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Phone : (033) 26610332
FAX : 033 26610240
Website : www.uluberiacollege.org
e-mail : uluberia_college@rediffmail.com
ULUBERIA, HOWRAH - 711315

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Criteria 3- Research, Innovations and Extension

Key Indicator 3.2- Innovation Ecosystem

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Report on publication of e-journals by departments

Debasish Pal
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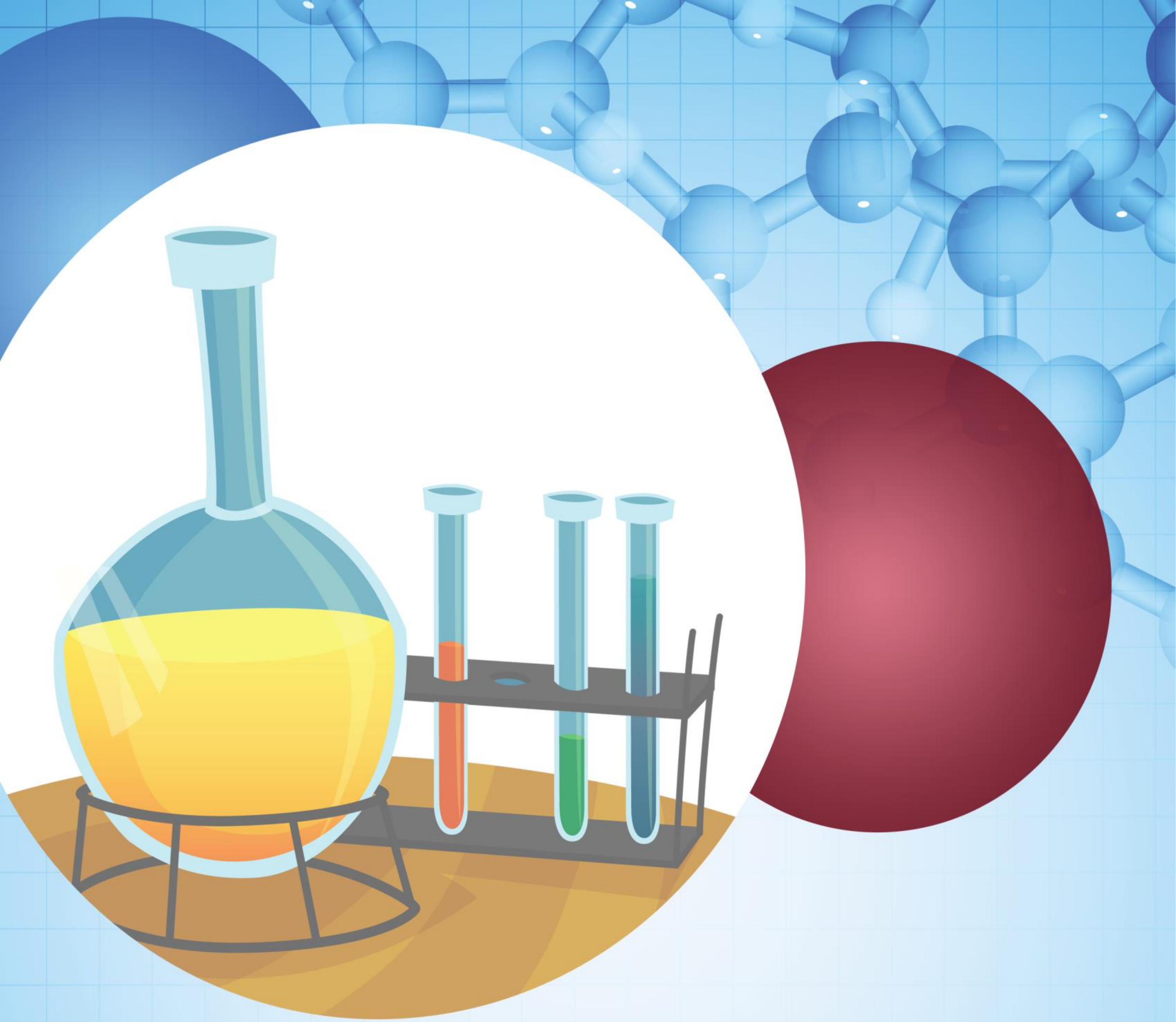

CHEMISTRY OUTLOOK

2023

EDITION

ULUBERIA COLLEGE
DEPARTMENT OF CHEMISTRY

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CONTENT

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Carbonic Anhydrase

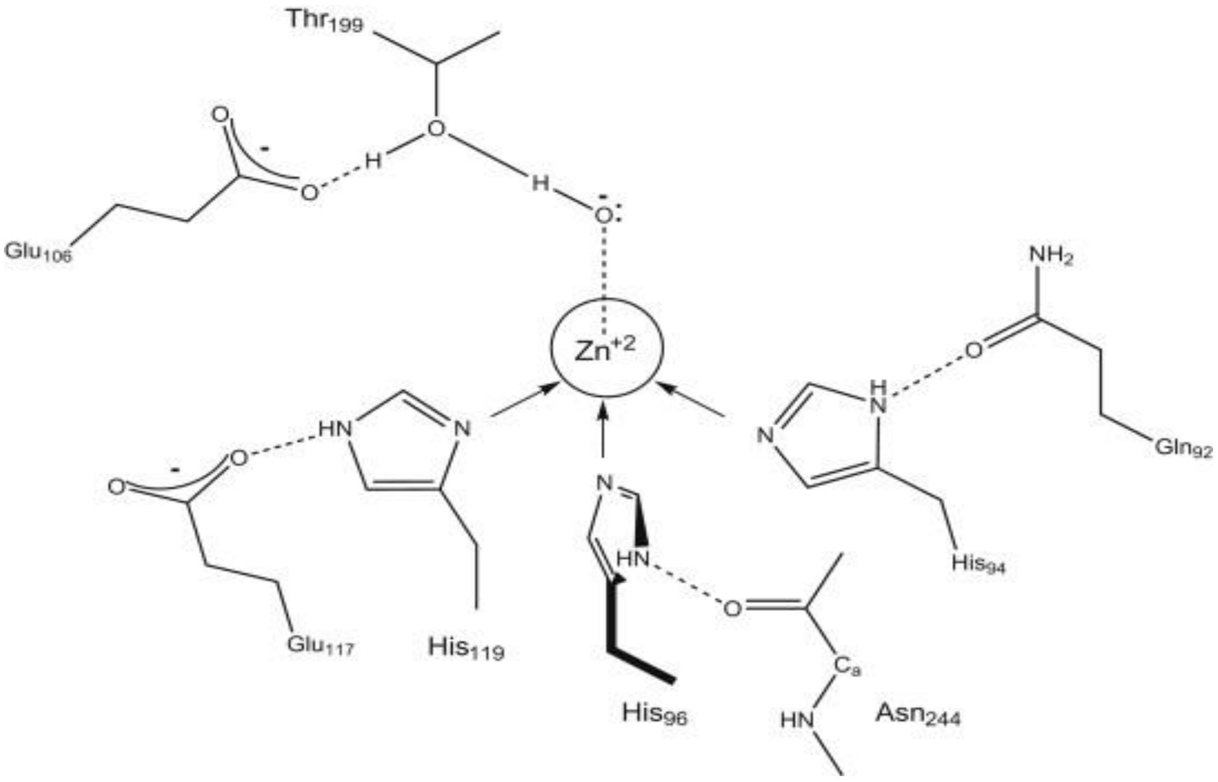
Tanushree Das

Sem-6, Department of Chemistry, Uluberia College.

Carbonic anhydrase, enzyme found in red blood cells, gastric mucosa, pancreatic cells, and renal tubules that catalyzes the interconversion of carbon dioxide (CO_2) and carbonic acid (H_2CO_3). Carbonic anhydrase plays an important role in respiration by influencing CO_2 transport in the blood. The enzyme also functions in the formation of hydrochloric acid by the stomach.

STRUCTURE

There are three evolutionarily unrelated CA families, designated alpha, beta, and gamma. All known CAs from the animal kingdom are of the alpha type. There are seven mammalian CA isozymes with different tissue distributions and intracellular locations,



MECHANISM OF SYNTHESIS

The **carbonic anhydrases** (or **carbonate dehydratases**) form a family of enzymes that catalyze the interconversion between carbon dioxide and water and the dissociated ions of carbonic acid (i.e. bicarbonate and hydrogen ions). The active site of most carbonic anhydrases contains a zinc ion. They are therefore classified as metalloenzymes. The enzyme maintains acid-base

The Bohr effect is a way to describe hemoglobin's oxygen binding affinity. The Bohr effect, described by Christian Bohr in 1904, refers to a shift in an oxygen dissociation curve that is caused by a change in concentration of carbon dioxide or a change in the pH. Essentially an increase in carbon dioxide results in lowered blood pH, which lowers oxygen-hemoglobin binding. The opposite is true where a decrease in the concentration of carbon dioxide raises the blood pH which raises the rate of oxygen-hemoglobin binding. Relating the Bohr effect to carbonic anhydrase is simple: carbonic anhydrase speeds up the reaction of carbon dioxide reacting with water to produce hydrogen ions (protons) and bicarbonate ions.

CARBONIC ANHYDRASE INHIBITORS

Acetazolamide, dichlorphenamide, and methazolamide are carbonic anhydrase inhibitors

Physiological Roles

Carbonic anhydrases (CAs, EC 4.2.1.1) are a family of metalloenzymes that catalyze the reversible hydration/dehydration of carbon dioxide/bicarbonate ion1,2. CAs are found in both prokaryotes and eukaryotes, and are involved in many physiological processes such as respiration, bone resorption, calcification and photosynthesis

1. ROLE OF CARBONIC ANHYDRASE IN EYE

Carbonic anhydrase plays an important role in The eye, where it is present in the lens, vitreous Body, cornea, and retina.

2. NERVOUS SYSTEM

In the nervous system, carbonic anhydrase serves many functions. In the choroid plexus, it Contributes to the production of cerebrospinal fluid. In the brain, it is found in oligodendrocytes and glial cells .

3. CO2 TRANSPORT IN BLOOD AND MUSCLES

4. VAS DEFERENS AND EPIDIDYMIS ACIDIFICATION

5. KIDNEY

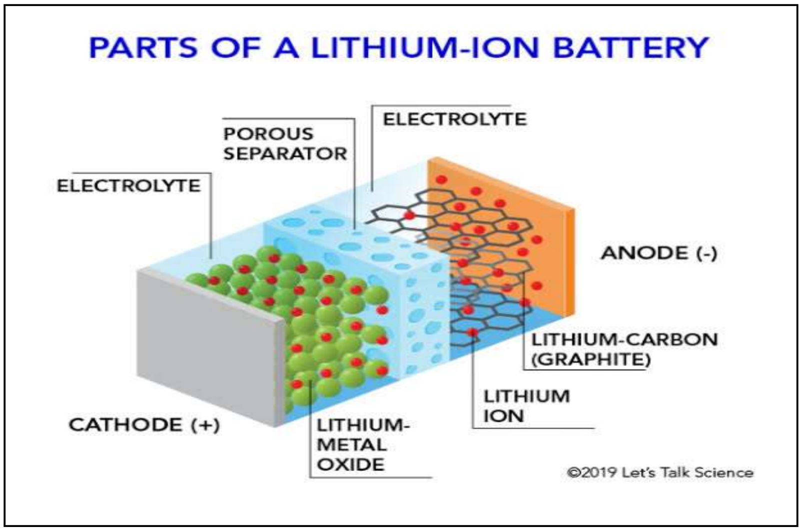
Carbonic anhydrase is expressed in most segments of the kidney. CAII and CAIV are predominate in human and rabbit kidneys, CAXII, and CAXIV are also present.

Lithium-ion Battery: The present and future prospects

Akash Hazra
6th sem , uluberia college

Lithium-ion batteries (LIBs) have been widely used in portable electronics, electric vehicles and grid storage due to their high energy density, high power density, and long cycle life. Since Whittingham discovered the intercalation electrodes in the 1970s, Goodenough et al. developed some key cathode materials (layered, spinel, and poly anion) in the 1980s and the 1990s, and Yoshino created the first safe, production-viable LIB with the combination of $LiCoO_2$ as the cathode and carbon /graphite as anode. In 2012 John Goodenough Goodenough ,Rachid Yazami and Akira Yoshino received the 2012 IEEE Medal for environment and safety technology for developing the lithium-ion batteries.Goodenough,Whittingham and Yoshino were awarded the 2019 Nobel Prize in Chemistry "**for the development of lithium-ion batteries".** Much progress in LIBs has been made in terms of cost, energy density, power density, safety, and cycle life. For example, the cost of LIBs has dropped from over $1,000/kWh in the early 2000 to $200/kWh currently. At the same time, the specific energy density of LIBs has been increased from 150 Wh/kg to 300 Wh/kg in the past decades . Although beyond LIBs, solid-state batteries (SSBs), sodium-ion batteries, lithium-sulfur batteries , lithium air batteries , and multivalent batteries have been proposed and developed . LIBs will most likely still dominate the market at least for the next 10 years . Currently , most research studies on LIBs have been focused on diverse, active electrode materials and suitable electrolytes for high cutoff voltage applications, especially the nickel-rich and/or cobalt-free cathode materials and Si or Li metal anode materials and their associated electrolytes. Progress in LIB manufacturing lags behind and not much progress have been made, although manufacturing contributes about 25% of the cost of LIBs. Currently, the manufacturing of LIBs still needs to go through the slurry mixing ,coating , drying, calendaring, slitting, vacuum drying, jelly roll fabrication (stacking for pouch cells and winding for cylindrical and prismatic cells),welding, packaging electrolyte filling, formation , and ageing , a multi-staged process being adopted by industry. Lithium-ion batteries (LIBs) have been widely used in portable electronics, electric vehicles, and grid storage due to their high energy density, high power density, and long cycle life.

Lithium is an unstable element that's why we use it with oxygen in our cathode. Lithium oxide (Lio2) is used as cathode . Anode can be of graphite or carbon, which is coated by active material, conductive additive and a binder. Graphite is of stable structure and less reactive which helps in storing lithium ions, without getting reacted with it. Lithium hexafluorophosphate can be used as salt because of its temperature range and conductivity . Vinylene carbonate and cyclic sulphate can be used as additives in lithium ion batteries.



During discharging (uses) of battery, positively charged Lithium ions (Li+) move from negative anode to positive cathode. They do this by electrolyte until they reached the positive electrode. There, they are deposited. The electrons, on the other hand moves from the anode to cathode. During charging of battery lithium ions are stored in anode, which are released from the cathode. At the discharge state when conduction wire connects the cathode, lithium ions flow back to the cathode through the electrolyte. Movement of lithium ions generate a flow of electrons from one side to another. Electrons separated from lithium ions starts moving and generate electricity . The following equations exemplify the chemistry.

The positive electrode (cathode) half reaction with the lithium-doped cobalt oxide substrate is

$$CoO_2 + Li^+ + e^- \rightleftharpoons LiCoO_2$$

The negative electrode (anode) half reaction for the graphite is

$$\mathrm{LiC6} \rightleftharpoons C_6 + Li^+ + e^-$$

The full reaction (left to right: discharging, right to left: charging) being

$$\mathrm{LiC6} + CoO_2 \rightleftharpoons Li_2O + CoO$$

Lithium ion batteries have been undergoing rapid development in the global market due to its superior performance. However, the soaring number of lithium ion batteries in the market presents serious disposal challenges at the end of the life. Moreover, continuous mining process is harmful for environment and also mining process are very costly. As the area of further research in the field of recycling of waste lithium - ion battery, could be used as follows:

- shorten battery recycling process while retaining a high percentage purity of sorted materials.
- Introduction of more automated and software controlled pretreatment process of recycling lithium - ion battery

Debasish Pal

Molecular Docking: A theoretical approach to predict the druggability of a molecule

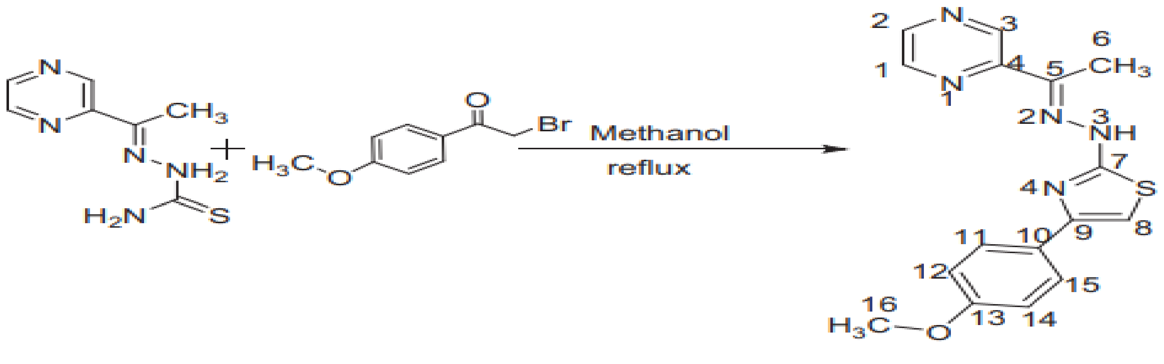
Subhadip Adhya,Uluberia College,Semester:6

Introduction: Molecular docking is a technique that helps to study and explains the properties of biomolecules.There are several stages in the docking process. Docking methods are used to place small molecules in the active site of the enzyme. Molecular docking is considered the most widely used computational method in the field of computer-aided drug design (CADD). The docking method uses a computer model to visualize the binding mode and the interaction between the complex and the DNA to design the drug. The advancement of docking study will open a new avenue in the field of the interface of research in chemistry and biology.

Docking is a method that predicts the preferred orientation of one molecule relative to another when the ligand and target are bound together to form a stable complex.The protein-ligand docking procedure can be typically divided into two parts**. (1) Rigid body docking 2) Flexible docking.**

Model of Molecular Docking: There are three Important models such as lock and key theory, induced fit theory and ensemble model.

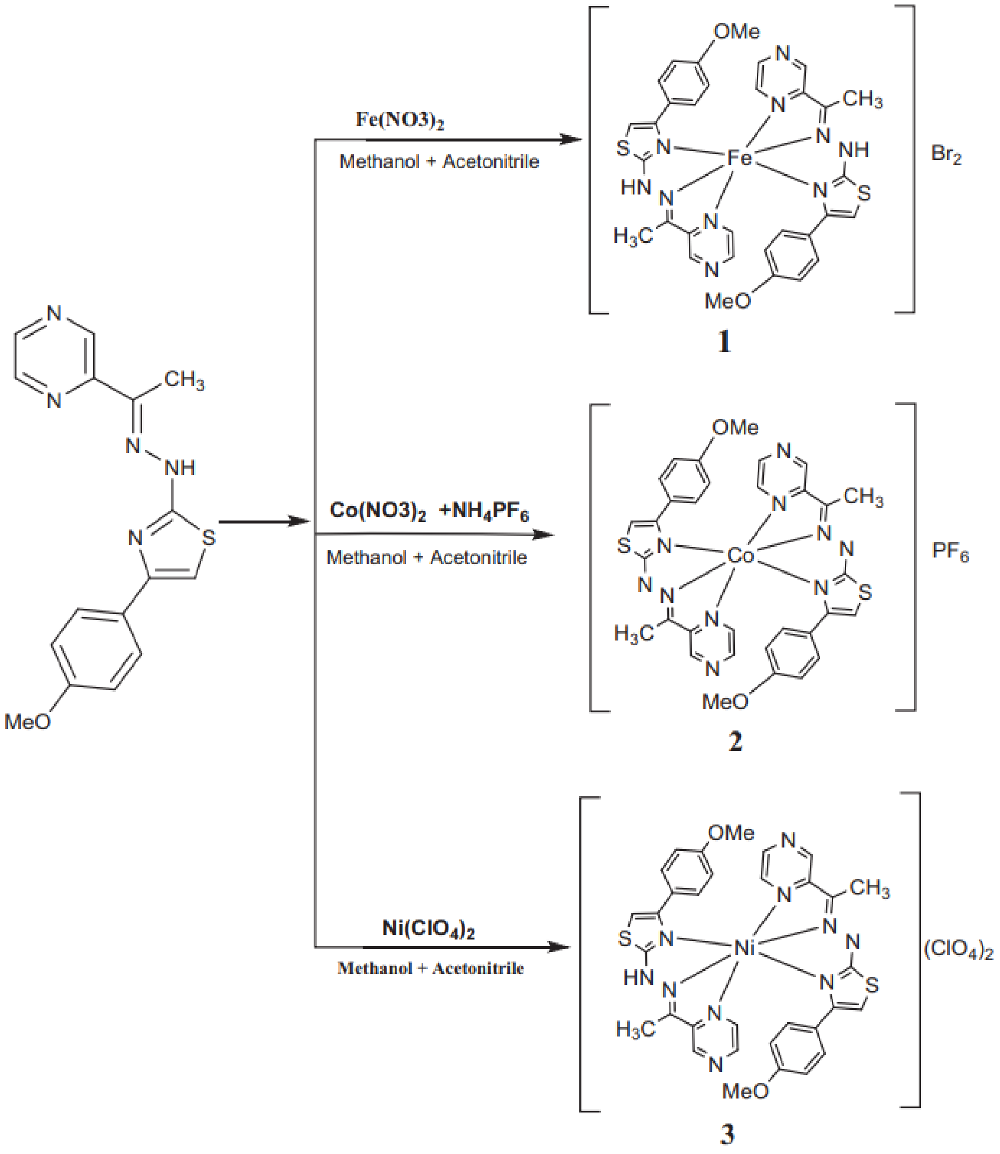
Experiment: The ligand (Pyzth) was synthesized by the following method.



L=PyztH

In brief the present ligand (PyztH) was prepared by the condensation of 2-bromo-1-(4-methoxyphenyl)ethen-1-one and 2-(1-(pyrazine-2-yl)ethylidene)hydrazine-1-carbothioamide. An anhydrous methanolic solution of 2-bromo-1-(4-methoxyphenyl)ethen-1- one (10 mmol) was added dropwise to a methanolic solution (20 mL) of 2-(1-(pyrazine-2-yl)ethylidene)hydrazine carbothioamide (10 mmol, 1.942 g) with constant stirring at RT. After the complete addition, the reaction mixture was refluxed in a water bath for three hours. An orange yellow precipitate was obtained, which was filtered off and washed 2 to 3 times with aqueous methanol. The crude product was recrystallized with a methanol and acetonitrile mixture. A light orange transparent micro-crystalline product was obtained by diffusion of methanol into the mixture.

The newly synthesized ligand 4-(4-methoxyphenyl)-2-(2-(1-(pyrazine2yl) ethylidene) hydrazinyl) thiazole (PyztH) and it’sFe (II) (**1**), Co (II)(**2**) and Ni (II) (**3**) complexes are discussed.



Conclusion: Molecular docking study shows significant interaction with DNA base pair. Finally, this study helps to design new compounds with pyrazine-thiazole framework as anticancer and antimicrobial agents for future therapy**.** Molecular docking is an inexpensive, safe and easy-to-use technology that helps study, interpret, explain and find molecular features using three-dimensional structures.

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CHEMICAL FOOD CONTAMINANTS: SOURCES AND DETECTION

Name: **Tuhina Mondal**
Semester: **6**
College: **Uluberia College**

With the development in international food trade, there have been emerging risks in the food chain. Food contamination can be caused by several factors in a complex food chain. This article provides a comprehensive review of known chemical contaminants from the production of raw materials to the consumption of food products as well as sources and detection measures. Chemical contaminants can cause acute or chronic human health effects from direct contact. Chemical food contamination examples - Inorganic contaminants such as heavy metal contamination (e.g., mercury, lead, cadmium, and arsenic), Intentionally present preservatives to improve shelf life or food quality (e.g., Lead Chromate, saccharine, Metanil Yellow etc.),Industrial chemicals (e.g., Pesticides, dry soil enhancers, herbicides, and fertilizers) . Apples, corn, oranges, rice, and wheat are among the agricultural commodities consumed in large amounts by children.

Fig: Organophosphate Spray in agricultural field

Food packaging processes can introduce toxic contaminants in food, thus causing public health problems. In some cases, individuals or a group of people deliberately contaminate food production as a form of terrorism or sabotage. This intentional adulteration can lead to wide-ranging health problems and issues for your food business. Examples: Lead Chromate, Metanil yellow etc.

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Now we can detect of chemical contaminants in food by simple experiments in our laboratory. One of them is detection of added starch and cereal flours safety precautions.Take about 3 ml of well mixed milk in a test tube. Boil the milk over a burner.Cool to room temperature (25±2°C) Add 2-3 drops of 1% iodine solution .Appearance of blue or bluish black color which disappears on boiling indicates the milk is adulterated with either starch or cereal flours.

The chemistry behind this color change due to charge transfer. The colors are caused by so-called charge transfer (CT) complexes. Molecular iodine (I_2) is not easily soluble in water, which is why potassium iodide is added. Together, they form polyiodide ions of the type I_n^-, for example, I_3^-, I_5^-, or I_7^-. The negatively charged iodide in these compounds acts as charge donor, the neutral iodine as a charge acceptor. Electrons in such charge-transfer complexes are easy to excite to a higher energy level by light. The light is absorbed in the process and its complementary color is observed by the human eye.In the case of the aqueous solution of polyiodides, the absorptions of the different species lead to an overall brownish color. Once amylose is added, it forms another CT complex, Here, the amylose acts as a charge donor and the polyiodide as an acceptor. This complex absorbs light of a different wavelength than polyiodide, and the color turns dark blue.

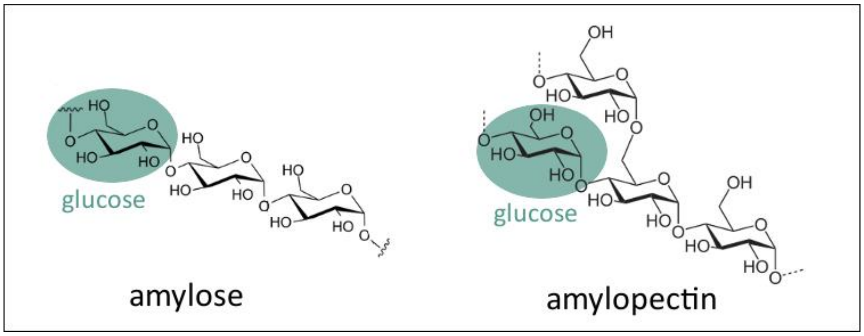

Fig:Amylose and Amylopectin

The chemical contamination of food has emerged as a serious concern with potential health hazards in their wake. As the technology advances, the detection of such contaminants becomes easier. However, there are several contaminants that are still unknown and research continues in this regard.

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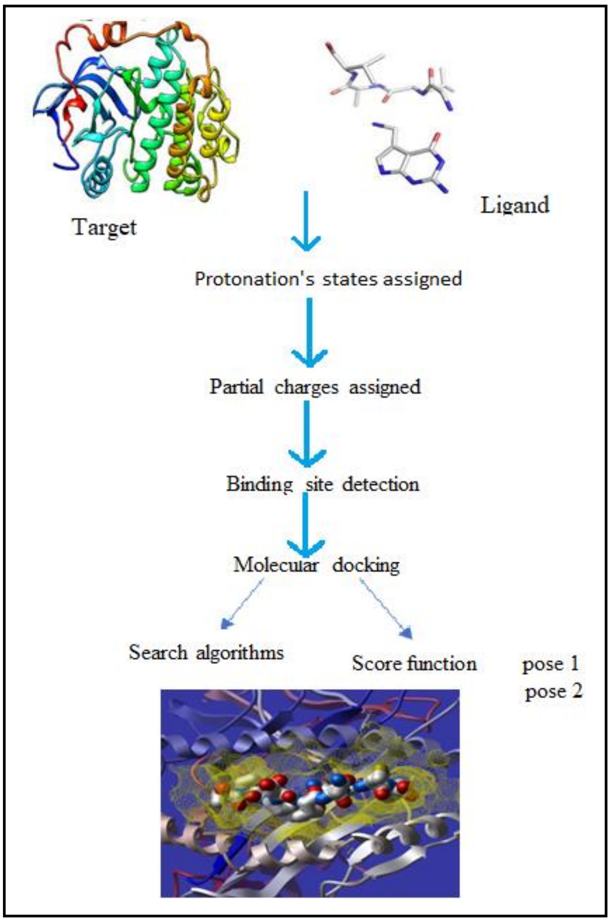
Molecular docking-A handful technique for drug discovery:

Soumya Saha

Uluberia College, 6th sem

Now-a-days molecular docking is performed to know the interactions of a drug molecule with protein/DNA or protein-protein. Molecular docking is held by the computational technical tool. Through this technique, one concept is understood, and that is how the target and the ligand interact with each other. The theoretical approach is a very powerful tool to discover many drugs. Nowadays molecular docking helps interdisciplinary research in science and technology. In this review, we present an overview of the method and attempt to summarise recent developments regarding four main aspects of molecular docking approaches: (i) the available benchmarking sets, highlighting their advantages and caveats, (ii) the advances in consensus methods, (iii) recent algorithms and applications using fragment-based approaches, and (iv) the use of machine learning algorithms in molecular docking. And a case study of docking of a newly synthesized compound is discussed to shed light the possible interactions between the molecule and DNA.

Molecular docking is a method that analyses the poses (conformations and orientations) of molecules in the binding site of a macromolecular target. Searching algorithms generate possible poses, which are ranked by scoring functions [1]. Various software namely AutoDock, AutoDock Vina, DockThor, GOLD, FlexX, and Molegro Virtual Docker were developed. The first step in a docking calculation is to obtain the large target structure (protein, DNA, or RNA). The structures of these macromolecules can be readily retrieved from the Protein Data Bank (PDB) [2], which provides access to 3D atomic coordinates obtained by experimental methods. However, it is not unusual that the experimental3D structure of the target is not available. In order to overcome this issue, computational prediction methods, such as comparative and ab initio modelling can be used to obtain the three-dimensional structure of proteins.



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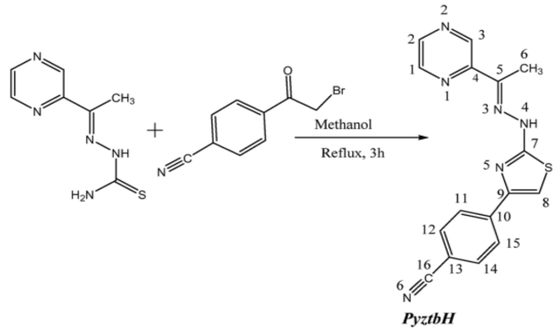
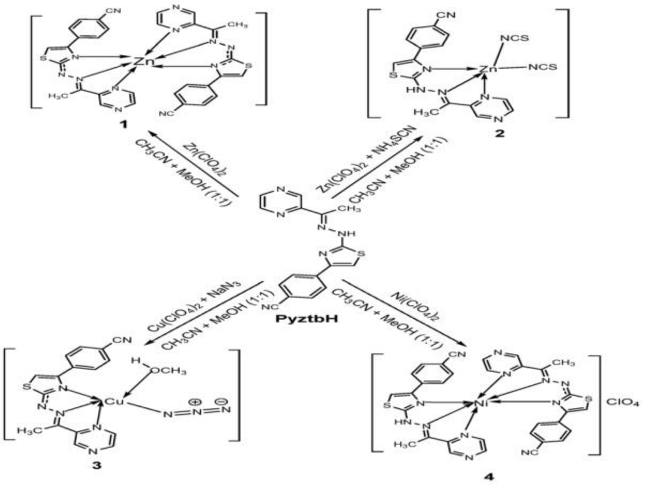
Newly Synthesized Drug:

The ligand (PyztbH) was prepared by the condensation of 4-(2-bromoacetyl)benzonitrile and 2-(1-(pyrazin-2-yl)ethylidene)hydrazine-1 carbothioamide. An anhydrous methanolic solution of 4-(2-bromoacetyl)benzonitrile (10 mmol) was added dropwise to the methanolic solution (20 mL) of 2-(1-(pyrazin-2-yl)ethylidene)hydrazine carbothioamide (10 mmol, 1.942 g) with constant stirring at room temperature. The crude product recrystallized with methanol and acetonitrile (1 : 1) solution whereupon a greenish-yellow transparent crystalline compound of PyztbH was obtained. Yield: 3.124 g (73.79%).

Synthesis of [Zn(Pyztb)2] (1), A methanolic solution of Zn(ClO4)2_6H2O (0.37 g, 1.0 mmol) was added dropwise to a methanol and acetonitrile (1 : 1) mixture (20 mL) of PyztbH(0.32 g, 1.0 mmol) with constant stirring for a period of 2 h. The resulting solution was filtered off using Whatman 41 filter paper .Yellowish-brown crystals were obtained by the slow evaporation ofthe filtrate. Yield is 0.245 g.



Scheme 1 Synthesis of **PyztbH** and molecular drawing with atom number.



Scheme 2 Synthetic route and molecular structures of **1**, **2**, **3** and **4**.

Synthesis of [Zn(PyztbH)(SCN)2] (2), Addition of Zn(ClO4)2_6H2O (0.37 g, 1.0 mmol) in methanol (20 mL) to a diluted methanol acetonitrile (1 : 1) solution (30 mL) of PyztbH(0.32 g, 1.0 mmol) resulted in a greenish-yellow solution which was then refluxed for 1 h. An aqueous solution (30 mL) of NH4SCN(0.3 g, 2.0 mmol) was then added to the reaction mixture and the reflux was continued for another 3 h. The colour of the solution changed to deep orange. The yellowish-brown transparent crystals of 2were separated out from the solution at room temperature. Yield is 0.225 g.

Synthesis of [Cu(Pyztb)(N3)(MeOH)] (3) . A methanolic solution (20 mL) of Cu(ClO4)2_6H2O (0.33 g, 0.9 mmol) was added dropwise to the methanolic solution (10 mL) of NaN3(0.09 g, 0.6 mmol). The mixture was stirred at 70 1C for 30 min. The resulting light blue solution was then added to the hot acetonitrile–methanol (1 : 1) solution (30 mL) of PyztbH (0.288 g,0.9 mmol). The reflux was continued for 2 h at water bath temperature. The solution was allowed to cool at room temperature where upon a precipitate was obtained which was filtered and washed with methanol and finally dried in air. The violet crystals suitable for X-ray crystallography were obtained from the slow vaporation of the filtrate. Yield: 0.222 g.

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Synthesis of complex $[Ni(Pyztb)(PyztbH)]ClO_4$ (4) . A stoichiometric mixture of $Ni(ClO_4)_2\_6H_2O$ (0.365 g, 1.0 mmol) and PyztbH (0.32 g, 1.0 mmol) was dissolved in the methanol and acetonitrile mixture (1 : 1) (20 mL). The resulting wine-red colour solution was heated for 2 h. The colour of the solution changed to deep red. Dark brown crystals were obtained from the slow evaporation of the red solution. The crystals were filtered off and washed with methanol and dried in air. Yield:0.25 g.

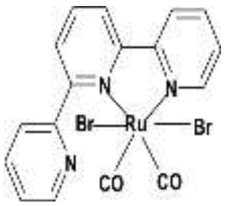
Molecular docking has been established as a pivotal technique among computational tools for structure-based drug discovery. Here we addressed key aspects of the methodology and discussed recent trends in the literature for advancing and employing the technique for successful drug design for the first learner. Benchmarking sets and the various metrics available are crucial for validating the performance achieved by new docking software but must be carefully chosen since no single one can be regarded as the absolute best for molecular docking. A significant improvement in the performance of all docking software can be achieved by employing multiple SFs for consensus posing and/or scoring. As reviewed here, there is a large discussion of protocols for consensus docking to be analysed by the user. The ligand, PyztbH, and its metal complex of Zn(II), Cu(II), and Ni(II) have been docked for verification. It was found that all the metal complexes showed prominent antitumor activity against a panel of human cancer cells of different tissue origins.

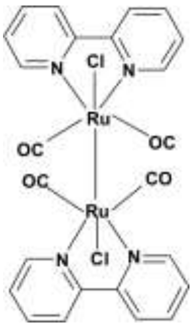
Retrospection of coordination chemistry of few Group 8 metal-carbonyl complexes of imine functions.

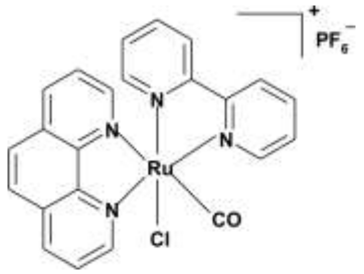
Mayuree Banerjee

Uluberia College, 6th sem student

Ruthenium polypyridine and phenanthroline complexes have been studied extensively because of their photocatalytic, photochemical, biological and electrochemical properties. The recent interest has been developed around the photochemical and redox activation of the substituted clusters $[M_3(CO)_{10}(\alpha\text{-diimine})]$, which has led to the discovery of a variety of biradical, zwitterionic, radical anionic and dianionic open structure intermediates, formed upon electron transfer-induced cleavage of an M-M(α-diimine) bond. Os carbonyl diimine complexes have very similar electrochemical properties to Ru carbonyl diimine complexes. Some representative examples of ruthenium and osmium carbonyl diimine system are given below.







Synthesis of Ru and Os diimine compounds viz. *trans*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$, *cis*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$, *cis*-(CO)-$[Ru^{II}(bpy)(CO)_2(COOMe)Cl]$, $[Ru^{I}(bpy)(CO)_2Cl]_2$, $[Ru^{I}(bpy)(CO)_2(COOMe)Cl]_2$, $[Os(bpy)(CO)_2Cl_2]$, $[Os(dmbpy)(CO)_2Cl_2]$, $[Os(bpy)(CO)_2Br_2]$, $[Os(bpy)(CO)_2I_2]$ is discussed in this work. Some synthesis are as follows,

Synthesis of *cis*-(CO)-$[Ru^{II}(bpy)(CO)_2(COOMe)Cl]$

This compound was obtained as side product during preparation of complexes *trans*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$ and *cis*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$. *cis*-(CO)-$[Ru^{II}(bpy)(CO)_2(COOMe)Cl]$ Complex was isolated by evaporation of the mother liquor (from 1 and 2) to dryness, followed by chromatography on a column packed with alumina under pressure and eluted with CH_2Cl_2 and CH_2Cl_2/0.5-1% methanol (R_f = 0.15 (alumina), 98/2 CH_2Cl_2/ MeOH as eluent), 15-18% respectively from the preparation of complex *trans*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$ and *cis*-(Cl)-$[Ru^{II}(bpy)(CO)_2Cl_2]$.

Synthesis of $[Os(bpy)(CO)_2I_2]$

$[Os(bpy)(CO)_2I_2]$ is synthesized (following above method) in an autoclave from compound HI (2 mL) is added to the vessel along with 2 mL water. The same temperature program is used as in the synthesis of compound. The total yield is ca. 40%.

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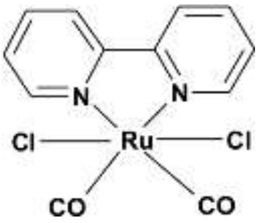
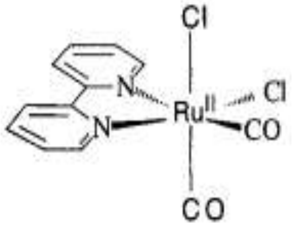
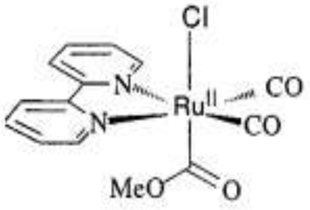
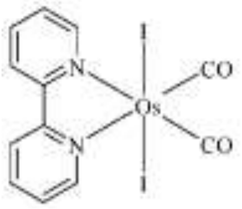
Structures of some of the synthesized compounds are given below.









Electrochemical properties

For Ruthenium complexes : Electrochemical reduction of the *trans*-(Cl) isomer leads to deposition on the working electrode of an electroactive polymeric film having the generic chemical structure $[Ru^0(bpy)(CO)_2]_n$ and containing metal-metal bonds.

For Os complexes : Two reversible redox systems, characteristic of the corresponding polymer electroactivity regularly appear in the CV of complexes $[Os(bpy)(CO)_2Br_2]$ and $[Os(bpy)(CO)_2I_2]$ during repeated potential scans between −0.6 V and −1.80 V. This electrochemical process does not depend on the nature of the halide ligands in $[Os(bpy)(CO)_2Br_2]$ and $[Os(bpy)(CO)_2I_2]$.

Luminescence Properties

The $[Os(NN)(CO)_2X_2]$ complexes possess luminescent properties at RT, unlike the corresponding ruthenium complexes. The extent of the luminescence lifetimes measured for complexes consists of a few dozen of nanoseconds at RT. A much higher luminescence lifetime (240 ns) and quantum yield ($\phi = 0.15$) have been determined for 4 by Chen et al. at RT in degassed CH_2Cl_2. The luminescence lifetime of was also significantly reduced in comparison with 1.

Catalytic activities of Ru & Os imine compounds

The catalytic efficiency of Ru and Os carbonyl complexes of 1-alkyl-2-(arylazo)imidazoles, 1-alkyl-2-(naphthyl-α/β-azo)imidazole and 1-alkyl-2-{(*o*-thioalkyl)phenylazo}imidazole in presence of NMO, Bu^{t}OOH and H_2O_2 in the oxidation of primery, secondary and tertiary alcohols to their corresponding aldehydes and ketones. Where ruthenium catalysts show higher conversion compared to osmium.

The discussed properties of the Os and Ru diimine complexes provide a valuable synthetic route in present researches.

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Application of Schiff base as a fluorescence sensor

Ritesh Patra
Uluberia College , Uluberia ,Howrah ,711315

Schiff bases are obtained from condensation of primary amines with carbonyl compounds. There are several applications of Schiff bases which include not only antimicrobial or antifungal activity but also in chemosensor for detection of metal ions and toxic anions.

Schiff bases are condensation products of primary amines and carbonyl compounds and they were discovered by a German Chemist . Nobel prize winner. Hugo Schiff. Structurally schiff base (also known as imine or azomethine) is an analogue of a ketone or aldehyde which the carbonyl group (C=O) has been replace by an imine or azomethine group. A Schiff's base is a type of chemical compounds containing a carbon nitrogen atom connected to aryl group or alkyl group (R) but not hydrogen. The Schiff base is synonymous with an azomethine. These compounds were named after Hugo Schiff on honor and have the following the general structure.

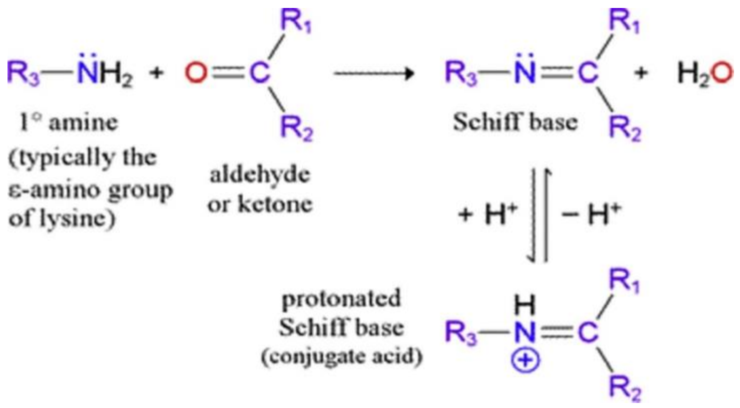


Fig 1 : Synthetic route of Schiff base

Where R stands for a phenyl or alkyl group which makes the Schiff base a stable imine. This kind of ligands is able to coordinate metal ions through the imine nitrogen and another group. Usually linked to the aldehyde.

Detection of metal ions:

A novel sensor, 7-Hydroxy-4-methylcoumarin-8-carbaldehyde-(rhodamine) hydrazone have synthesized (An, et al., 2013) and investigated as a fluorescence chemo sensor for Ca^{+2} in acetonitrile. The compound was found preferential binding to Ca^{+2} ions in presence of excess of other competitive ions with associated changes in its optical and fluorescence spectral behavior.

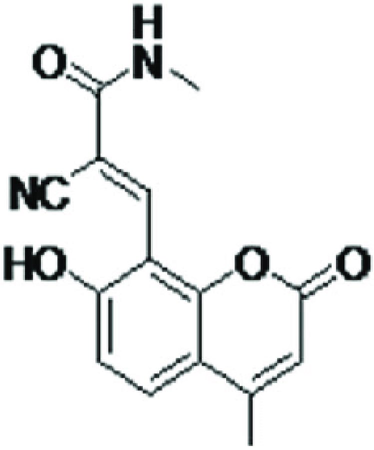


Fig 2 Chemical structure of sensor .

Nowadays, researchers are using Schiff base metal ion complexes for productive purposes owing to their outstanding applications in optoelectronic systems. However, with the increase in their concentration due to industrialization and urbanization, metal ions have shown toxic effects on human health and the environment. Therefore, their detection is crucial, which is challenging .

Although fluorescent-based Schiff base sensors encounter many challenges in terms of both exploratory and practical application, by taking into consideration the above-mentioned aspects in the sensor design and application-oriented research work, we believe that fluorescent Schiff base sensors can be utilized as important materials in the upcoming days and their commercial availability will be expected in the future.

CAPILLARY ELECTROPHORESIS AND IT'S APPLICATIONS

NAME – MONIDEEPA MAJI

ULUBERIA COLLEGE

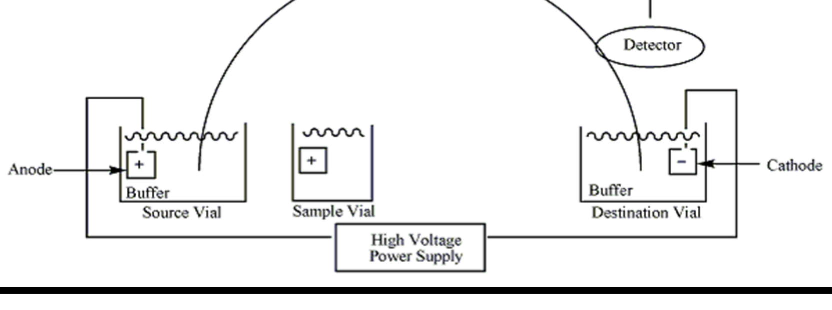
SEMESTER – VI

CHEMISTRY

CE is a family of electro kinetic separation method Perform in Submilliter diameter. It is based on the Principle of electro Phones. The driving Force for the use of CE at the Present time are simplicity, speed, high resolution and low operating cost. Many general application areas are identified which are expected to have a great impact on bal routine clinical analysis by CE.

Capillary electrophoresis is anatet technique that Saparates ions, based on their electrophoretie mobility with the help an art aflued voltage. Hear the separation and quantification of a wide variety of molecules are based not only on charge, but also on size hydrophobicity and" Stereospecif stereo specificity. To determination the number, amount and mobility of Components in a given sample or to separate them. To often obtain information about the electrical double & layers Surrounding the Particles. The developed methods for amplification and detection which has a great impact on forensic Science.

A capillary electrophoresis System



It is used in Analysis of DNA and RNA. Protein characterization. Enzyme analysis. Single cell analysis. Counter-ion analysis in drug discovery and CE become an established analytical tools in the clinical laboratory, Forensic, and biopharmaceutical companies. It is the most efficient separation technique available for Analysis of both large and small molecule.DNA analysis, protein identification, inorganic metals and ions can be detected easily by this method.

Glass Material and Their Advanced Applications

Mamin Mollah

Uluberia college,6th semester student

Abstract

The present review summarizes the progress made in the area of glass science and also propose new definition of glass. The applications of glasses in everyday life and especially glasses used for light emitting devices, optical displays, optical fibers, amplifiers, lasers which are of special interest. Among these materials rare earth ions doped glasses are of great important to optoelectronics and are widely used in optical fiber amplifiers and solid state high power lasers for telecommunications and light emitting diodes. Optical fiber revolutionized the glass industry and is been used as sensing applications which depends upon light wavelength, fiber parameters, fiber geometry, and metal layer properties. Even smart glasses play a vital role in the medical field.

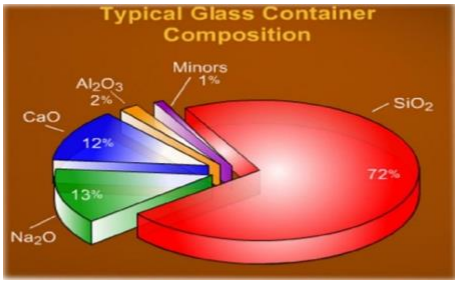
1. What is Glass?

Several theoretical and empirical models have been proposed to explain the definition of glass in the literature for almost a century and even more, invoking control parameters such as density, temperature, gas like or solid like structures, specific molecular shape and interactions.

"Glass is an amorphous solid which exhibits glass transition temperature by arresting the kinetics below supercooled liquid region when bypassed crystallization"

RAW MATERIALS USED IN MANUFACTURING OF GLASS

1)Sodium as Na_2CO_3 (used in soft glass)***2***)Potassium as K_2Co_3 (used in hard glass)***3***)Calcium as lime stone , chalk and lime ***4)***Lead as litharge , red lead (flint glass)***5***)Zinc is zinc oxide (heat and shock proof glass)***6)***Borates are borax , Boric acid(heat and shock proof glass)



VARIOUS TYPES OF GLASS:-

Sodalime or soft Glass,Borosilicate / pyrex / Jena Glass,Lead Glass or Flint Glass,Aluminosilicate Glass,Toughened Glass,Potash lime or hard Glass,Wired Glass,Coloured Glass,Laminated Glass.

Sodalime or soft Glass

- About 90% of all glass is sodalime glass made with silica(sand) Carbonate and soda ash.
- The approximate composition is $Na_2CO_3.CaO.6SiO_2$.
- They are low cost , resistant to water but not to acids.

Borosilicate / pyrex / Jena Glass

- It is common hard glass containing silica and boron with small amount of alumina and less alkaline solids.
- The borosilicate glass is made by adding the boric oxide to the
- traditional glassmaker frit of the silicate soda , sand or to the ground lime.

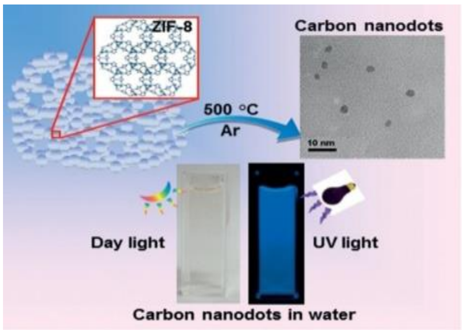
Simple Method of Conversion of Metal-Organic Framework to Fluorescence Carbon Nanodots

Monidipa Maity

6th Semester

Uluberia College, Uluberia, Howrah

Highly photoluminescent carbon nanodots (CNDs) were synthesized for the first time from metal–organic framework (MOF, ZIF-8) nanoparticles. Carbon nanodots are now a days considered as the rising star in the nanocarbon family due to their sustainable, compatible, cost-effective, and benign nature. Light-emitting quantum-sized carbon nanodots (CNDs) have attracted tremendous attention because of numerous possible applications in drug/gene delivery, bioimaging, photocatalysis, energy conversion, optoelectronics, sensing, and other directions. CNDs exhibit several promising advantages, such as excellent chemical stability, up-conversion emission, pH-sensitivity, and resistance to photobleaching compared with semiconductor quantum dots and rare-earth and organic fluorescent materials. Arc-discharge, laser-ablation, electrochemical synthesis, microwave synthesis and combustion/thermal routes have been used to synthesize CNDs, of which thermal route was regarded as efficient way. More importantly, although CNDs have been demonstrated as probes in cellular imaging, clear evidence to ensure their biosafety is highly desired, which can be achieved, as shown in this work. Recently, it has been demonstrated that metal–organic frameworks (MOFs), also called as porous coordination polymers (PCPs), can be used as templates/precursors to prepare porous carbons through thermal conversion.



Schematic illustration for the formation of carbon nanodots (CNDS) derived from ZIF-8 NPs and their aqueous dispersion under visible and UV lights

Herein, for preparation of the fluorescent CNDs, NPs of the zeolitic imidazolate framework, ZIF-8 [Zn(MeIM)$_2$; MeIM = 2-methylimidazole] were used which were prepared by using a sonochemical. The powder X-ray diffraction (PXRD) pattern of ZIF-8 NPs confirmed the preserved ZIF-8 framework, and the transmission electron microscopic (TEM) displayed the morphology of resultant ZIF-8 particles with a size of 20–100 nm. The carbonization temperature is a crucial factor for getting CNDs from ZIF-8 NPs.

Debasish Pal
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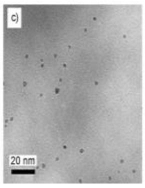
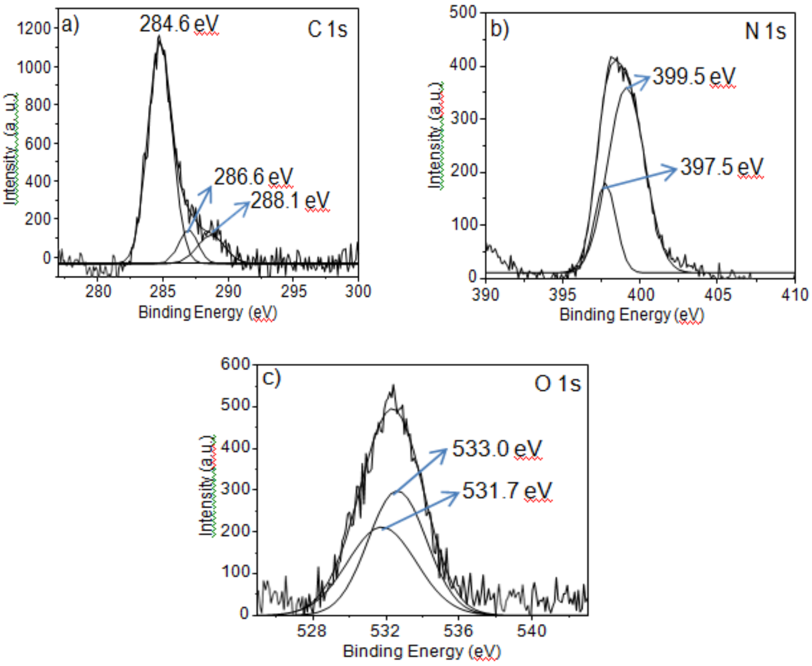


TEM images of CNDs

Again, X-ray photoelectron spectroscopic (XPS) measurements were carried out to probe the composition of the CNDs, which clearly revealed the presence of nitrogen and oxygen in the CNDs. From the C1s, N1s, O1s spectrum it is considered that the CNDs contains C—C, C—O, C=N, N—H, C=O and C—OH/C-O-C groups. The presence of these functional groups imparts excellent solubility to the CNDs in water without further chemical modification.



XPS spectra of CNDs at (a) C 1s, (b) N 1s and (c) O 1s levels.

To better understand the characteristics of CNDs, from the photophysical studies, the observed lifetimes of CNDs are 1.60 and 3.12ns. The lifetime of CNDs nanoseconds suggests that the synthesized CNDs are most suitable for optoelectronic and biological application.

(a) **(b)**

CND marked "T" letter on ordinary paper under a) daylight and b) UV light (λ_{ex}=385nm)

Thus, a facile methodology to use MOF nanoparticles (NPs) as a precursor to prepare carbon nanodots with intrinsic fluorescence properties is reported. The synthesized CNDs showed emission maximum 412 nm when excited at 330 nm, and showed a bright blue color under UV irradiation (385 nm).

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SYNTHESIS, CHARACTERISATION AND PROPERTIES OF AZOIMINE COMPLEXES OF SOME RUTHENIUM(Ru) AND OSMIUM (Os) CARBONYL COMPOUNDS

Suman Samui

Uluberia College, 6th Sem

$[Ru(CO)_2Cl_2(\alpha/\beta\text{-NaiR})]$ and $[Ru(CO)_2I_2(\alpha/\beta\text{-NaiR})]$ are synthesized by the reaction of $[Ru(CO)_2Cl_2]_n$ or $[Ru(CO)_4I_2]$ with α/β-NaiR (1-alkyl-2-(naphthyl-α/β-azo)imidazole (α-NaiR/ β-NaiR, where, R = Me, CH_2CH_3 and CH_2Ph)) and have been characterized by spectroscopic data. Catalytic activity of these compounds is investigated to the oxidation of $PhCH_2OH$ to PhCHO, 2-butanol (C_4H_9OH) to 2-butanone, 1-phenylethanol (PhC_2H_4OH) to acetophenone, cyclopentanol (C_5H_9OH) to cyclopentanone and cyclohexanol to cyclohexanone by N-methylmorpholine-N-oxide (NMO), H_2O_2 or Bu^tOOH in CH_2Cl_2 and NMO shows highest yield.

Synthesis of $[Ru(CO)_2Cl_2(\alpha\text{-NaiMe})]$ and $[Ru(CO)_2I_2(\alpha\text{-NaiMe})]$

To a 20 mL acetonitrile suspension of $[Ru(CO)_2Cl_2]_n$ (100 mg, 0.43 mmol) 15 mL acetonitrile solution of α-NaiMe (103.63 mg, 0.44 mmol) was added and the reaction mixture was refluxed for 6h under N_2 atmosphere. The colour of the solution changed from orange to dark red. The solvent was removed under reduced pressure. The dark red dry mass was then dissolved in minimum volume of CH_2Cl_2 and subjected to chromatography separation on a silica gel column (60-120 mesh). The desired red band of complex was eluted by 1:10 CH_2Cl_2-MeCN mixture. Slow evaporation of the solvent the red crystalline complex was obtained. The yield was 141.92 mg. The another complex was prepared by the reaction of $[Ru(CO)_4I_2]$ 100 mg, 0.21 mmol) with α-NaiMe (51.82 mg, 0.22 mmol) following the same procedure as of. The purification was carried out by column chromatography. Yield was 73.79 mg (69%).

The complexes show two equally intense υ(CO) bands at 1995-2006 and 2048-2065 cm^{-1} which supports the cis-$Ru(CO)_2$ configuration. Infrared spectra of the complexes also exhibit υ(C=N) at 1542–1563 cm^{-1} and υ(N=N) at 1355–1365 cm^{-1}. The azo (–N=N–) stretching is significantly shifted to lower frequency region compared to free ligand value (1400–1410cm^{-1}), which supports $d\pi(Ru) \rightarrow \pi^*(N=N)$ back donation in the complexes.

The complexes and show moderately intense band at 473 nm and 485 nm respectively corresponds to HOMO-1→LUMO, mixed MLCT and XLCT transitions. The band at 411 nm and 367 nm for and respectively has ILCT/XLCT character. In addition the intense bands at 390-310 nm for the complexes are purely intra-ligand charge transfer transitions (ILCT).

We cannot determine the x-ray crystallographic structure of α-isomer, but we can determine the x-ray crystallographic structure of β-isomer by x-ray crystallographic analysis. The molecular structures of [Ru(CO)$_2$Cl$_2$(β-NaiMe)] and [Ru(CO)$_2$I$_2$(β-NaiEt)] are shown in **Figures 1** and **2**, respectively.

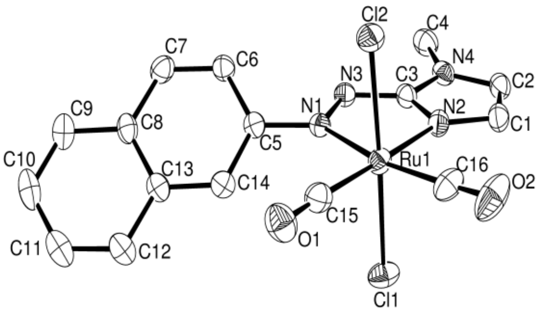
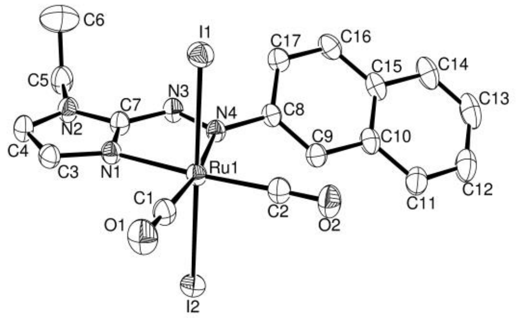
	

Figure 1. Ortep structure of [Ru(CO)$_2$Cl$_2$(β-NaiMe)]	**Figure 2.** Ortep structure of [Ru(CO)$_2$I$_2$(β-NaiMe)

The complexes catalyse the oxidation of PhCH$_2$OH to PhCHO, C$_4$H$_9$OH to C$_4$H$_7$O (2-butanone), PhC$_2$H$_4$OH to PhCOCH$_3$ (acetophenone), C$_5$H$_9$OH to C$_5$H$_8$O (cyclopentanone) and CyCH-OH to CyC=O (cyclohexanone) with high yields. The aldehyde or ketone formed after 1 h of reflux was determined by GC and there was no detectable oxidation in the absence of ruthenium complex. Results of the investigations suggest that the complexes are able to react efficiently with NMO or peroxides (H$_2$O$_2$/ Bu^{t}OOH) to yield a high valent ruthenium-oxo species, which is capable of oxygen atom transfer to alcohols.

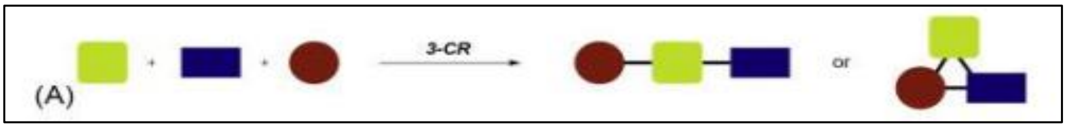
Ruthenium/ Osmium(II)-CO complexes of azoimine functions from 1-alkyl-2-(naphthyl-α/βazo)imidazoles (α/β-NaiR) are structurally and spectroscopically characterized. The catalytic activity of the complexes has been examined and thus scope of catalytic reaction has unveiled new defining area.

REVIEW ON TYPES OF THREE COMPONENT REACTIONS

Payel Mondal

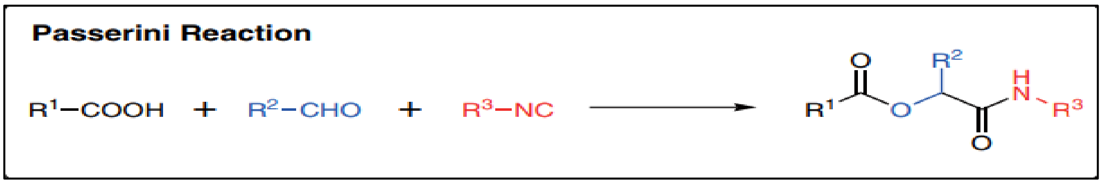
Uluberia college 6th sem (Chemistry Honours)

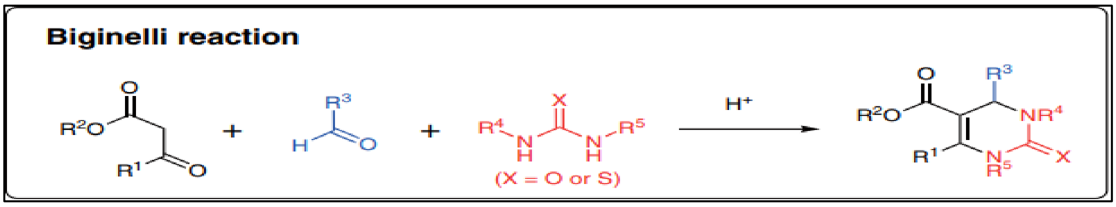
Multicomponent reaction (MCR) is a synthetic methodology in which three or more reactants come together in a single reaction vessel to form a new product. The characteristic aspect of MCRs is that the final products contain almost all portions of substrates, generating almost no by-products. That makes MCRs an extremely ideal and eco-friendly reaction system. Target compounds can be obtained in one pot with much fewer steps. Therefore, MCRs have been paid much attention in various research fields, such as discovery of lead compounds in medicinal chemistry, or combinatorial chemistry. Three component interaction is included in the preparation of the pharmaceutical compounds, as they need the shortest steps and the fastest results, so such interactions are used in the preparation of many drugs and the simplest examples are tramadol and some anesthetics used in surgical processes. Three-component reactions have emerged as useful methods because the combination of three components to generate new products in a single step is extremely economical, among the multi-component reactions. Multi-component reactions (MCRs) are a promising and vital field of chemistry because the synthesis of complicated molecules can be achieved in a very fast, efficient, and timesaving manner without the isolation of any intermediate. As a result, it requires minimum effort, which minimizes the environmental loading and is acceptable from a 'Green Chemistry' point of view.



All components in MCRs might assemble in linear form (like the **Mannich reaction**) or undergo further cyclization (like the **Hantzsch dihydropyridine** synthesis) to provide complex molecules in a single step from simple building blocks. In figure 3CR shows there are three reactants in the reaction pot – Three component reactions.

Three component name reactions are **Biginelli Condensation**, **Hantzch Reaction, Strecker Reaction**, **Mannich Reaction, Passerini Reaction**, **Kabachnik-Fields Reaction, Petasis Reaction**. Like -





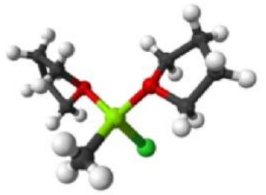
There are many example of three component reactions: Microwave assisted three component Reaction, Three component reaction of iodobenzene**,** alkynes and diaziridinone**,** Synthesis Of a-Aminophosphonates and Related Phosphonates By Three Component Reactions, Synthesis of HomoallylicAmines by Three Component Reactions, etc. Three-component chemical reactions include the interaction of three raw materials (nucleophile and electrophile) to form a single compound that changes the arrangement of atoms in chemical molecules. Chemical reactions usually involve breaking or forming chemical bonds. These are the most versatile method for the synthesis of complicated molecules in a one pot, fast, efficient and time saving manner. These represent a very interesting organic synthetic methodology due to its features, such as the use of convergent one-pot reactions, atoms economy, steps with high chemical yields, less aggressive reactions conditions to the environment, accessible and cheap substrates, easy operation and, a considerable advantages of this methodology, the ability to quickly build a library of varied and structurally complex compounds. The creation and understanding of new MCRs is certainly a great intellectual challenge and it is worthwhile to engage in it for several reasons.

Grignard Reagent

Aritra Das

6th Semester student of Uluberia College, Department of Chemistry

A Grignard reagent or Grignard compound is a chemical compound with the genericFormula R−Mg−X, where X is a halogen and R is an organic group, normally an alkyl or aryl.Two typical examples are methylmagnesium chloride Cl−Mg−CH3 and phenylmagnesium Bromide (C6H5)−Mg−Br. They are a subclass of the organomagnesium compounds.



Usually Grignard reagents are written as RMgX, but in fact the magnesium(II) centre is tetrahedral when dissolved in Lewis basic solvents, as shown here for the bis-adduct of methylmagnesium chloride and THF.

Grignard compounds are popular reagents in organic synthesis for creating new carbon-carbon

Bonds. For example, when reacted with another halogenated compound R'−X' in the presence of A suitable catalyst, they typically yield R−R' and the magnesium halide MgXX' as a byproduct; And the latter is insoluble in the solvents normally used. In this aspect, they are similar toOrganolithium reagents.Pure Grignard reagents are extremely reactive solids. They are normally handled as solutions inSolvents such as diethyl ether or tetrahydrofuran; which are relatively stable as long as water is Excluded. In such a medium, a Grignard reagent is invariably present as a complex with theMagnesium atom connected to the two ether oxygens by coordination bonds.The discovery of the Grignard reaction in 1900 was awarded with the Nobel prize in 1912.

Grignard reagents are prepared by treating an organic halide (normally organobromine) with magnesium metal. Cyclic or acyclic ethers.Are required to stabilize the organomagnesium compound. Water and air, which rapidly destroy the reagent by protonolysis or oxidation,Are excluded using air-free techniques.Although the reagents still need to be dry, ultrasound can allow Grignard reagents to form in Wet solvents by activating the magnesium such that it consumes the water.As is common for reactions involving solids and solution, the formation of Grignard reagents is often subject to an induction period.During this stage, the passivating oxide on the magnesium is

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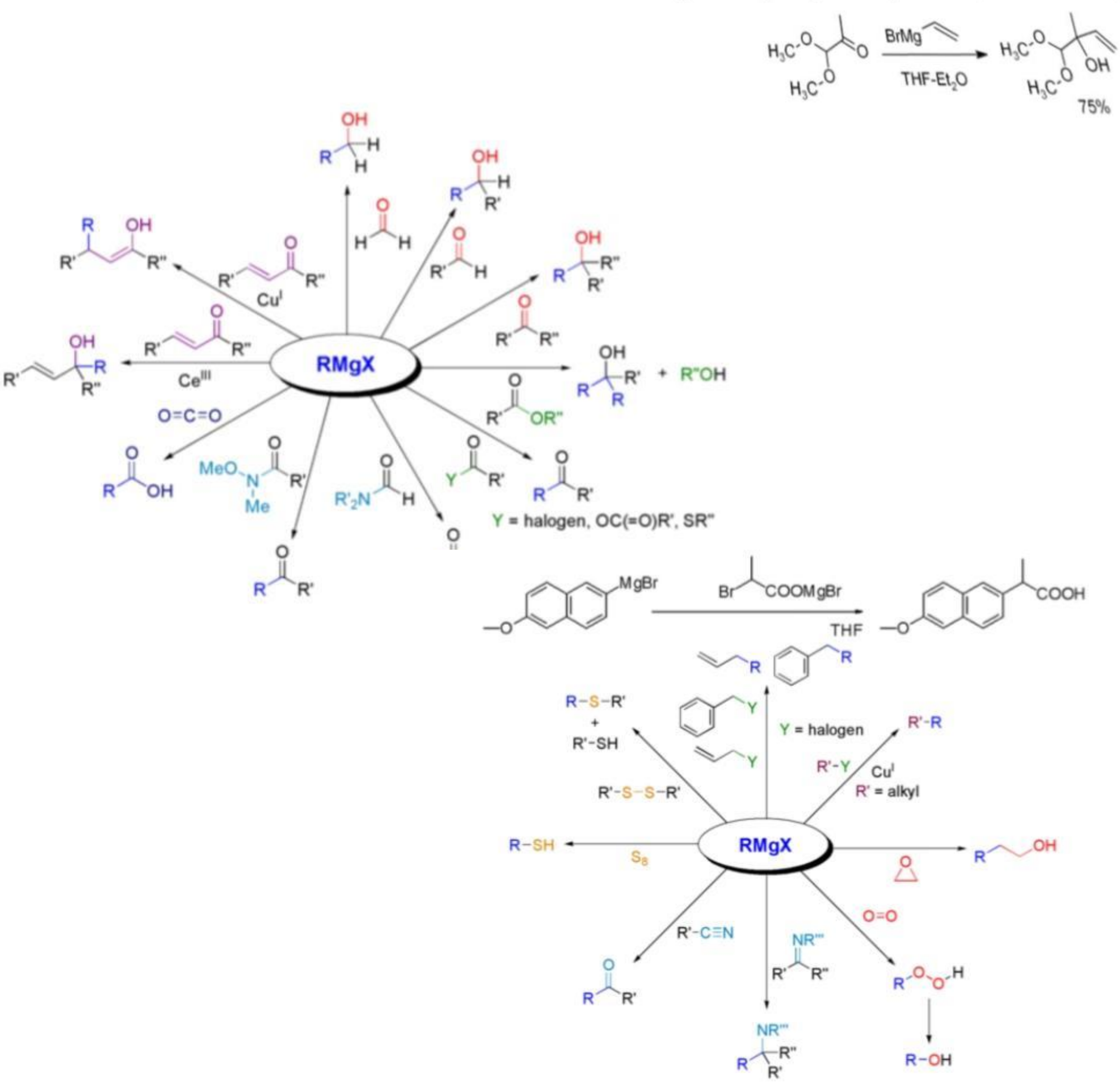
removed. After this induction period, the reactions can be highlyExothermic. This exothermicity must be considered when a reaction is scaled-up from laboratory to production plan



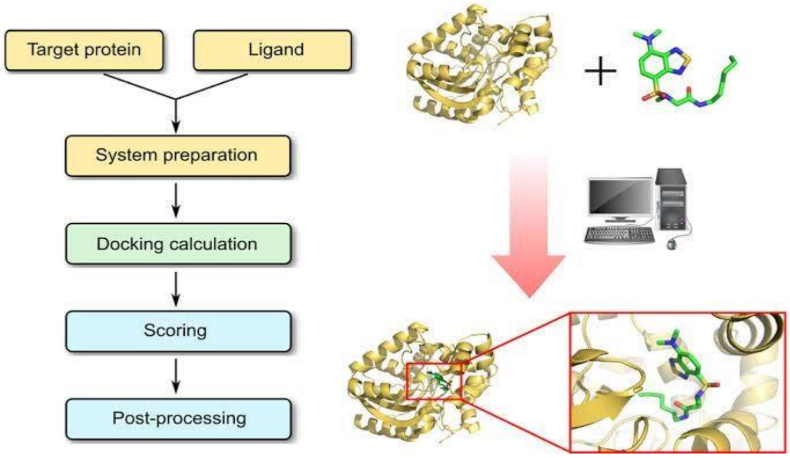
Grignard reagents serve as a base for protic substrates (this scheme does not show workup conditions, which typically includes water).Grignard reagents are basic and react with alcohols, phenols, etc. to give alkoxides (ROMgBr). The phenoxide derivative is susceptible.To formylation paraformaldehyde to give salicylaldehyde. To form salicyladehyde.

"An awesome computational Technique to Drug Discovery: A Case Study of Molecular Docking of Newly Synthesized Compounds"

SHREYA PARAL

UIUBERIA COLLEGE,6th Sem (Chemistry Honours)

Molecular docking is a computational method used to predict the binding mode and affinity of a small molecule ligand to a biomolecular target, such as a protein or nucleic acid. The process involves predicting the interactions between the ligand and the target based on their 3D structures, and can be useful in drug discovery and design.



Molecular docking is the process that involves placing molecules in appropriate configurations to interact with a receptor. Molecular docking software uses various algorithms and scoring functions to predict the most likely binding pose of the ligand and estimate the binding energy between the ligand and the target. The results can be used to guide the design of new drugs or to understand the mechanism of existing drugs. Here we report the basic techniques of the docking process and study the docking results of newly synthesized compounds.Molecular docking is a natural process which occurs within seconds in a cell.Molecular docking study is a popular technique to estimate the interaction between synthesized compounds and protein or DNA for rational drug design.Molecular docking has become an increasingly important tool for drug discovery. In this review, we present a brief introduction of the available molecular docking methods, and their development and applications in drug discovery.

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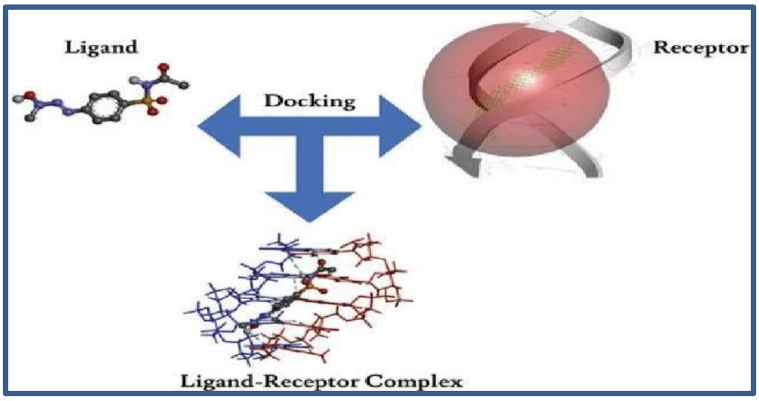
The relevant basic theories, including sampling algorithms and scoring functions, are summarized. The differences in and performance of available docking software are also discussed. Flexible receptor molecular docking approaches, especially those including backbone flexibility in receptors, are a challenge for available docking methods. A recently developed Local Move Monte Carlo based approach is introduced as a potential solution to flexible receptor docking problems. Three application examples of molecular docking approaches for drug discovery are provided.The aim of molecular docking is to give a prediction of the ligand-receptor complex structure using computation methods. Docking can be achieved through two interrelated steps: first by sampling conformations of the ligand in the active site of the protein; then ranking these conformations via a scoring function. Ideally, sampling algorithms should be able to reproduce the experimental binding mode and the scoring function should also rank it highest among all generated conformations. From these two perspectives, we give a brief overview of basic docking theory.Structure-based virtual screening is a key, routine computational method in computer-aided drug design



Such screening can be used to identify potentially highly active compounds, to speed up the progress of novel drug design. Molecular docking-based virtual screening can help find active compounds from large ligand databases by identifying the binding affinities between receptors and ligands. In this study, we analyzed the challenges of virtual screening, with the aim of identifying highly active compounds faster and more easily than is generally possible. We discuss the accuracy and speed of molecular docking software and the strategy of high-throughput molecular docking calculation, and we focus on current challenges and our solutions to these challenges of ultra-large-scale virtual screening.

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