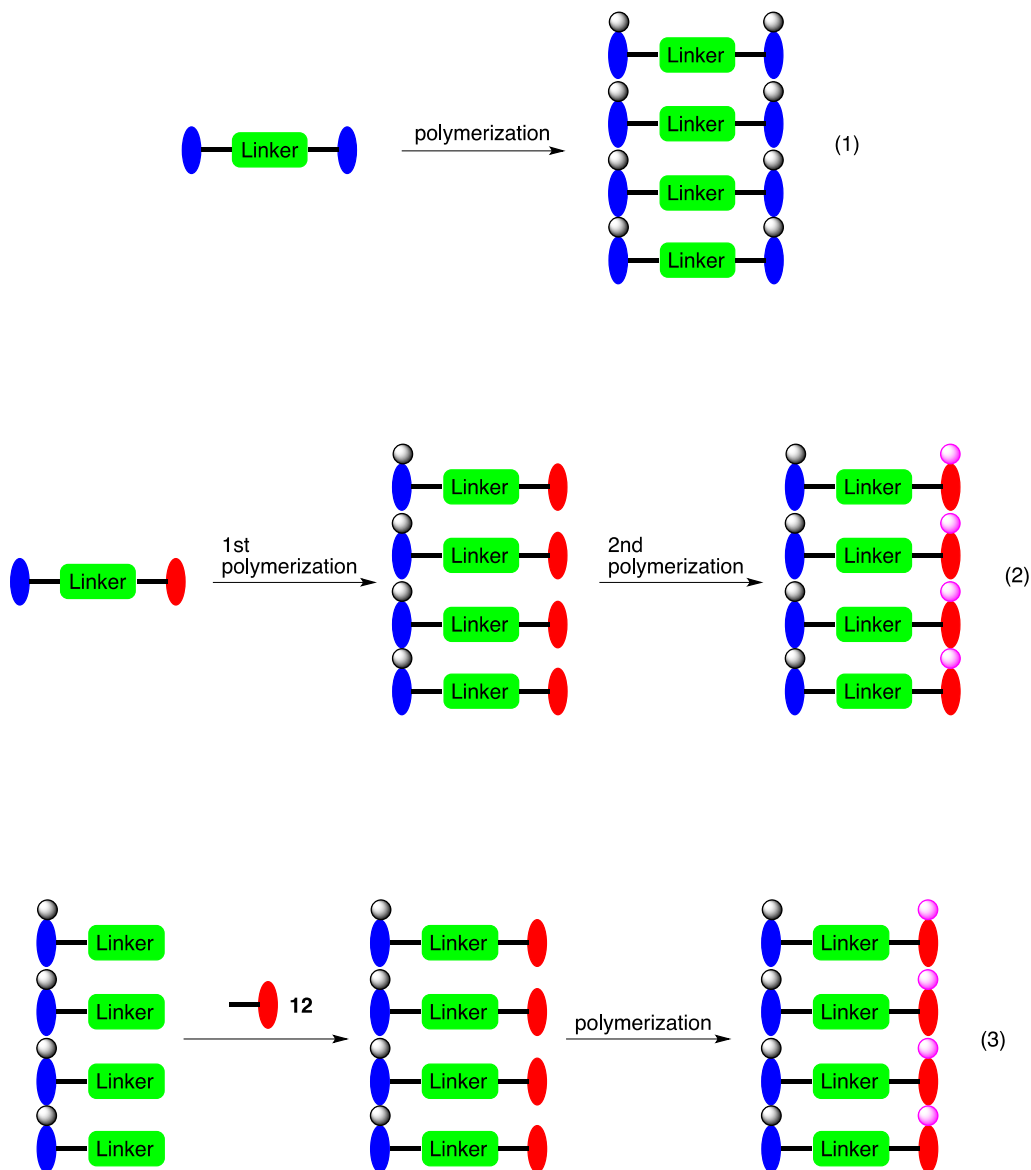
Tien-Yau Luh

Department of Chemistry, National Taiwan University, Taipei, Taiwan 106

Ladderphane **1** is defined as a polymer that consists of multiple layers of cyclophanes, where the tethers are part of the polymeric backbones.¹ A DNA molecule can be considered as a special kind of ladderphane, where the base pairs are connected through hydrogen bonds and linked perpendicularly to the deoxyribose phosphates backbones. The sugar-phosphate backbones have isotactic stereochemistry. The spacing separating adjacent base pair layers is about 3.4 Å and this distance suggests that there should be strong interactions between adjacent layers of base pairs. These characteristics could offer useful clue for the design and synthesis of double stranded DNA-like polymeric ladderphanes.



Three approaches have been executed for the synthesis of polymeric ladderphanes. The first method involves double polymerization of a monomer containing two polymerizable groups linked by a rigid linker. The ladderphanes thus obtained are symmetric. The second and third protocols are for the synthesis of unsymmetric ladderphanes where the two polymeric backbones are not same, but complementary. The latter method has been used for replication to synthesize a range of condensation polymers with well-controlled degree of polymerization and narrow polydispersity.



Several important features are worthy to comment. The polymeric backbones can be polynorbornene or polycyclobutene and are obtained by ring opening metathesis polymerization reactions. It is important to note that they should have homogeneous stereochemistry (tacticity). The linkers are relatively rigid and can be planar aromatic, antiaromatic, metallocycle or three-dimensional organic or organometallic moieties, whose span must be smaller than that of the monomeric species of the polymeric backbone. These polymers can form highly ordered assembly on graphite surface as revealed by STM images. Since the adjacent linkers in these polymers are in close

proximity (4.5-5.5 Å), significant interaction between these adjacent linkers may take place. Various interesting photophysical properties (fluorescence quenching, excimer formation, electron hopping etc) will be discussed.

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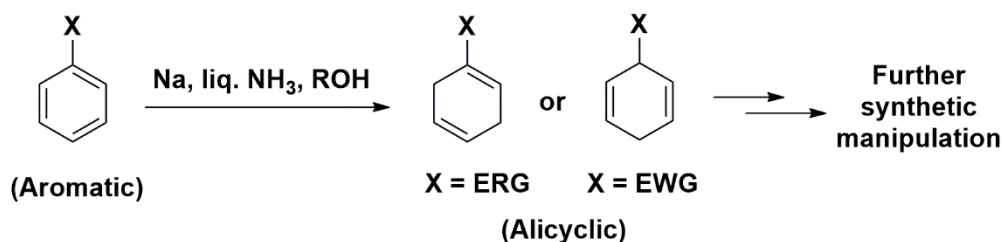
Abstract for Poster Presentation

Birch Reduction of Aromatic Compounds: Applications in Synthetic Organic Chemistry

Kaushik Basu

Department of Chemistry, St. Paul's C. M. College, Kolkata

It was 1946 when Arthur J. Birch, an organic chemist from down under, then working at the Dyson Perrins Laboratory, Oxford University, reported a remarkable partial hydrogenation of aromatic nucleus induced by sodium in liquid ammonia (scheme 1). This reaction came to be known as the Birch Reduction. This reduction of aromatic compounds to their dihydro derivatives by dissolving metals is one of the most powerful synthetic methods available to organic chemists. In one simple reaction it builds a bridge between aromatic and alicyclic molecules, thereby allowing us to tap into the huge reserve of aromatic chemistry readily available for the construction of alicyclic structures. It also facilitates to carry through a protracted synthesis a moiety which is inert towards an extensive array of reagents, but which is readily damasked by the reductive process into a range of useful functionalities. Depending upon the substituents present in the aromatic ring, the reduction shows excellent regioselectivity which serves as a valuable tool to address selectivity issues in synthesis. The products of Birch reduction are also amenable to further synthetic manipulation. Asymmetric variation of Birch Reduction has contributed to expand its application further into the realm of synthetic organic chemistry. In this presentation some novel synthetic applications of this name reaction will be highlighted.



Scheme 1: Birch Reduction of aromatics to dihydro derivatives

References:

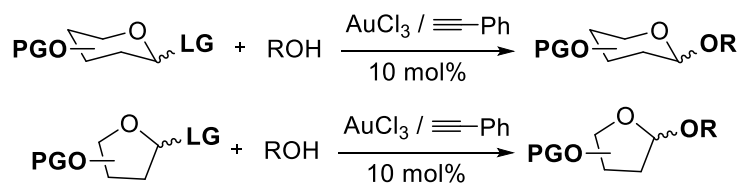
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Au(III) Catalysed Glycosylation Reactions from Simple to Modified Glycosyl Donors

Dr. Asadulla Mallick

Assistant Professor, Ramakrishna Mission Vidyamandir, Belur Math

The majority of carbohydrates are not found in their free forms in nature; monosaccharides are linked through glycosidic bonds to other monosaccharides, or to aglycons such as lipids, peptides, or proteins to form oligosaccharides or glycoconjugates. Depending on the nature of the linkage, they can be classified as *N*-, *O*-, *C*-, or *S*-linked glycosides. Among all *O*-Linked glycosides are most common and most important. As a consequence, the synthesis of biologically important oligosaccharides and glycoconjugates has been a prime concern for chemists, and a large number of glycosylation methods have been developed for these purpose.¹ Different kinds of glycosyl donors have been introduced like thioglycosides, glycosyl sulfoxides, glycosyl sulfones, trichloroacetimidates, *n*-pentenyl glycosides to achieve glycosylation reactions. However, the use of Au(III) catalysed glycosylation reaction has been reported very few in the current years. In this context, we recently developed²⁻⁵ a new relay catalyst system comprising Au(III) chloride and phenylacetylene, which was able to activate glycosyl trichloroacetimidates,² 1-*O*-acetyl furanose,³ 1-*O*-acetyl pyranose⁴, 1,2-Orthoesters³ and glycosyl sulfoxides⁵ as glycosyl donors.



LG = -OAc, -SOPh, 1,2-orthoester

PG = protecting group

Scheme: Au(III) catalysed glycosylation reactions with different donors

The donor glycosyl sulfoxides were activated with milder Au (III) reagent at room temperature. Further, the α or β selectivity in the final product were nicely maintain by using modified 1,2-orthoester as donor.

References:

1. *Handbook of Chemical Glycosylation*, Ed.: A. V. Demchenko, Wiley-VCH, Weinheim, Germany, **2008**.
2. Comparative study of AuCl₃ and AuCl₃-Phenylacetylene catalyzed glycosylations using glycosyl trichloroacetimidates. Rashmi Roy, Ashok kumar Palanivel, Asadulla Mallick and Yashwant D. Vankar *Eur. J. Org. Chem*, **2015**, *18*, 4000-4005, DOI:10.1002/ejoc.201500137
3. Au^{III}-Halide/Phenylacetylene-Catalysed Glycosylations Using 1-*O*-Acetylfuranoses and Pyranose 1,2-Orthoesters as Glycosyl Donors. Asadulla Mallick, Yakkala Mallikharjunarao, Parasuraman Rajasekaran, Rashmi Roy, Yashwant D. Vankar
4. Gold(III) Chloride and Phenylacetylene: A Catalyst System for the Ferrier Rearrangement, and *O*-Glycosylation of 1-*O*-Acetyl Sugars as Glycosyl Donors” Rashmi Roy, Parasuraman Rajasekaran, Asadulla Mallick, Yashwant D. Vankar *Eur. J. Org. Chem*, **2014**, *25*, 5564–5573, DOI:10.1002/ejoc.201402606
5. AuCl₃-AgOTf promoted *O*-glycosylation using anomeric sulfoxides as glycosyl donors at room temperature. Ashokkumar Palanivel, Ande Chennaiah, Sateesh Dubbu, Asadulla Mallick, Yashwant D. Vankar. *Carbohydr. Res.*, **2017**, *437*, 43-49, DOI: 10.1016/j.carres.2016.11.012

Metal–Organic Frameworks in Macromolecular Gel Matrices

Ashesh Garai[†], William Shepherd, Jia Huo and Darren Bradshaw

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([†] Present address: Rammohan College, 102/1 Raja Rammohan Roy Sarani, Kolkata-700009)

Gelatin is used as both a matrix and macromolecular additive for growing metal–organic frameworks (MOFs) crystals, ZIF-8 and HKUST-1. These MOFs are readily prepared within the cheap, non-toxic hydrogel medium. ZIF-8@gelatin composites are readily dispersed in water to form colloidal MOFs dispersion stable for several months. The matrix also has a significantly more pronounced effect on the crystal growth and morphology of HKUST-1. Gelatin plays a vital role to tune the particle size and morphology of the MOFs depending on the method of synthesis and the amount of gelatin used in the synthesis.

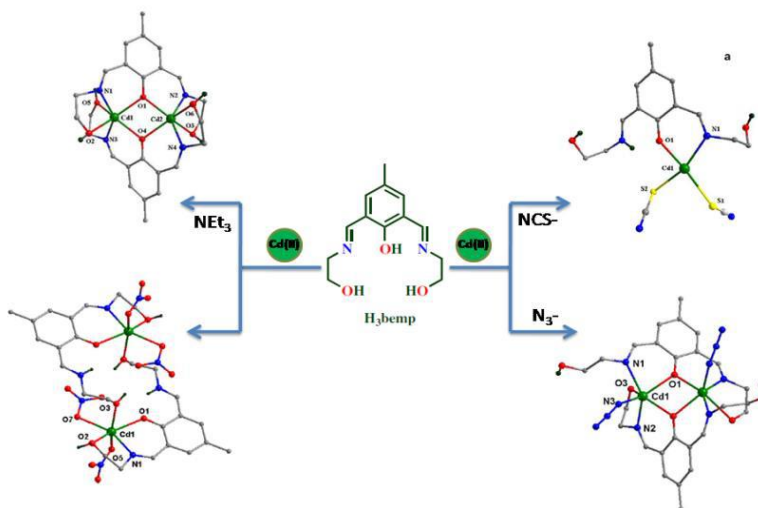
Syntheses, Characterization, and Photophysical Studies of Cadmium (II) Complexes Derived from Binucleating Schiff Base Ligand 2,6-bis[(2-hydroxy ethylimino)methyl]-4-methylphenol

Avijit Sarkar¹ and Debashis Ray²

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A series of dinuclear cadmium (II) complexes (**1-4**) with 2, 6-bis[(2-hydroxy ethylimino)methyl]-4-methylphenol have been synthesized and characterized by X-ray crystallography, spectroscopic and analytical techniques. Different reaction condition and varying anion coordination changes the different coordination geometry around the Cadmium (II) center. The photoluminescence behavior of the ligand and cadmium (II) with varying anions have been investigated in a PBS buffer (5 mM in pH = 7.1) at 25 oC. The H3bemp molecule registers as a highly selective fluorescent probe for Cd²⁺ and is accounted by the formation of [Cd₂(H₂bemp)₂](NO₃)₂ (**1**) in solution. The quantum yield of the ligand is 0.201 and it increases more than 4-fold (0.851) in the presence of the cadmium (II) ion. In presence of anion NCS⁻, complex **1** showed coordination induced fluorescence enhancement, whereas the other anions NO₃⁻ and N₃⁻ anions quench the emission intensities significantly.



Helical Chains of Ternary Copper(II) Complexes of Mono-Anionic Glutamate: Anion-Directed Variation in the Molecular and Supramolecular Structures

Chaitali Biswas

Assistant Professor, Sarojini Naidu College for Women, 30, Jessore Road, Kolkata – 700028, India. E. mail: mail2_chaitali@yahoo.co.in

Two new polynuclear copper(II) complexes of singly deprotonated L-glutamic acid (L-glu), $\{[\text{Cu}(\text{bipy})_2][\text{Cu}(\text{bipy})(\text{L-glu})\text{H}_2\text{O}]_2(\text{BF}_4)_4 \cdot (\text{H}_2\text{O})_3\}_n$ (**1**), $\{[\text{Cu}(\text{bipy})(\text{L-glu})\text{H}_2\text{O}][\text{Cu}(\text{bipy})(\text{L-glu})(\text{ClO}_4)](\text{ClO}_4) \cdot (\text{H}_2\text{O})_2\}_n$ (**2**) (bipy = 2,2'-bipyridine), were synthesized in acidic pH (ca. 2.5) and characterized structurally. In both complexes, L-glutamic acid acts as a bidentate chelating ligand, leaving the protonated carboxylic acid free. The structural analyses show that in both of them two different type of species $[\text{Cu}(\text{bipy})_2](\text{BF}_4)_2$ and $[\text{Cu}(\text{bipy})(\text{L-glu})\text{H}_2\text{O}]\text{BF}_4$ for **1** and $[\text{Cu}(\text{bipy})(\text{L-glu})\text{H}_2\text{O}]\text{ClO}_4$ and $[\text{Cu}(\text{bipy})(\text{L-glu})(\text{ClO}_4)]$ for **2** coexist in the solid state. In complex **1**, the $[\text{Cu}(\text{bipy})(\text{L-glu})]_2^+$ units are joined together by syn-anti carboxylate bridges to form an enantiopure (M) helical chain and the $[\text{Cu}(\text{bipy})_2]^{2+}$ represent a very rare example of the four-coordinate distorted tetrahedral geometry in that species. In complex **2**, the $[\text{Cu}(\text{bipy})(\text{L-glu})(\text{ClO}_4)]$ units are joined together by weakly coordinating perchlorate ions to form a polymeric chain whereas the $[\text{Cu}(\text{bipy})(\text{L-glu})\text{H}_2\text{O}]^+$ units remains as mononuclear species. The different coordination ability of the two very similar counter anions along with their involvement in the H-bonding network seems to be responsible for the difference in the final polymeric structures in the two compounds. Variable-temperature (2-300 K) magnetic susceptibility measurement shows negligible coupling for both the complexes.

**Photobehavior and Docking Simulations of Drug within
Macromolecules: Binding of an Antioxidative Isoquinolindione to a
Serine Protease and Albumin Proteins**

Dr. Dipak Kumar Rana

Department of Chemistry, Saldiha College, Saldiha, Bankura- 722173, E-mail:

[*drpcju@yahoo.co.in*](mailto:drpcju@yahoo.co.in)

The principal intent of the present contribution is to decipher the binding domain and structural changes of trypsin (TPS), a proteolytic globular enzyme and two serum proteins, namely, bovine serum albumin (BSA), human serum albumin (HSA) association with a newly synthesized bioactive isoquinolindione derivative (ANAP) by employing steady state, time resolved fluorescence and circular dichroism (CD) techniques. Intramolecular charge transfer emission (ICT) of ANAP is found to be responsible for the commendable sensitivity of the probe as an extrinsic fluorescent marker to the protein environments. A sharp distinctive feature of determined micropolarities in proteinous media clearly demarcates the differential extent of hydrophobicity around the encapsulated ANAP. A proficient efficiency tunable fluorescence (Förster type) resonance energy transfer (FRET) from the excited tryptophan to ANAP reveals that ANAP binds in the close vicinity of the tryptophan residue in protein. Molecular modeling simulation has been exploited for evaluating the probable interaction site of ANAP in proteinous assembly which shows subdomain IIA are earmarked to possess affinity for ANAP in serum albumins whereas S1 binding pocket in TPS has been found potential binding region for ANAP.

Introduction of Ruthenium Analogues: Alternative of Pt-based Anticancer Drugs

Dr. Arup Mandal

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Email: mandalarup86@gmail.com

Platinum-based drugs have become a mainstay of cancer therapy; approximately half of all patients undergoing chemotherapeutic treatment receive a platinum drug. The widespread use of platinum agents in the treatment of cancer began with the discovery of the antineoplastic activity of cisplatin by Barnett Rosenberg in the 1960s. But when cisplatin, the first discovered anticancer drug, failed to reach its maximum expectation then researchers were eager to find new analogues so that it can cover all the deficiencies shown by cisplatin. In this abstract, by the survey of lot of papers, the target is to show how Ru-analogues had been introduced as alternatives.

The platinum-group metals constitute a family of six chemically related elements which can be divided into the denser platinum, iridium, osmium and the lighter palladium, rhodium and ruthenium. Ruthenium complexes seem to be less toxic, a number of ruthenium compounds have some biological demands. In the search for drugs with improved clinical effectiveness, reduced toxicity and a broader spectrum of activity, other metals than platinum have been considered, such as rhodium and ruthenium. Ruthenium complexes are very promising, especially from the viewpoint of overcoming cis-platin resistance with a low general toxicity. Ruthenium has found its way into the clinic, where its properties are exploited for very miscellaneous uses. The radio physical properties of Ru can be applied to radio diagnostic imaging.^[1, 2] Ruthenium(II) and ruthenium(III) complexes have similar ligand-exchange kinetics to those of platinum(II) complexes. This property makes them the first choice in the search for compounds that display similar biological effects to platinum(II) drugs.^[3, 4] The range of accessible oxidation states of ruthenium under physiological conditions makes this metal unique amongst the platinum group. One more property of ruthenium that makes it very appreciated in medicinal chemistry is its tendency to selectively bind biomolecules, which partly accounts for the low toxicity of ruthenium drugs.^[3, 4] Transferrin and albumin are two proteins used by mammals to solubilize and transport iron, thereby reducing its toxicity. The ability of some ruthenium drugs to bind to transferrin has been proven.^[5-9]

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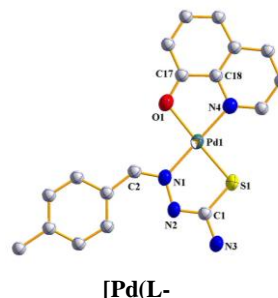
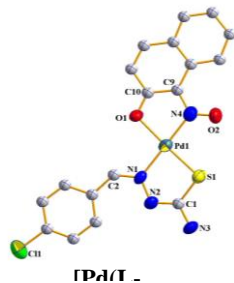
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Synthesis of Palladium Complexes Containing Mixed-Ligands. Structures and Application as Catalysts in Suzuki and Buchwald Coupling Reactions

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Reaction of a 1:1 mixture of 4-R-benzaldehyde thiosemicarbazone (denoted in general as **HL-R**; where H stands for the dissociable acidic proton and R (R = OCH₃, CH₃, H, Cl and NO₂) for the substituent) and 1-nitroso-2-naphthol (abbreviated as **Hnn**) with an equivalent quantity of Na₂[PdCl₄] in ethanolic medium affords a group of mixed-ligand complexes of type [Pd(L-R)(nn)]. Similar reaction of a mixture of **HL-R** and quinolin-8-ol (**Hq**) with Na₂[PdCl₄] affords another family of mixed-ligand complexes of type [Pd(L-R)(q)]. Crystal structures of [Pd(L-Cl)(nn)], [Pd(L-CH₃)(q)] and [Pd(L-Cl)(q)] have been determined. In all the complexes the thiosemicarbazones are coordinated to the metal center, via dissociation of the acidic proton, as monoanionic bidentate N,S-donors forming five-membered chelate rings. In the [Pd(L-R)(nn)] complexes the 1-nitroso-2-naphtholate anion is coordinated as a N,O-donor forming five-membered chelate ring. Similarly in the [Pd(L-R)(q)] complexes the quinolin-8-olate anion is bound to the metal center in N,O-mode forming five-membered chelate ring. Catalytic activity of the [Pd(L-R)(nn)] and [Pd(L-R)(q)] complexes has been examined towards some C-C and C-N coupling reactions and, both are found to show remarkable, as well as comparable, catalytic efficiency.



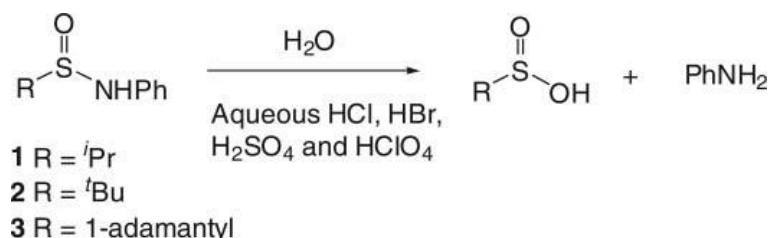
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J. Dutta; S. Datta; D. K. Seth, S. Bhattacharya, *RSC Advances*, **2012**, 2, 11751.

Hydrolysis of *N*-Phenylalkanesulfinamides in Aqueous Mineral Acids

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The acid-catalyzed hydrolysis of *N*-phenylalkanesulfinamides (RSONHPh; **1**, R = *i*Pr; **2**, R = *t*Bu; **3**, R = 1-adamantyl) has been studied in aqueous mineral acids. Hydrolysis was found to proceed *via* a slow spontaneous (uncatalyzed) pathway, an A-2 (bimolecular) acid-catalysis pathway, and an acid-dependent nucleophilic catalysis pathway, the last of which predominates in hydrobromic and hydrochloric acid solutions. A mechanistic switch over from A-2 to A-1 was detected for compounds **2** and **3** in concentrated sulfuric acid. Order of catalytic activity, effect of added salts, Arrhenius parameters, kinetic solvent isotope, and solvent effects are all consistent with the proposed mechanisms.

Quantum Dot: A Role of Confinement Potential

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In recent years, significant progress has been made in the fabrication of low dimensional structures thereby reducing the effective dimensions from 3D bulk materials to quasi 2-D quantum wires and even to quasi 0-D quantum dots. The quantum confinement effects in such systems of reduced space dimensions have attracted considerable attention. Maksym and Chakraborty worked out the energy levels and found an incredibly rich structure. In quantum dots the electron energy levels are quantized and the behavior is similar to that of an atom. The presence of discrete energy levels and even the manifestations of the shell structure which was predicted and experimentally observed for quantum dots, give grounds for treating them as artificial atom. The confinement potentials in quantum dots can be exploited to describe typical features of transport processes and spin oscillations in magnetic field. The main components responsible for the formation of the confinement potential in a quantum dot include the external voltage applied to the layered nano structure and properties of contacts having various geometries and connecting the quantum dot with ambience. Quantum mechanical effects play a significant role in the description of the mechanism of quantum dot formation. However, the form of the confinement potential may be strongly affected under certain experimental conditions.

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Temperature Dependence and Temperature Compensation of Kinetics of Circadian Oscillation

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Based on the distribution of activation energies around the experimental mean and averaging of rate constants we propose a theoretical scheme to examine the temperature dependence and temperature compensation of time periods of chemical oscillations. The critical width of the distribution is characteristic of endogeneous oscillations for compensating kinetics as observed in circadian oscillations, while the vanishing width corresponds to Arrhenius temperature dependent kinetics of non-endogeneous chemical oscillation in Belousov-Zhabotinskii reaction in a CSTR or glycolysis in cell-free yeast extracts. Our theoretical analysis is corroborated with experimental data.

Interplay Between Photoinduced Electron Transfer and Energy Transfer in Aza-Crown Ethers of Varying Cavity Dimension

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Photophysical studies involving intramolecular photoinduced electron transfer (PET) in supramolecular systems having F–S–R configuration (where F represents a fluorophore that is linked to the receptor R through a spacer S) are of current interest in many laboratories for their potential use as molecular sensors, molecular switching devices and logic processors as well as to understand the mechanism of PET. At the same time, Photoinduced energy transfer (ET) from donor ligands to acceptor lanthanide ions in lanthanide chelate complexes and in macrocyclic polyether complexes of lanthanides have attracted the interest of researchers due to their importance as model systems to study ion transport phenomena and to understand metal ion induced conformational changes in proteins where the metal ions may be replaced by lanthanide ions. The aza-crown ethers when attached to suitable fluorophores can act as excellent systems to study both PET as well as energy transfer phenomena. The lone pairs on the nitrogen atom of the aza-crown receptor moiety could be involved in PET to the photoexcited fluorophore resulting in quenched emission of the fluorophore. At the same time, the aza-crown ethers can effectively bind alkali metal and rare earth ions in their cavity and under suitable conditions energy transfer between the fluorophores and the rare earth ions may be studied.

We have investigated two derivatives of N-(β -ethylnaphthalene) aza-crown systems having different cavity dimensions (L1 and L2). The aza-crown moiety is attached to β -position of naphthalene moiety by one $>CH_2$ unit in both the derivatives. Both the systems exhibit photoinduced electron transfer (PET) at room temperature resulting in almost switching “off” of the naphthalene emission but causing the appearance of a new solvent sensitive red shifted broad structure less emission which is

assigned to exciplex formation. The efficiency of PET and the formation of exciplex is found to more effective in the system L2 which has a larger cavity dimension suggesting a more favourable 'in line approach' of the donor N atom and the acceptor naphthalene unit in L2 compared to that in L1. In both systems, complexation of alkali metals, rare earth ions and protons by the aza-crown moiety results in switching "on" of fluorescence emission of the naphthalene unit due to blocking of PET.

At low temperature (77K) both the systems exhibit phosphorescence emission from the T1 state of naphthalene. In the complex of the ligands with Eu^{+3} , the phosphorescence emission from the naphthalene units is quenched with simultaneous increase of the Eu^{+3} emission indicating that there is energy transfer from the naphthalene moiety to the Eu^{+3} states.

Stochastic Optimization and DFT based study of Structure and Spectroscopy of Water-Chloride Clusters

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Structures and IR spectral features of $(\text{H}_2\text{O})_n\text{Cl}^-$ clusters have been explored in the size range $n=1-6$. Good quality structures being found out by exploring a suitable empirical potential energy surface and using stochastic optimization technique (Genetic Algorithm) to explore the surface. These structures are then further subjected to quantum chemical DFT calculation to obtain the final structure and IR spectra. Red shifted peaks increases with increase the size of cluster from $n=2-6$.

Keywords: Genetic Algorithm, DFT, IR spectra

Synthesis of Hydrogel from Melamine and Citrazinic Acid: A Supramolecular Platform for Anion Recognition & Iodine Adsorption

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A new two-component hydrogelator has been synthesized from citrazinic acid and melamine following an intimate grinding-mixing protocol (GMP). The powdered mixture upon sonication, for few second, in a suitable solvent/mixed-solvent system finally results in a gel matrix. Different micro-analytical studies (FTIR, Powder XRD, FESEM, TEM, Rheology etc.) have been conducted for complete characterizations of the gel sample. The gel shows entangled network morphology. A thorough and complete solvent dependent gelation investigation suggests that water must be present as the sole solvent or one of the members of other mixed-solvent system to successfully result in gel formation. Citrazinic acid, is decorated with ureidopyrimidone functionality and melamine is enriched with amino-pyridine functionality. Therefore, the necessary non-covalent interactions (like hydrogen bonding and π - π stacking) become a part-and-parcel, bringing a nanofibrous gel material in existence. Again, it is worth mentioning that here GMP plays a key role to strongly initiate and improvise solid state self-assembly. Different non-covalent interactions procure the suitable hydrogen-bonded motif which presumably propagates upon activation in solution phase after mild sonication favouring spontaneous formation of fibrous architectures. It was also noticed that without grinding, the solid state interactions are jeopardized and only partial gel structure prevails. Finally the available porosity in the gel framework and the enriched π -electron density within, make the gel a suitable host for adsorption of guest molecules. We studied the reversible adsorption-desorption equilibrium of molecular iodine within the dried-gel matrix. The guest entrapment into the host occurs both from the solution and also from gas phase iodine. The complete analysis suggests that our material presents a high storage capacity of this halogen species.



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Mapping Out Reaction Paths for Conformational Changes in $(\text{MgO})_n$ Clusters: A Study Based On A Stochastic Procedure

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Clusters can exhibit enormous structural diversities and in most cases with the increase in size, the number of conformers that can be supported by the potential energy surface describing the system also increases at a rapid rate. In the present work, this issue has been addressed from the angle of finding out transformation pathways or the so called reaction paths for interconversion among isomers in $(\text{MgO})_n$ clusters, where 'n' denotes the size. Clusters with ten different values of 'n' starting from 6 and ending at 16 have been studied. For each of these sizes, effort has been made to identify the transition state geometry which connects two minimum configurations. Structural similarities or dissimilarities between the various conformers have been discussed so as to see if any basic units gets repeated with increase in size of the clusters. The entire study has been conducted using the stochastic optimisation principle of simulated annealing and an adequately defined objective function which can uniquely guide the search towards a first order saddle point or the transition state on a potential energy surface.

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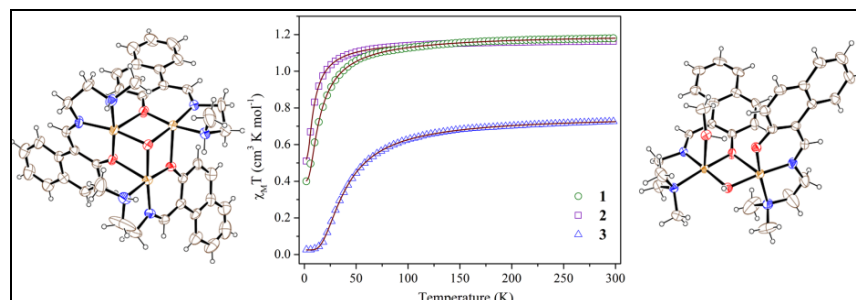
[‡]Electronic Address: pinakc@rediffmail.com (+919830480149)

Role of Steric Crowding of Ligands in the Formation of Hydroxido Bridged Di- and trinuclear Copper(II) Complexes: Structures and Magnetic Properties

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Three new Cu(II) complexes (**1-3**) have been synthesized using naphthaldehyde based N₂O donor Schiff bases and structurally characterized by single crystal X-ray crystallography. Complexes **1** and **2** are discrete trinuclear with [Cu₃O₄] core and complex **3** is discrete dinuclear. We have rationalize these differences taking into account of the role of steric crowding of ligands due to the presence of difference substituent on the N atom of amine group (H, methyl or dimethyl) of diamine. We got trinuclear complexes (**1** and **2**) for less sterically hindered substituents where more sterically demanding substituents (dimethyl) yielded the dinuclear complex **3**. Such rationalization is expected to help in designing the tailored synthesis of the complexes of this ligand with various metal ions. Variable temperature magnetic susceptibility measurements of all complexes in 2-300 K temperature range indicate antiferromagnetic coupling interactions between Cu(II) centres with $J = -8.85 \text{ cm}^{-1}$, -4.86 cm^{-1} and -50.60 cm^{-1} for **1-3** respectively. Density Functional Theory has also been performed in order to estimate the exchange coupling constants in these three complexes. Theoretically calculated J values are in well agreement with the experimental values. While investigating the magneto structural correlation of these type of [Cu₃O₄] cores, all previous attempt was made to explain the exchange coupling constants (J values) on the basis of distances of bridging μ_3 -OH from Cu₃ plane, we have first time correlate exchange coupling interactions (J values) with the Cu-O(H)-Cu bond angles. Magnetostructural correlations of [Cu₃O₄] structured complexes reported in literature, show that the larger Cu-O(H)-Cu bond angles favor larger antiferromagnetic contributions and ferromagnetic coupling is dominated if the angle is less than the critical value of $\sim 103^\circ$. The Cu-O(H)-Cu average bond angle in complexes **1-2** are 105.86° and 103.62° respectively, higher than critical angle (103°) which suggests for a moderate/weak antiferromagnetic interaction.



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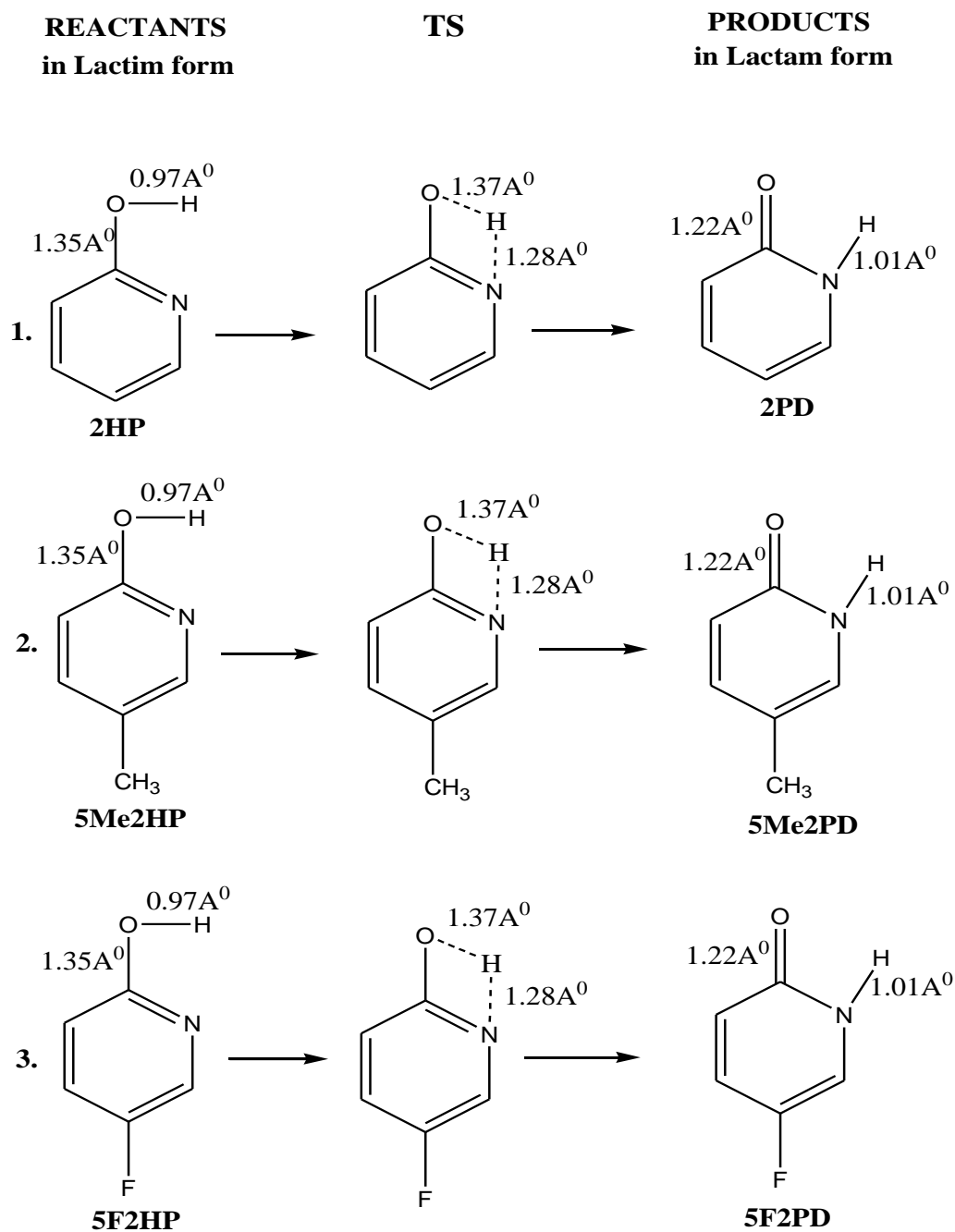
Computation of Global Reactivity Descriptors for Enol–keto Tautomerizations of 2-Hydroxy Pyridines

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The keto-enol tautomeric equilibrium is one of the most important processes in chemical and biological system where proton transfers occurs. It is indeed shown by the nucleic acid bases e.g., cytosine, thymine, uracil and it has been related to the appearance of DNA and RNA mutations induced by proton transfer reactions. One of the model systems of this type of equilibrium in heterocyclic compounds is the pair 2-hydroxypyridine/2-pyridone (2HP/2PD) where a hydrogen atom is transferred between the N and O sites of the molecule.

Density functional theory (DFT) based calculations on a series of intra-molecular proton-transfer reactions e.g. 2-hydroxy pyridine (2HP), 5-Methyl-2-hydroxy pyridine (5Me2HP) and 5-fluoro-2-hydroxy pyridine (5F2HP) are performed to understand the variation of the quantum chemical reactivity parameters along the proton transfer coordinate. Variations in optical gap and first hyper-polarizability which are measures of non-linear optical parameters are also computed. The average polarizability, first hyper-polarizability, chemical hardness, ionization potential and optical gap show their optimum value at the same IRC point which corresponds to the transition state (TS) for all the three titled intra-molecular proton transfer systems. The maximum polarizability and minimum chemical hardness at the transition state (TS) are due to greater extents of charge transfer which arise from smaller optical gap.



Scheme-1: Optimized structure of reactants, transition states (TS) and products for enol→ keto tautomerizations using DFT-B3LYP/6-31G (d) level of theory.

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Functions and Uses of Biodegradable Macromolecule and Macromolecular Composites

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Research and development is only a portion of the work that is done in order to introduce them use of biodegradable polymer materials. The design of such materials usually begins with a conceptual application. Many materials that have been developed and commercialized are applied in more than one of these categories. Biopolymers that may be employed in packaging continue to receive more attention than those designated for any other application. All levels of government, particularly in China and Germany, are endorsing the widespread application of biodegradable packaging materials in order to reduce the volume of inert materials currently being disposed of in landfills, occupying scarce available space. It is estimated that 41% of plastics are used in packaging, and that almost half of that volume is used to package food products. The renewable and biodegradable characteristics of biopolymers are what render them appealing for innovative uses in packaging. The end use of such products varies widely. The starch material is treated by an acetylation process, chemical treatments, and post-extrusion steaming. Mechanical properties of the material are adequate, and true biodegradability is achieved. The biopolymer materials suited for packaging are often used in agricultural products. From an agricultural standpoint, biopolymers which are compostable are important, as they may supplement the current nutrient cycle in the soils where the remnants are added. The medical world is constantly changing, and consequently the materials employed by it also see recurrent adjustments. The biopolymers used in medical applications must be compatible with the tissue they are found in, and may or may not be expected to break down after a given time period. Reported that researchers working in tissue engineering are attempting to develop organs from polymeric materials, which are fit for transplantation into humans. The plastics would require injections with growth factors in order to encourage cell and blood vessel growth in the new organ. Work completed in this area includes the development of biopolymers with adhesion sites that act as cell hosts in giving shapes that mimic different organs.

Analysis of AID-AID Interaction in Living Cells

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Activation-induced cytidine deaminase (AID) is essential to somatic hypermutation (SHM) and class switch recombination (CSR), which are required for antibody gene diversification. AID induces SHM and CSR by initiating antibody gene locus (IgH) specific DNA breaks. The structural properties of AID involved in regulation of CSR, SHM or its cytidine deaminase (CDA) activity in the cell are yet to be explored. Although CDA family of enzymes can be found in nature as monomeric, dimeric or tetrameric forms, it remains to be solved in the case of AID. Since dimerization/oligomerization of AID demonstrated by biochemical assays is controversial, we applied BiFC (Bimolecular Fluorescence Complementation) assay to investigate the interaction of AID in live cells. The fluorescence reconstitution signal unequivocally demonstrates that AID-AID interaction takes place in the cells. The characteristic of AID-AID interaction is also distinguishable from the homomeric interaction patterns of the related APOBEC family members. Utilizing this assay system we analyzed various AID mutants specific to SHM or CSR as well as mutants associated with typeII hyper IgM syndrome. It appears that the C-terminus and the N-terminus of AID as well as the overall structural integrity are crucial for efficient interaction signal generation in living cells.

Role of Induction Period in Determination of Reaction Pathway for a Nano-Catalyzed Reduction of Thiazine Dye

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Palladiumnano-particles (Pdn) catalyze the reduction of the thiazine dye, methylene green (MG) by hydrazine (N_2H_4) in buffer media (pH = 6.0–8.0) at room temperature. The observed rates, k_o increase with increase in [Pdn], [N_2H_4] and pH but decrease with increase in ionic strength of the reaction medium, I . This catalysis reaction proceeds through an initial induction period (t_0 , s) and $1/t_0$ accounts for the rate of surface restructuring process. Observations that $1/t_0$ only depends upon the [N_2H_4] suggest that the active reductant $N_2H_5^+$ is only adsorbed on the Pdn surface before reducing MG through a transient association of the reactants. Moreover the nature of this association changes around the inversion temperature, $T_{inv} \approx 304$ K.

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Supramolecular Hydrogen Bonded Interactions in Mixed-ligand Complexes of Palladium(II) and Platinum(II)

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It seems of interest to continue the synthetic chemistry of substituted pyrazoles. A few examples of mononuclear complexes: $[\text{Pd}(\text{Hpz})_4]\text{Cl}_2$, $[\text{Pd}(\text{dmpz})_2(\text{Hdmpz})_2]$, $[\text{Pt}(\text{pz})_2(\text{Hpz})_2]$, $[\text{Pt}(\text{Hpz})_4]\text{Cl}_2$, binuclear complexes: $[\text{Pd}_2(\mu\text{-dmpz})_2(\text{dmpz})_2(\text{Hdmpz})_2]$, $[\text{Pd}_2(\mu\text{-3-}t\text{Bupz})_2(3\text{-}t\text{Bupz})_2(\text{H}_3\text{-}t\text{Bupz})_2]$, $[\text{Pd}_2((\mu\text{-pz})_2(\text{Hpz})_4)(\text{BF}_4)_2]$ and trinuclear complexes: ($[\{\text{Pd}(\mu\text{-pz})_2\}_3]$, $[\{\text{Pd}(\mu\text{-4-Mepz})_2\}_3]$, $[\{\text{Pt}(\mu\text{-pz})_2\}_3]$) containing only pyrazoles (HRpz) and/or pyrazolates (Rpz) as ligands have been reported till now. Report had been made previously of an unsymmetrical binuclear Pd(II) complex $[(\text{Hdmpz})_2\text{Pd}_2(\mu\text{-dmpz})_2(2,6\text{-dipicolinate})]$ [1] where the terminal Hdmpz ligands bonded to one Pd(II) center act as a hydrogen bond donor and a free-carboxylate group of the 2,6-dipicolinate moiety acts as the hydrogen bond acceptor. The hydrogen bonds of the type N–H---O form a 1D *zigzag* network.

With an aim to construct such hydrogen bonded supramolecular networks, attempts have been made to synthesize mixed-ligand Pd(II) and Pt(II) complexes with another kind of substituted pyrazole 3,5-diphenylpyrazole (Hdppz) and carboxylic acids such as iminodiacetic acid (H_2ida) and 2,6-pyridinedicarboxylic acid (2,6- H_2dipic). The structural features of a dppz bridged binuclear Pd(II) complex $[\text{Pd}_2(\mu\text{-dppz})_2(\text{Hida})_2]\cdot\text{CH}_3\text{OH}\cdot 2\text{H}_2\text{O}$ (**1**) and a mononuclear one $[\text{Pt}(\text{Hdppz})(2,6\text{-dipic})]\cdot\text{CH}_3\text{OH}$ (**2**) are reported herein [2].

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Sequence and molecular analysis of Taxol-binding site of β -tubulin

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Taxol is an important cancer chemotherapeutic agent for treatment of advanced ovarian, lung and breast carcinoma. But clinical resistance against paclitaxel becomes an increasingly significant problem. It is known that increased expression of β_{III} tubulin isotypes inhibits cell proliferation and confers resistance to paclitaxel. Similarly, tubulin from *Saccharomyces cerevisiae* also shows weak binding affinity for paclitaxel. The aim of the work was to understand these two apparently unconnected experimental data in the light of paclitaxel bound tubulin structure and sequence variations among a large collection of β -tubulin. To assess the contribution from the tail region, we performed paclitaxel induced polymerization assay with C-termini depleted tubulin and thereby judge that C-termini have no found effect on paclitaxel-induced polymerization. We have considered 74 eukaryotic β -tubulin sequences. Multiple sequence alignments were performed using the program ClustalW to identify the PBS residues in different sequences. Subsequently, principal component analysis was performed in the multi-dimensional sequence-space. We have identified two major axes (PC). Structural consequences along PC axes have been identified that are associated with residue changes. It also clearly shows how evolution brings about correlated changes at the PBS. Here we focus on deciphering the mechanisms, specifically identifying residues and their interactions, responsible for paclitaxel resistance of yeast tubulin and the β_{III} tubulin. The molecular mechanisms behind paclitaxel-resistance, mediated through key residues, were identified from structural consequences of characteristic mutations that confer paclitaxel-resistance. Specifically, Ala 277 in β_{III} isotype was shown to be crucial for paclitaxel-resistance. The present analysis captures the origin of two apparently unrelated events through two common collective sequence vectors.

Methanol-triggered Vapochromism of a Ni(II)-quinonoid Complex with Solid-state Spin Switching

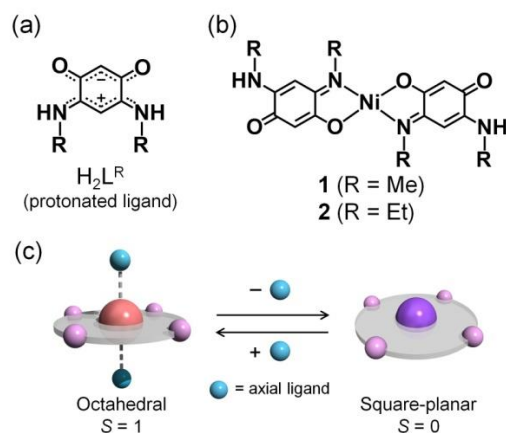
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Highly methanol-selective vapochromic response has been brought out by a Ni(II)-quinonoid complex, which exhibits an reversible structural transformation between square-planar and octahedral geometry followed by remarkable color change as well as the coordination induced spin-state switching (CISSS) in solid-state at ambient conditions. Such system has high potential for applications in molecular spintronics as well as chemical sensor i.e. smart responsive material.



Scheme 1. Structures of (a) H_2LR and (b) Ni(II) complexes **1** and **2**. (c) A schematic illustration of coordination-induced spin-state switching of Ni(II).

An Adaptive Mutation Simulated Annealing Based Investigation of Coulombic Explosion and Identification of Dissociation Patterns in $(\text{CO}_2)_n^{2+}$ Clusters

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We have shown the advantages of Adaptive Mutation Simulated Annealing (AMSA) over conventional Simulated Annealing (SA) in studying the Coulombic explosion of $(\text{CO}_2)_n^{2+}$ clusters for $n = 20 - 68$, where 'n' is the cluster size. We have demonstrated how AMSA itself can overcome the predicaments which can arise in conventional SA and carry out the search for better results by adapting the parameters dynamically during the simulations so that the search process can come out of high energy basins and not go astray. This technique also has in-built properties for getting more than one minimum in a single run. For a $(\text{CO}_2)_n^{2+}$ cluster system we have found the critical limit to be $n_c = 43$, above which the attractive forces between individual units become greater in value than that of the large repulsive forces and the clusters stay intact as the energetically favoured isomers. This result is in good concurrence with earlier studies. Moreover, we have studied the fragmentation patterns for the entire size range and we have found fission type fragmentation as the favoured mechanism nearly for all sizes.

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Predicting Stability Limits for Pure and Doped Dicationic Noble Gas Clusters Undergoing Coulomb Explosion: A Parallel Tempering Based Study

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We have used a replica exchange Monte-Carlo procedure, popularly known as Parallel Tempering, to study the problem of Coulomb explosion in homogeneous Ar and Xe dicationic clusters as well as mixed Ar–Xe dicationic clusters of varying sizes with different degrees of relative composition. All the clusters studied have two units of positive charges. The simulations reveal that in all the cases there is a cutoff size below which the clusters fragment. It is seen that for the case of pure Ar, the value is around 95 while that for Xe it is 55. For the mixed clusters with increasing Xe content, the cutoff limit for suppression of Coulomb explosion gradually decreases from 95 for a pure Ar to 55 for a pure Xe cluster. The hallmark of this study is this smooth progression. All the clusters are simulated using the reliable potential energy surface developed by Gay and Berne (Gay and Berne, *Phys. Rev. Lett.* 1982, 49, 194). For the hetero clusters, we have also discussed two different ways of charge distribution, that is one in which both positive charges are on two Xe atoms and the other where the two charges are at a Xe atom and at an Ar atom. The fragmentation patterns observed by us are such that single ionic ejections are the favored dissociating pattern.

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1. S. Ghorai, P. Chaudhury, *J. Comput. Chem.* 2017, DOI: 10.1002/jcc.25156

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Synthesis, Characterization and Antimicrobial Study of Some Lanthanide-crown ether Complexes by IR and ¹H-NMR

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The crown ethers are excellent hosts for accommodating metal ions via ion-dipole interaction. A large number of lanthanide-crown ether complexes have been studied by single-crystal X-ray diffraction methods. Crown ethers have a lower coordination power towards lanthanides but they have selectivity to the best-fit metal ions.¹ The present paper describes preparation, characterization and antibacterial study of some new lanthanide-crown ether complexes with 1,4,7,10,13,16,-hexaoxacyclooctadecane (18C6) and 2,3,11,12-dibenzo-1,4,7,10,13,16,-hexaoxacyclooctadeca-2,11-diene (db18C6) having general formula of [Ln.L.(Pic)₃].nH₂O, where Ln³⁺ = Pr³⁺/Nd³⁺, L = 18C6/db18C6 and Pic = Picrate anion. The crown ethers display ν(-CH₂-) stretching vibrations at 2922±10 cm⁻¹ and these are little affected on bonding with lanthanide ions. The crown ethers in uncoordinated state display ν(C-O-C) stretching vibration band near 1115±10 cm⁻¹. This ν(C-O-C) vibration band shifted to lower frequency by 14-60 cm⁻¹ in almost all complexes suggesting involvement of crown ether oxygen in bond formation with lanthanide ion. Some complexes are hygroscopic in nature and thus their IR spectrum displays a broad band of water molecules around 3345-3420 cm⁻¹, with maxima near 3405±10 cm⁻¹. In the far-IR region new bands are found in the 425-580 cm⁻¹ region, which may be assigned to the ν(Ln-O_{crown}) stretching frequency.²

Small but noticeable changes were observed in the chemical shift of 1-H in 18C6 and, 1-H as well as 2-H, in dibenzo18C6. After formation of the [Ln.L.(Pic)₃].nH₂O complex. The proton chemical shift δ(-CH₂-O-) shows significant downfield shifts [Δδ(-CH₂-O-)=0.08-0.20 ppm], indicating metal-ligand bond formation. The degree of downfield shift shows the relative strength of the complexes. The ¹H-NMR spectrum of db18C6 shows peaks at, δ₁=3.9-4.1 ppm, (16H, 8 -CH₂O-), δ₂=6.8-7.0 ppm, (8H, aryl -CH-), in CDCl₃. Possible reasons for this downfield shift are the conformational change in the macrocyclic skeleton during complexation which could affect the electron density on the hydrogens through the Fermi Contact term.³ The shift of -CH₂- signals in complexes from free crown ether unambiguously suggests the coordination of crown ethers with lanthanide ion. The bonding pattern and structure of complexes were suggested from elemental analysis, molar conductivity, IR, UV-Vis and ¹H-NMR spectral analysis.

Antibacterial and antifungal activities of the ligand and its complexes were carried out against Staphylococcus aureus, Pseudomonas aeruginosa, Bacillus subtilis, Escherichia coli bacteria and Aspergillus niger, Candida albicans fungi by ditch plate method. 10-15 ml nutrient agar and sabouraud's dextrose agar is used as medium for antibacterial and antifungal activities respectively. The antimicrobial activity was estimated on the basis of size inhibition zone.

(Key Words : 18C6, DB18C6, TNPH)

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Mechanistic Studies on the Anti-oxidant Activities of Mercaptan Compounds

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In acid-media ($[H^+] = 0.01\text{--}0.06\text{ M}$), two of the mercaptan compounds, D-penicillamine (PEN, $L_P H_2$) and captopril (CAP, $L_C H_2$) exist in several proton-dependent forms which can reduce the superoxo complex, $[(en)(dien)Co^{III}(O_2)Co^{III}(en)(dien)]^{5+}$ (**1**) to the corresponding peroxo $[(en)(dien)Co^{III}(O_2)Co^{III}(en)(dien)]^{4+}$ (**2**) complex. The observed first-order rate constants, $k_{o,P}$ and $k_{o,C}$ for PEN and CAP increase with the increase in $[T_{PEN}]$ and $[T_{CAP}]$ (which are the analytical concentrations of the respective compounds) but decrease with increase in the media-acidity ($[H^+]$) and the media ionic strength (I). The protolytic equilibria in aqueous solution allow several potentially reducing forms to coexist for both PEN ($L_P H_3^+$, $L_P H_2$, $L_P H^-$ and L_P^{2-}) and CAP ($L_C H_2$, $L_C H^-$, L_C^{2-}) but the kinetic analyses reveal that the order of reactivity for the species are $L_P H_3^+ \sim L_P H_2 \lll L_P H^-$ and $L_C H_2 < L_C H^- \lll L_C^{2-}$ respectively. The predominance and higher reactivities of the anionic species, $L_P H^-$ and L_C^{2-} are supported by the negative slopes of the plots of $k_{o,P}$ or $k_{o,C}$ vs. I . Moreover, a large value of k_H/k_D for PEN suggests an inner-sphere electroprotic reaction pathway while the absence of such effect for CAP strongly supports an outer-sphere electron transfer reaction.

Reference:

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Effect of pollutant on Biodiversity

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In this study, we show that how biodiversity affected by chemical pollutants. Society has benefited tremendously from chemical use. Chemical pollution introduces chemicals into the natural environment, negatively affecting the air, water and soil. The class of chemical pollutants called greenhouse gases may contribute to global warming. Greenhouse gases released as a result of human activities include carbon dioxide, methane, nitrous oxide and fluorinated gases. Methane and nitrous oxide are released mostly through agricultural activities. Impacts on biological diversity must be accounted for when tallying the costs and benefits of chemical use in society.

Keywords: Chemical pollutant, biodiversity, global warming, greenhouse gas

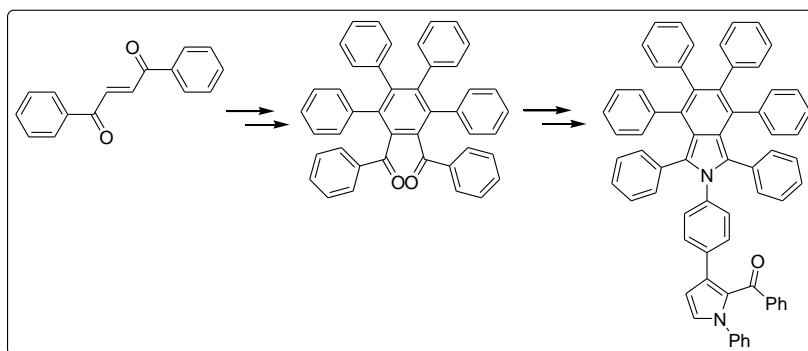
Copper Catalyzed Synthesis of Pyrrole Derivative: Used as Organic Light-Emitting Diode

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Electroluminescent (EL) devices based on organic small molecules and conjugated polymers are a new and exciting form of emissive display technology which holds great potential for flat-panel display applications.¹ Among numerous heterocycles, the pyrrole moiety has always been one of the most prominent since it is found in natural products² and electrically conducting materials such as polypyrroles.³ Previously we have developed an efficient synthesis of pyrrole derivative using copper (I) catalyst.⁴ Using this methodology here we are trying to synthesize a new compound which is a highly phenylated isoindole with good thermal and chemical stabilities.⁵ Its bulky structure leads to good film-forming properties of the compound via thermal evaporation. Aside from the high hole mobility, the compound possesses other important attributes required for a good hole transporting host material for applications in organic electroluminescence. In the present work, we report the development of a new HTM with better thermal stability based on a highly phenylated isoindole.



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Synthesis of Imidazolidine Spacer Based Multidentate Ligands and Its Hydrolysis During Complexation: Role of Azide Binding

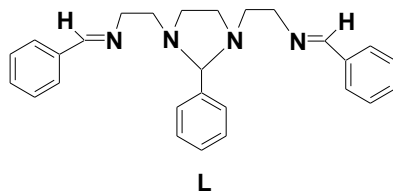
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Among various products from the condensation of aromatic aldehydes with both primary and secondary amino groups is a binucleating Schiff base ligand with spacer imidazolidine rings. Schiff base reactions in 3:1 mole ratio between aldehydes and triethylenetetramine (trien) yield tetraaza μ - bis(bidentate/tetradentate) acyclic ligands L and $H_3L_1^x$ (subscript I for imidazolidine; $x = 1,2$). Reaction of $H_3L_1^x$ with cobalt salts give mononuclear complexes $[Co^{III}L_1]Cl \cdot 2H_2O$ and $[Co^{III}L_2]ClO_4 \cdot H_2O$ of hydrolyzed ligands H_2L^x .



Expected dicobalt complexes were not obtained due to the coordination induced hydrolytic cleavage of backbone imidazolidine rings. Both *mer*- and *fac*- ON_2 binding modes of the two halves of the hexadentate ligands have been identified. Both the ligands initially bind two Co^{2+} centers in solution and coordination driven imidazolidine ring hydrolysis takes place with increase in coordinated nitrogen atom basicity. Imidazolidine nitrogen donors present in binucleating ligands are soft bases compared to the secondary amine nitrogens in hexadentate ligands.

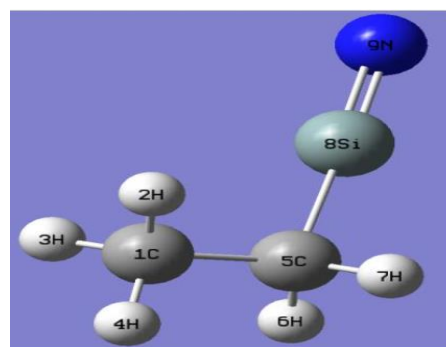
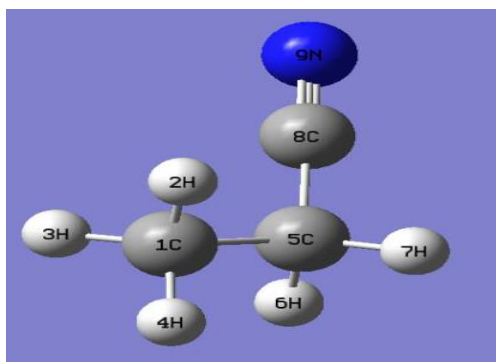
Density functional and ab initio study of Ethylsilanitrile and Propanenitrile

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During last two decade, there have been rapid developments in the field of silicon chemistry from both experimental and theoretical points of view. Herbst *et al.* investigated the gas phase chemistry of silicon in dense interstellar clouds using a pseudo-time-dependent model. The fractional abundances of silicon bearing neutral molecules with respect to H₂ have been predicted. The detection of SiH₄, SiN and CH₃ interstellar medium and subsequent detection of CH₃CN, CH₂CHCN, CH₃CH₂CN and HC₄CN indicate there is a possibility that these molecules react with each other to form CH₃SiN and SiH₃SiN and their isomers. Bhaskar et al. studied the optimized structure, relative energies, dissociation energies and thermochemistry of CH₃SiN and SiH₃SiN molecules. This is corroborated with the pseudo-time-dependent model of Herbst *et al.* where various Si- containing molecules have been formed by reactions. In this work we have studied the optimized structure, relative energies of CH₃CH₂SiN and its isomer and the dissociation channel of CH₃CH₂NSi. The optimized structure, relative energies of CH₃CH₂CN and its isomer and the dissociation channel of CH₃CH₂CN have also been studied in B3LYP, B3PW91, MP2 and QCISD methods. In dissociation channels the fragmented atoms and molecules are in their ground state.



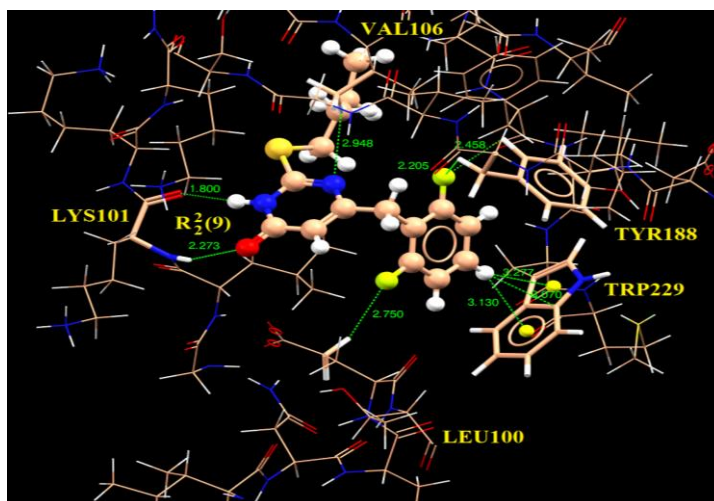
Study of HIV-1 Reverse Transcriptase Non-Nucleoside Inhibitors Activity of a Series of DABO Derivatives through 3D-QSAR and Docking Studies

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In the present study, we have explored the utility of a set of dabo molecules for their anti-HIV activity. 3D QSAR (CoMFA & CoMSIA) and docking analysis have been carried out for the chosen set of molecules. CoMFA analysis reveals that electrostatic field is more important than the steric field in case of anti HIV activity of dabo molecules. CoMSIA analysis also indicates the same trend like the CoMFA analysis. A docking analysis has been performed which show that hydrogen bonding as well as π -stacking interactions are important for binding of the molecules with the HIV protein 1RT1. The docking analysis reveal that the core moiety of the dabo molecules have a nice donor acceptor complementary for binding the Lysine residue through a cyclic hydrogen bonding motif.



N-Arylation of Tertiary Amines under Mild Conditions

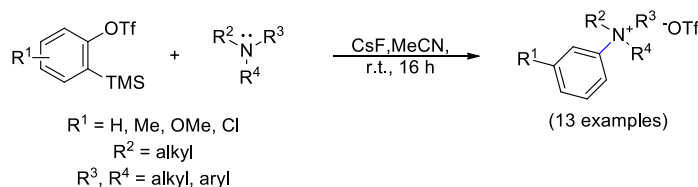
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Abstract: Quaternary ammonium salts are important industrial chemicals that are used as antimicrobials,¹ surfactants,² antistatic agents,³ and more. In addition, these onium salts play a significant role as phase-transfer catalysts⁴ and in anion-exchange membranes,⁵ and constitute biologically relevant functional groups, playing essential roles in alkylation reactions⁶ and in natural products.⁷ A transition-metal-free procedure for the *N*-arylation of tertiary amines to sp³ quaternary ammonium salts has been described. The presented conditions allow for the isolation of trialkylaryl, dialkyldiaryl, and novel triarylalkyl ammonium salts, including *N*-chiral quaternary ammonium salts. The reaction works at room temperature, open to air with electron rich or -poor benzyne precursors and different tertiary amines, allowing the synthesis of a broad range of *N*-aryl ammonium salts that have applications in a variety of fields.



Key Words: Tertiary amine, benzyne, *N*-arylation, quaternary ammonium salt.

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