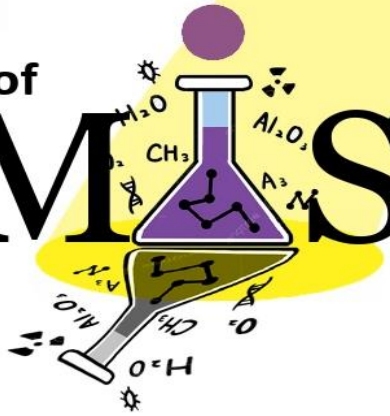
St. Paul's Cathedral
Mission College

Exploring

The World Through Molecules

By the Department of

CHEMISTRY



STUDENTS' SEMINAR 2025

Date

13/06/2025

Students' Seminar 2025

on

Chemistry: Exploring the World through Molecules

Organizing Committee

- **Secretary:** Dr. Kalyan Kumar Mandal (Head of the Department)
- **Convener:** Dr. Biswajit Pal

Members:

- Dr. Anil Kumar Barik
- Dr. Ankan Sanyal
- Dr. Jaydip Gangopadhyay
- Dr. Kaushik Basu
- Dr. Jishnunil Chakraborty
- Mr. Ratikanta Pradhan
- Mr. Goutam Manna
- Mr. Kamaljit Singh
- Mr. Pabitra Routh

Events of the Seminar

1. Welcome address by Dr. Kalyan Kumar Mandal, HOD
2. Speeches of Teacher-in-charge, Vice-Principal, IQAC Coordinator and Bursar.
3. Address by Dr. Biswajit Pal, Convener
4. Presentation of Semester IV Students
5. Presentation of Semester II Students
6. Vote of Thanks by Dr. Kaushik Basu

Welcome Address by Head of the Department

On behalf of all the learned members of Department of Chemistry, SPCMC, I, Dr. Kalyan Kumar Mandal cordially welcome you all in this Students' Seminar, entitled, "Exploring the World through Molecules".

It's a pleasure to see most of the departmental students participating in the seminar. As the Head of the Department of Chemistry, I'm incredibly proud to host this event, which promises to be both insightful and engaging. This seminar provides a fantastic opportunity to delve deeper on a topic that is both fascinating and relevant to our modern world.

At our department, we are committed to providing a stimulating and supportive environment for learning and research. We encourage all our students to actively participate in seminars, workshops, and research projects, as these experiences are crucial for developing a strong foundation in chemistry and preparing for future careers.

I encourage you all to actively participate in the discussions, ask questions on the deliberation presented by your fellow speakers.

In this seminar, most of the students of our department have responded spontaneously, and I strongly believe that they will present their themes in an elegant manner. The choice of the topics and preparation of the slides are mostly done by themselves. However, we, the teachers, extended our support wherever they sought, and this interactive exchange proved beneficial for both of us.

As this seminar is designed to enrich the students in various capacities, studying a concept is only the inception of the assimilation process. Through the sound knowledge on the subject accompanied with a good articulation power will help you presenting yourself in front of audiences in your future endeavour. This is surely going to build your identity. Participating actively in the seminar will boost your confidence as well. I also like to urge that, those who have not shown interest presently for some reasons will come up as strong contenders for appraisal, in near future.

Once again, welcome, and I wish you all an enriching and productive seminar.

Dr. Kalyan Kumar Mandal
Head of the Department,
Department of Chemistry,
St. Paul's Cathedral Mission College

From Convener's Desk……

The seminar, "Chemistry: Exploring the World through Molecules" highlights the basic role of chemistry in realizing and shaping our world, from the tiniest molecules to the vastness of the universe. With a view to understand how the studies on materials and their transformation lead to advancement of chemistry in diverse field, the necessity of such seminar arises to be organized. The seminar will also shed a light on the importance of chemistry in various sectors, including medicine, materials science, environmental sustainability, and eventually showcase how chemical principles are applied to solve real-world problems.

The core chemical concepts, such as atomic structure, chemical bonding, molecular interactions, and reaction mechanisms, providing a solid foundation for understanding the molecular world are supposed to be covered in such seminar that emphasizes the interdisciplinary areas related to chemical sciences.

It will also underscore the role of chemistry in developing innovative solutions for challenges related to energy, healthcare, and environmental protection for sustainable future.
By showcasing the relevance and excitement of chemistry, the seminar aims to foster a deep sense of appreciation for the field and encourage students to pursue careers in chemistry or related areas in future. Participants will gain a comprehensive understanding of fundamental chemical principles. They will be exposed to cutting-edge research and potential career paths in chemistry. They will be inspired to explore the world through the lens of molecules and contribute to future scientific advancements.

Dr. Biswajit Pal
Convener of the Seminar,
Department of Chemistry
St. Paul's Cathedral Mission College, Kolkata

Message from IQAC Coordinator

The Internal Quality Assurance Cell (IQAC) of the College believes in promoting holistic development of the students and the Annual Students' Seminar, organized by all departments of the College, is a part of this initiative. The Student Seminar organized by the Department of Chemistry under the aegis of the IQAC provided a platform to the students of the Chemistry Department to showcase their academic curiosity, research aptitude and presentation skills. It encouraged them to engage in critical thinking and relate their theoretical understanding of the subject to the real world. I extend my best wishes to all the student participants and faculty mentors who contributed to the success of this event. Their dedication and enthusiasm reflects the commitment of this institution to academic excellence.

Dr. Jaya Mukherjee
IQAC Coordinator,
St. Paul's Cathedral Mission College

CONTENTS

Beyond Petroleum: The Science and Scope of Bioplastics

Nilanjan Basak, Subhrojit Nandy, Gourab Das

Semester IV

Abstract

In recent years, bioplastics are becoming increasingly prominent owing mainly to scarcity of oil, increase in the cost of petroleum-based commodities, and growing environmental concerns with the dumping of non-biodegradable plastics in landfills. In the present paper, we first discuss the definition and basic facts as well as the major advantages of bioplastics, then the main differences between plastics and bioplastics in packaging are briefly reviewed. Finally, possible future developments of bioplastics are prospected.

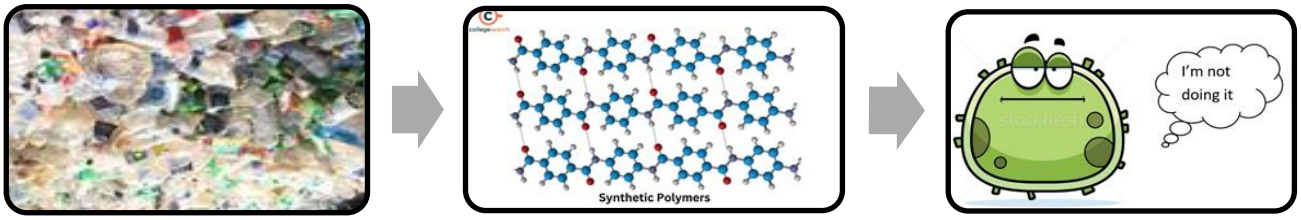
Introduction:

Synthetic plastics, though widely used for their durability and versatility, pose a significant threat to our environment and health. These petroleum-based plastics are **non-biodegradable**, meaning they persist in the environment for hundreds of years. Over time, they break down into **microplastics**—tiny plastic particles that contaminate our water, food, and even the air we breathe. These microplastics accumulate in the bodies of humans and animals, leading to serious ecological and health concerns.

Globally, over **400 million metric tons of plastic waste** are produced every year. A large portion of this waste ends up in **landfills**, and eventually finds its way into the **oceans and seabeds**, where it severely damages both **terrestrial and marine ecosystems**. One of the key reasons behind this persistence is the presence of **strong carbon–carbon bonds** in synthetic plastics, which makes them **resistant to microbial degradation**.

In light of these challenges, **bioplastics** have emerged as a promising alternative. Derived from renewable resources, many bioplastics are designed to be **biodegradable or compostable**, offering a more sustainable and eco-friendly solution to the global plastic crisis. Bioplastics are a class of materials derived from **renewable biological sources** such as **corn starch, sugarcane, potato starch, or even microorganisms**. Unlike traditional plastics, some bioplastics can break down naturally under suitable conditions, significantly reducing their environmental footprint. More importantly, their production taps into the principles of **green chemistry**, emphasizing **cleaner synthesis routes** and the use of **renewable feedstock**.

In this seminar, we will explore the **types of bioplastics**, understand the **chemical processes behind their synthesis**, evaluate their **benefits and limitations**, and discuss how **chemistry** is paving the way for a **greener, more sustainable future**.



What are Bioplastics?

Bioplastic is a biodegradable material that come from renewable source and can be used to reduce the problem of plastic waste that suffocates All earthly ecosystems and cause pollution in the biosphere.

Types of Bioplastics

Bioplastics can be broadly categorized based on their **origin (bio-based or fossil-based)** and **end-of-life behaviour (biodegradable or non-biodegradable)**. The main types used in the market today include:

1. Polylactic Acid (PLA)

- **Source:** Corn starch, sugarcane, or other carbohydrate-rich crops.
- **Properties:** Transparent, rigid, and compostable under industrial conditions.
- **Applications:** Food packaging, disposable cutlery, 3D printing filament, medical implants.
- **Synthesis:** Produced by the fermentation of sugars to lactic acid, followed by polymerization.

2. Polyhydroxyalkanoates (PHA)

- **Source:** Synthesized naturally by bacteria using sugars or lipids as carbon sources.
- **Properties:** Biodegradable, biocompatible, water-insoluble.
- **Applications:** Medical devices, agricultural films, packaging materials.
- **Note:** PHA includes many variants like PHB (Polyhydroxybutyrate) and PHV.

3. Starch-Based Bioplastics

- **Source:** Potato, corn, wheat, or cassava starch.
- **Properties:** Biodegradable, hydrophilic, low mechanical strength (usually blended with other polymers).
- **Applications:** Compostable bags, food trays, loose-fill packaging.
- **Note:** Can be processed into thermoplastic starch (TPS) by adding plasticizers.

4. Cellulose-Based Plastics

- **Source:** Cellulose derived from wood, cotton, or hemp.
- **Properties:** Biodegradable, flexible, transparent.
- **Applications:** Films, coatings, photographic films, and packaging.
- **Types:** Cellophane, cellulose acetate.

5. Bio-Polyethylene (Bio-PE) and Bio-PET

- **Source:** Ethanol from sugarcane or other plant materials.
- **Properties: Not biodegradable**, but identical in structure to conventional PE and PET.
- **Applications:** Bottles (like Coca-Cola's PlantBottle), food packaging, containers.
- **Advantage:** Can be processed using existing plastic manufacturing infrastructure.

6. Algae-Based Bioplastics (Emerging Technology)

- **Source:** Seaweed or microalgae.
- **Properties:** Potentially biodegradable, sustainable with low land and freshwater use.
- **Applications:** Packaging, films, cosmetics (still under research and development).

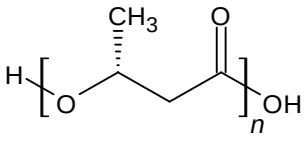
These different types of bioplastics are tailored to specific needs based on **durability, degradability, and functionality**, and their adoption is growing steadily across industries from **packaging and agriculture to healthcare and electronics**.

Main topic of concerns:

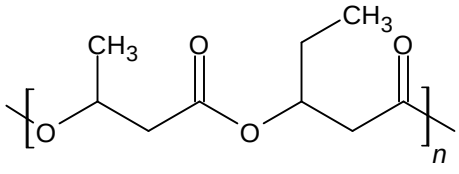
1. Polyhydroxyalkanoates (PHA)

Polyhydroxyalkanoates (PHAs) are a family of biodegradable polyesters naturally synthesized by various microorganisms through the fermentation of sugars or lipids. These biopolymers serve as intracellular carbon and energy storage compounds in bacteria. PHAs have garnered significant attention as sustainable alternatives to conventional plastics due to their biodegradability and biocompatibility.

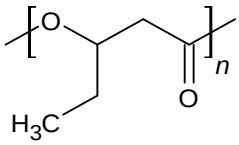
 Chemical Structure:



Poly-(R)-3-hydroxybutyrate



Poly(3-hydroxybutyrate-co-3-hydroxyvalerate)



Polyhydroxyvalerate

 Properties

- **Biodegradability:** PHAs are fully biodegradable under aerobic and anaerobic conditions, making them environmentally friendly.
- **Thermal Properties:** Melting points range from 40°C to 180°C, depending on monomer composition.
- **Mechanical Properties:** PHAs can exhibit a range of mechanical properties from rigid and brittle to flexible and elastic, based on their monomeric composition.
- **Barrier Properties:** PHAs have good resistance to moisture and aroma permeability, making them suitable for packaging applications.

 Applications:

- **Packaging:** Biodegradable films, containers, and bags.
- **Medical Devices:** Sutures, drug delivery systems, and tissue engineering scaffolds.
- **Agriculture:** Mulch films and controlled-release fertilizer coatings.
- **Textiles:** Fibres and non-woven fabrics.

The versatility of PHAs makes them suitable for a wide range of applications, particularly where biodegradability and biocompatibility are desired.

 Advantages:

- **Renewable Resources:** Produced from renewable feed stocks like sugars and lipids.
- **Biodegradability:** Decompose naturally without leaving harmful residues.
- **Biocompatibility:** Safe for medical and pharmaceutical applications.
- **Versatility:** Properties can be tailored by altering monomer composition.

 Disadvantages:

- **Production Cost:** Currently more expensive to produce than conventional plastics.
- **Thermal Stability:** Some PHAs have lower thermal stability, limiting processing options.
- **Brittleness:** Certain PHAs, like PHB, can be brittle, restricting their use in flexible applications.

2**. Starch-Based Bioplastics**

Starch-based bioplastics are one of the most widely used categories of bioplastics, accounting for nearly 50% of the global bioplastics market. Derived from renewable and abundant sources such as corn, potatoes, and cassava, starch bioplastics offer an eco-friendly alternative to conventional plastics. The production process typically involves gelatinizing starch and blending it with plasticizers like glycerol, glycol, or sorbitol to improve flexibility and processability. This mixture forms **thermoplastic starch (TPS)**, which can be moulded using traditional techniques such as extrusion, injection moulding, and solution casting. The physical and mechanical properties of starch-based plastics are largely influenced by the ratio of amylose to amylopectin; high-amylose starch imparts better strength but is harder to process due to its higher gelatinization temperature and viscosity.

To improve performance and compostability, starch is often blended with biodegradable polyesters such as polylactic acid (PLA), polycaprolactone (PCL), or BASF's Ecoflex (PBAT). These blends are commonly used in applications like food packaging, compostable bags, pharmaceutical capsules, and biodegradable agricultural films. Starch-based plastics can also be processed into paper-like films or used in lightweight, biodegradable packaging materials like packing peanuts. Additionally, **starch-based nanocomposites** have been developed, offering improved thermal stability, gas barrier properties, and moisture resistance.

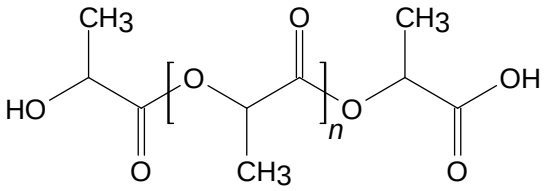
The primary advantages of starch-based plastics include their biodegradability, compostability, renewable sourcing, and lower carbon footprint compared to petroleum-based plastics. They are also non-toxic and safe for direct contact with food and pharmaceuticals. However, these bioplastics also have certain limitations. Pure starch materials are brittle and highly sensitive to moisture, and some blends with polyolefin may not be biodegradable. Furthermore, the durability and shelf-life of starch-based plastics can be lower than that of conventional plastics, and large-scale production may compete with food supply chains due to the agricultural sourcing of raw materials. Despite these challenges, starch-based bioplastics remain a promising solution in the global effort to reduce plastic pollution and transition towards more sustainable materials.




3. Polylactic Acid (PLA)

Polylactic Acid (PLA) is a biodegradable thermoplastic polyester derived from renewable resources such as corn starch, sugarcane, or cassava. It is synthesized through the polymerization of lactic acid monomers, which are produced via the fermentation of plant-based sugars.

 Chemical Structure:



 Properties:

- **Density:** 1.21–1.43 g/cm³
- **Melting Point:** 150–160°C (for comparison PET has 225°C MP)
- **Mechanical Properties:** Low tensile strength, low thermal expansion
-
- **Biodegradability:** Compostable under industrial conditions (under high temperature and pressure)

 Applications:

- **Packaging:** Biodegradable containers, films, and bottles.
- **Medical Devices:** Sutures, implants, and drug delivery systems due to its biocompatibility.
- **3D Printing:** Widely used as filament material in fused deposition modeling (FDM) printers.
- **Textiles:** Blended with other fibers for biodegradable fabrics.

 Advantages:

- **Renewable Resources:** Derived from plant-based materials, reducing reliance on fossil fuels.
- **Biodegradability:** Breaks down into lactic acid under composting conditions, minimizing environmental impact.
- **Low Toxicity:** Safe for use in medical and food-related applications.
- **Processability:** Compatible with existing plastic processing equipment.

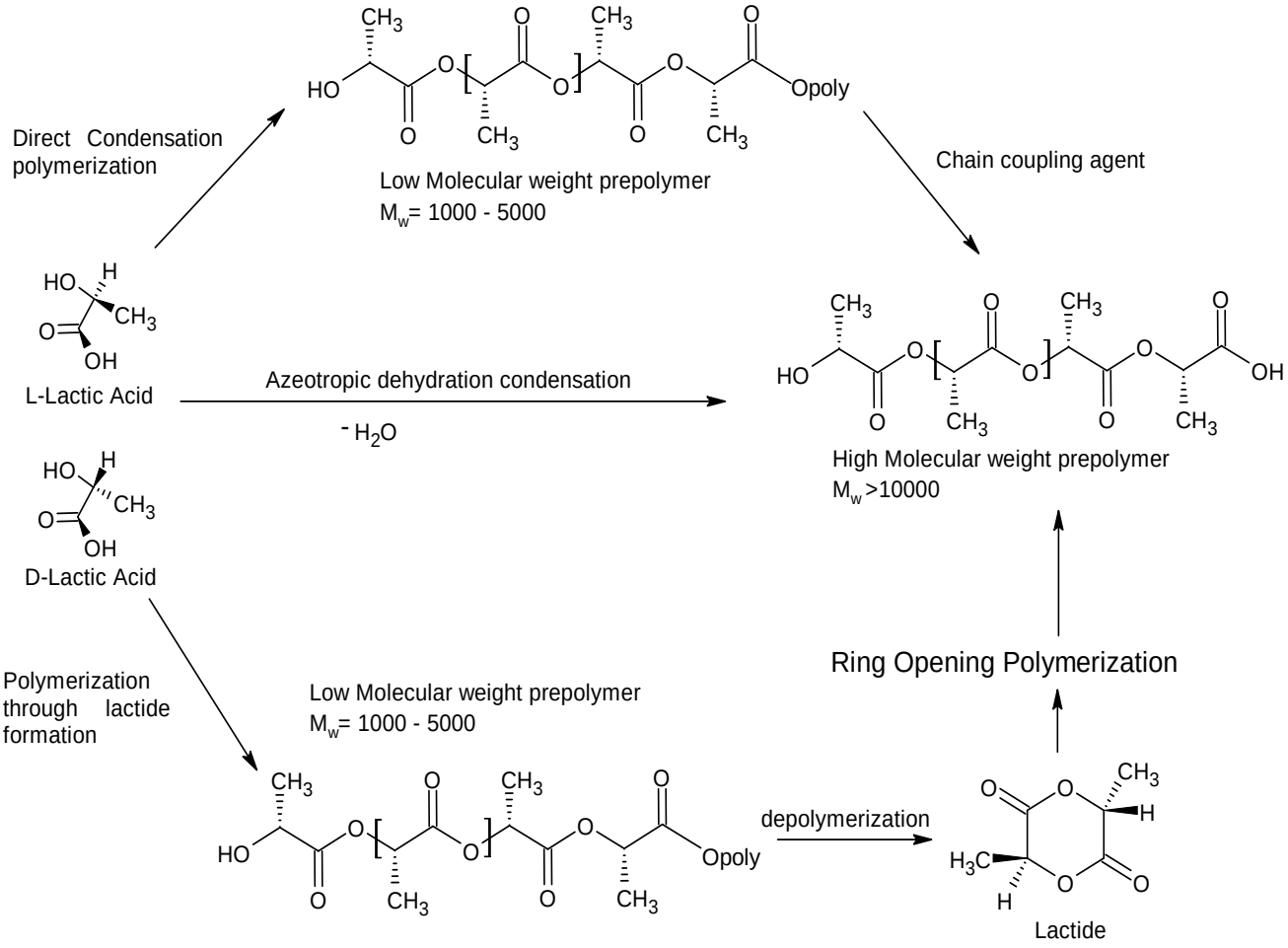
 Disadvantages:

- **Thermal Stability:** Lower heat resistance compared to some conventional plastics.
- **Mechanical Properties:** Brittle nature may limit its use in high-impact applications.

- **Composting Requirements:** Requires specific industrial composting conditions for effective degradation.
- **Cost:** Generally more expensive than petroleum-based plastics.

Synthesis Methods of PLA

Several industrial routes afford usable (i.e. high molecular weight) PLA. Two main monomers are used: lactic acid, and the cyclic di-ester, lactide. These monomers are typically made from fermented plant starch such as from corn, cassava, sugarcane or sugar beet pulp.



Precursors:

1. Lactic Acid

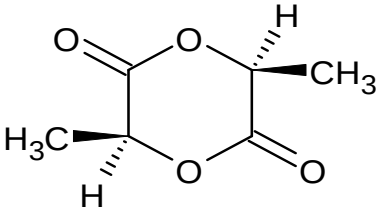
Lactic acid is mainly prepared in large quantities (around 200 kT per year) by the bacterial fermentation of carbohydrates. These fermentation processes can be classified according to the type of bacteria used: (i) the hetero fermentative method, which produces less than 1.8 mole of

lactic acid per mole of hexose, with other metabolites in significant quantities, such as acetic acid, ethanol, glycerol, mannitol and carbon dioxide; (ii) the homo-fermentative method, which leads to greater yields of lactic acid and lower levels of by-products, and is mainly used in industrial processes. The conversion yield from glucose to lactic acid is more than 90 per cent.

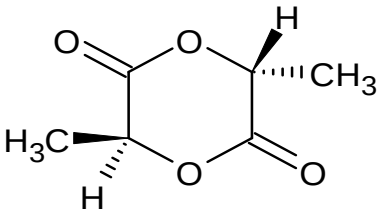
In general, the sources of basic sugars are glucose and maltose from corn or potato, sucrose from cane or beet sugar, etc. The processing conditions are an acid pH close to 6, a temperature around 40°C and a low oxygen concentration. The major method of separation consists in adding $CaCO_3$, $Ca(OH)_2$, $Mg(OH)_2$, NaOH, or NH_4OH to neutralize the fermentation acid and to give soluble lactate solutions, which are filtered to remove both the cells (biomass) and the insoluble products. The product is then evaporated, crystallized, and acidified with sulphuric acid to obtain the crude lactic acid. If the lactic acid is used in pharmaceutical and food applications, it is further purified to remove the residual by-products. If it is to be polymerized, it is purified by separation techniques including ultra-filtration, nano-filtration, electro-dialysis and ion-exchange processes.

2. Lactide

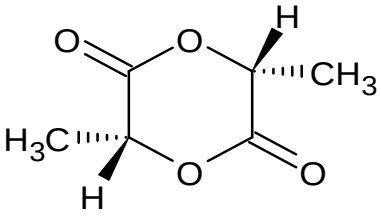
The cyclic dimer of lactic acid combines two of its molecules and gives rise to L-lactide or LL - lactide, D-lactide or DD-lactide, and meso-lactide or LD-lactide (a molecule of L-lactic acid associated with another one of D-lactic acid). A mixture of L- and D- lactides is a racemic lactide (rac lactide). Lactide is usually obtained by the depolymerization of low molecular weight PLA under reduced pressure to give a mixture of L- , D- and meso-lactides. The different percentages of the lactide isomers formed depend on the lactic acid isomer feedstock, temperature and the catalyst's nature and content. A key point in most of the processes is the separation between each stereoisomer to control the final PLA structure (e.g. by vacuum distillation) which is based on the boiling point differences between the meso- and the L- or D- lactide.



L-lactide



meso-lactide



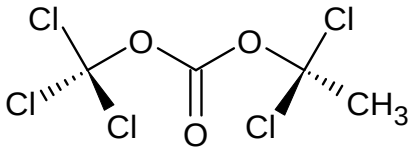
D-lactide

There are three primary methods for synthesizing PLA:

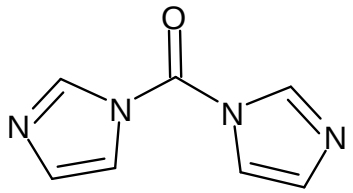
1. *Lactic acid condensation and coupling*

The condensation polymerization is the least expensive route, but it is difficult to obtain high molecular weights by this method. The use of coupling or esterification-promoting agents is

required to increase the chains length, but at the expense of an increase in both cost and complexity (multistep process). The role of chain coupling agents is to react with either the hydroxyl (OH) or the carboxyl end-groups of the PLA thus giving telechelic polymers. The disadvantages are that the final polymer may contain unreacted chain-extending agents, oligomers and residual metallic impurities from the catalyst. The chain coupling or chain-extending agents or adjuvant are bis (tri-chloromethyl) carbonate and carbonyl diimidazole, but they produce low PLA quality and reaction by-products (water & alcohols),that must be either neutralized or removed completely from high viscous reaction mixture, adding cost and complexity hence this route is not preferred in this research.



bis-(tricholoromethyl) carbonate



Carbonyl diimidazole

2. *Azeotropic dehydration and condensation*

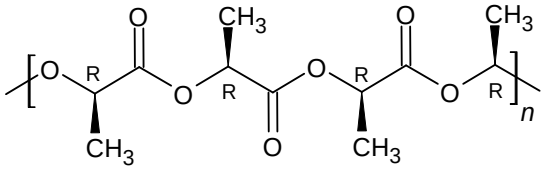
The azeotropic condensation polymerization is a method used to obtain high chain lengths without the use of chain extenders or adjuvents and their associated drawbacks. Mitsui Chemicals (Japan) has commercialized this process wherein lactic acid and a catalyst are azeotropically dehydrated in a refluxing, high boiling, aprotic solvent under reduced pressures to obtain high molecular weight PLA (Mw 300 000). A general procedure consists in the reduced pressure distillation of lactic acid for 2–3 h at 130°C to remove most of the condensation water. The catalyst and diphenyl ether are then added and a tube packed with molecular sieves is attached to the reaction vessel. The refluxing solvent is returned to the vessel by way of the molecular sieves during 30–40 h at 130°C. Finally, the ensuing PLA is purified.

This polymerization gives considerable catalyst residues because of its high concentration needed to reach an adequate reaction rate. This can cause many drawbacks during processing, such as degradation and hydrolysis. For most biomedical applications, the catalyst toxicity is a highly sensitive issue. The catalyst can be deactivated by the adding of phosphoric acid or can be precipitated and filtered out by the addition of strong acids such as sulphuric acid.

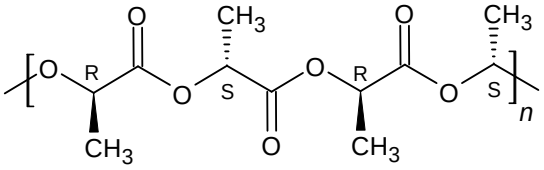
3. *Ring Opening Polymerization of Lactide*

The lactide method is the only method for producing pure high molecular weight PLA (Mw 100 000). The mechanism involved in ROP can be ionic (anionic or cationic) or coordination–insertion, depending on the catalytic system. It has been found that trifluoromethane sulphonic acid and its methyl ester are the only cationic initiators known to polymerize lactide. Lactide anionic polymerizations proceed by the nucleophilic reaction of the anion with the carbonyl group and the subsequent acyl–oxygen bond cleavage, which produces an alkoxide end-group, which continues to propagate. Some authors have shown that the use of alkoxides, such as potassium methoxide, can yield well-defined polymers with negligible racemization. Both the anionic and cationic ROPs are usually carried out in highly purified solvents, and although they show a high reactivity, they are susceptible to give racemization, transesterification and high impurity levels. For industrial and large commercial use, it is preferable to do bulk and melt polymerization with low levels of non-toxic catalysts.

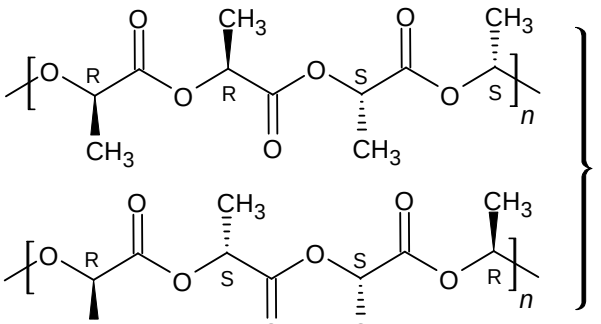
Stereo-Homogeneity of PLA blocks: Four different stereoisomers of PLA are possible and are shown below. Isotactic PLA is formed from either pure D or L-lactide, syndiotactic PLA has alternating configurations of the sequential stereocenters. However, atactic PLA has a random distribution of configurations about the stereocenters while its heterotactic counterpart has regions of stereo-homogeneity. Isotactic stereoblock PLA is similar to isotactic PLA but differs in that rac-lactide is used instead of pure L- or D-lactide.



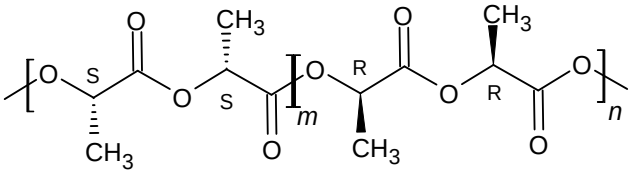
Isotactic



Syndiotactic



Heterotactic

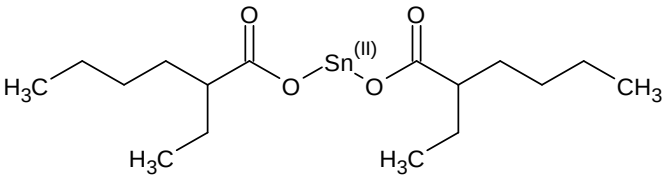


Isotactic Stereoblock

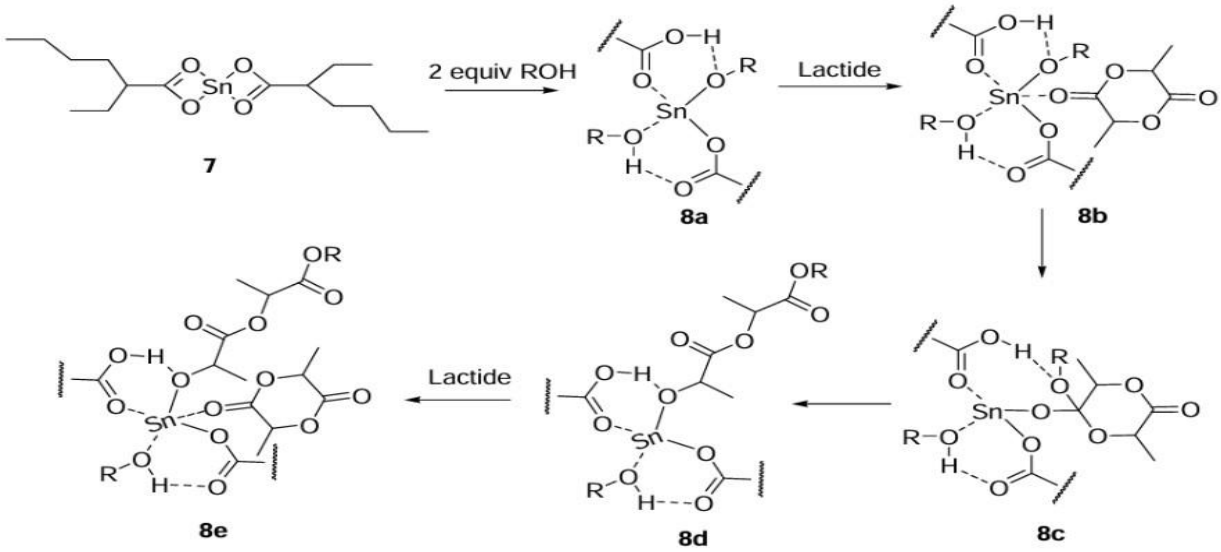
The synthesis:

Isotactic PLA is formed by the polymerization of either pure L or D-lactide. The coordination-insertion mechanism is proposed and shown in the following diagram. Molecular modeling suggests that two alcohols (these alcohols can be initiators such as MeOH or iPrOH or the propagating hydrolyzed lactide) exchange with the octoate ligands (8a) followed by the

coordination of lactide to the metal center (8b). Insertion of the alcohol (8c) followed by ring-opening (8d) generates a linear monomer (8e) and starts propagation. The ROP of neat lactide with $Sn(Oct)_2$ gives PLA having molecular weights up to 106 g/mol at 140 – 180 °C with catalyst concentration of 100-1000 ppm in 2-5 hours. A major drawback of the tin catalyst is the incorporation of the toxic metal on the polymer chain end and the resulting toxicity risk in biomedical applications.



Tin (II) bis-(2-ethylhexanoate)

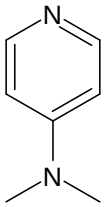


Why to use Stannous Octoate as the catalyst?

A systematic investigation has led to the wide use of tin compounds, namely tin(II) bis-2-ethylhexanoic acid (stannous octoate) as a catalyst in PLA synthesis. This is mainly due to its high catalytic efficiency, low levels of toxicity, food and drug contact approval and ability to give high molecular weights with low racemization.

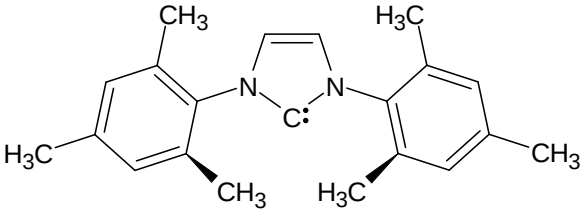
Use of Organic catalyst for the ROP synthesis of Lactide

An important consideration in the polymerization of lactide is the removal of metal contaminants, bound to the chain end before application in resorbable biomaterials. The application of organocatalysts to controlled lactide polymerization would be a highly viable alternative to organometallic approaches. Several organic compounds have demonstrated high activity and enantioselectivity in a number of common organic transformations. Some of them are: 4-(dimethylamino) pyridine (DMAP) and N-Heterocyclic carbene (NHC).



N,*N*-dimethylpyridin-4-amine

DMAP

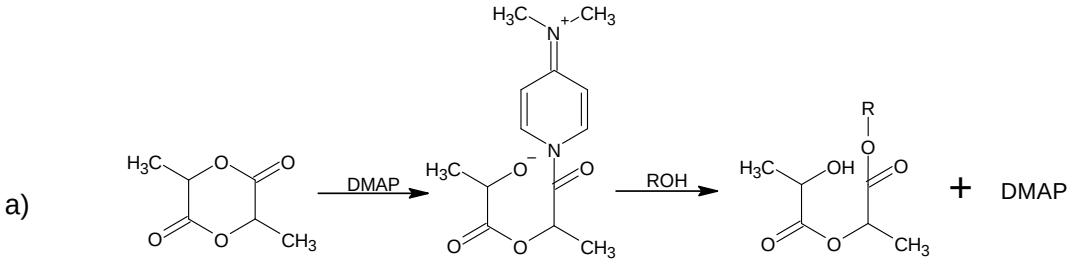


1,3-bis(2,4,6-trimethylphenyl)-1,3-dihydro-2*H*-imidazol-2-ylidene

NHC

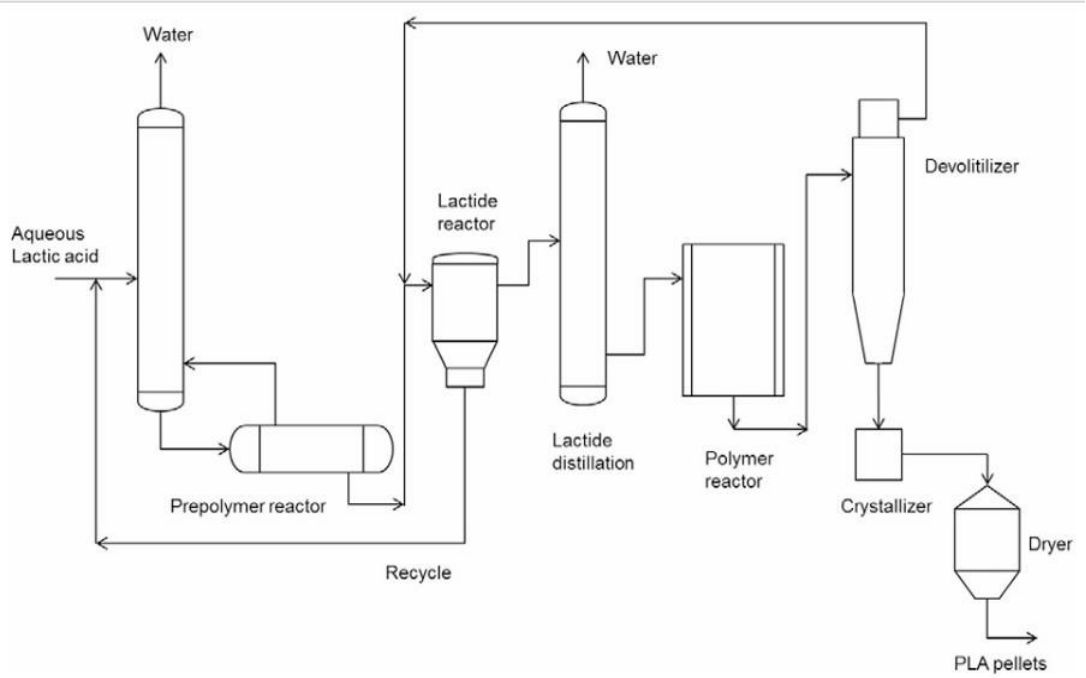
Mechanism:

Initiation occurs when alcohol reacts with the lactide-organic catalyst complex, leaving a terminal hydroxyl group to act as a nucleophile to react with additional lactide monomer. High conversions of up to 99% in 2 hours are obtained with NHC. These organic catalysts are relatively inexpensive and highly active, and they provide attractive substitutes for the ROP of lactide for biomedical and environmental applications.



Industrial Mass Production of PLA

In the first step, water is removed in a continuous condensation reaction of aqueous lactic acid to produce lowmolecular-weight prepolymer. Next, the prepolymer is catalytically converted into the cyclic dimer, lactide. The molten lactide mixture is then purified by distillation. Finally, highmolecular-weight PLA polymer is produced using a ring-opening lactide polymerization. After the polymerization is complete, any remaining lactide monomer is removed and recycled within the process.



Degradation of Bioplastics

1. Poly-Lactic Acid

Degradation leads to irreversible changes of the polymer until it gradually fails due to the loss of various properties. Such loss of properties can occur under different mechanisms, including chemical hydrolysis, microbial, photochemical, thermal, and enzymatic degradation, which mainly occur by main chain scission or side chain scission**s.**

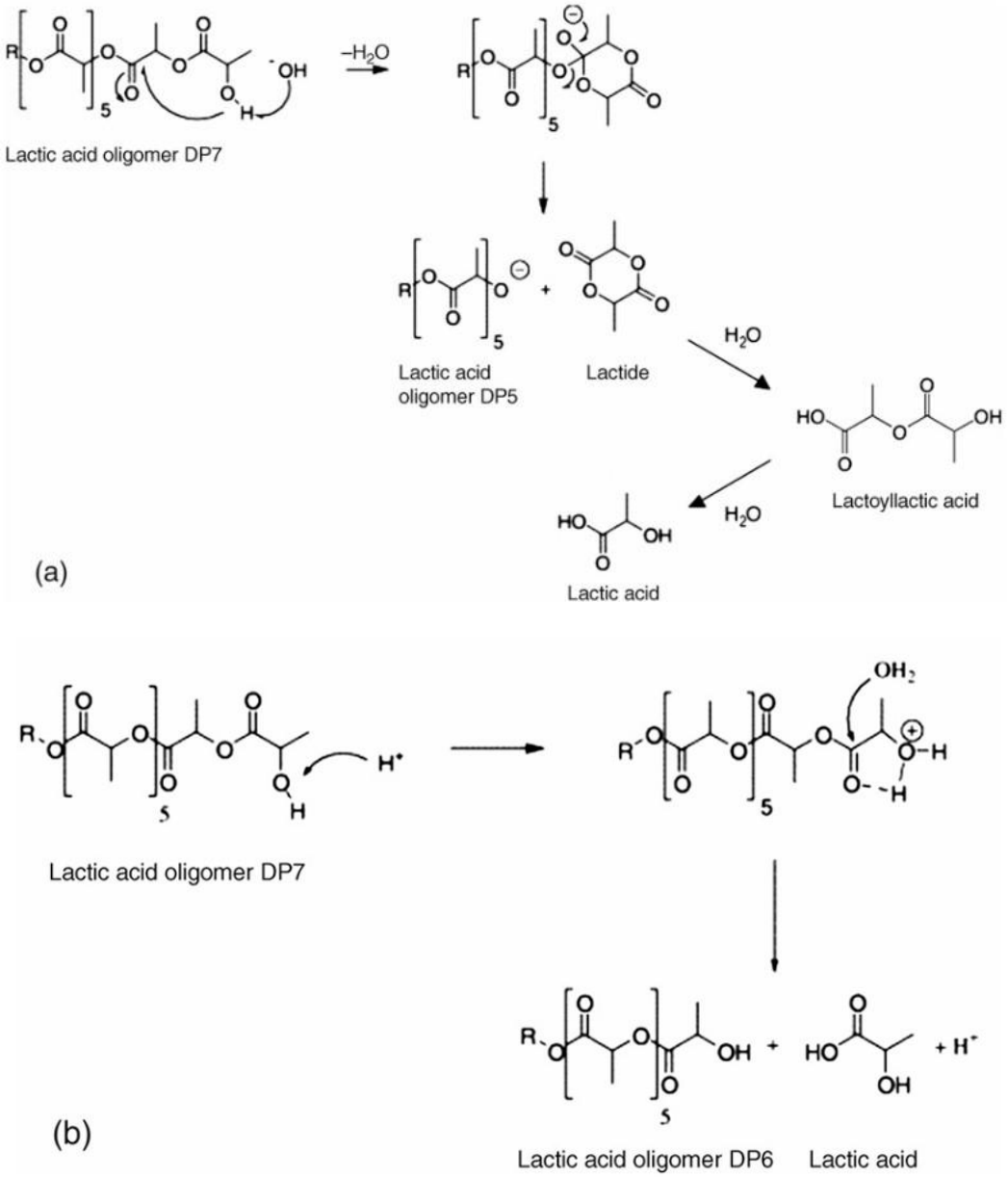
1. **Abiotic (Non-biological) Degradation –**

   a. **Hydrolysis**

Hydrolytic degradation takes place when PLA is exposed to moisture: the ester groups of the main chain of the polymer are cleaved, resulting in a decrease of molecular weight and the release of soluble oligomers and monomers. The products of the hydrolysis self-catalyze the reaction. Thus, hydrolysis of PLA starts by the diffusion of water molecules into the amorphous regions, which in turn initiates the cleavage of the ester bonds.

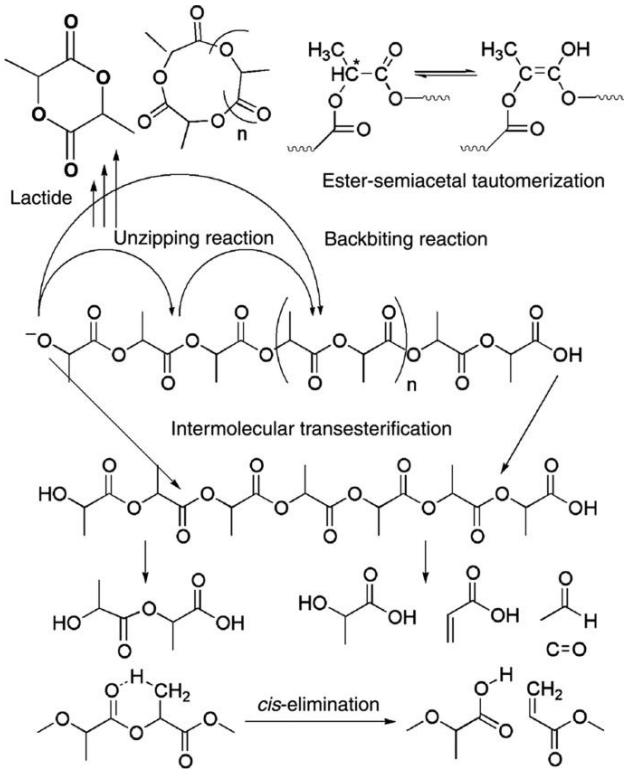
For example, PLA has been used in plasticulture as mulch films where PLA can be affected by a number of abiotic factors, such as temperature, pH, soil moisture, and UV radiation, which all play relevant roles in the degradation. During abiotic degradation, the mulch films are fragmented, the tensile strength of the material weakens, and as light reduction of Mw occurs, and then PLA is converted into CO_2, water, and inorganics. Hydrolysis is one of the mechanisms that helps degrade PLA in this environment. Temperature also plays a crucial role in the

hydrolysis of PLA in non-medical applications. The rate of degradation of PLA increases with temperature, resulting in faster cleavage of the ester bonds.



b. **Thermal Degradation:**

PLA is susceptible to thermal degradation during processing, leading to a decrease in Mw, thermal degradation of PLA can be attributed to the hydrolysis initiated by residuals of water during processing, unzipping depolymerization reaction, random main-chain scission, and intramolecular and intermolecular transesterification. Therefore, drying PLA resins before processing is highly recommended.



The dominant pathway of the PLA thermal degradation above 200 °C is intra- and intermolecular ester exchange, cis-elimination, radical and concerted non-radical reactions. McNeill and Leiper stated that the mechanism is based upon a hydroxyl end-initiated ester inter change, non-radical process. Aoyagi et al. and Abe et al. proposed that PLA not only follows one mechanism during pyrolysis but this thermodegradation also involves more than two pathways, such as random scission, unzipping depolymerization, and intermolecular transesterification. Thermal degradation of PLA is a complex phenomenon leading to the appearance of different compounds such as low molecular weight molecules and linear and cyclic oligomers with different M_w and lactide. Other degradation products have been detected such as CO, CO_2, acetaldehyde, and methyl ketone. PLA thermal degradation is influenced by several factors such as initial Mw, moisture, and residual polymerizing catalysts.

Kopinke showed that PLA in the presence of residual Sn from the polymerization process leads to a selective depolymerization step producing lactide. Cam and Marucci observed that the presence of residual metals assists thermal degradation in PLA, affecting the onset temperature in the order of Fe >Al>Zn>Sn. Furthermore, the presence of stannous octoate catalyst ($Sn(Oct)_2$) in a proportion of 0.5, 1, and 5 wt.%, accelerated the degradation of PLA. To improve the thermal stability of PLA the end groups of the polymer chain must be protected and it is famously done by the acetylation process, which not only achieves end-protection, but also is capable of removing residual metals that accelerate degradation of PLA.

2. **Biotic (Biological) Degradation – Biodegradation:**

PLA degradation upon disposal in the environment (environmental degradation) is more challenging because PLA is largely resistant to attack by microorganisms in soil or sewage under ambient conditions. The polymer must first be hydrolyzed at elevated temperatures (about 60 °C) to reduce the Mw before biodegradation can commence. Under conditions of high temperature and high humidity, as inactive compost, for example, PLA will degrade quickly and disintegrate within weeks to months. The primary mechanism of degradation occurs by a two step process starting also with hydrolysis, followed by bacterial attack on the fragmented residues. During the initial phases of degradation, the high Mw polyester chains hydrolyze to lower Mw oligomers.

As the average Mw reaches approximately ~10,000 Da, micro-organisms present in the soil begin to digest the lower Mw lactic acid oligomers, producing carbon dioxide and water. The rate of hydrolysis is accelerated by acids or bases and is dependent on moisture content and temperature. PLA products rapidly degrade in both aerobic and an aerobic composting conditions.

PLA undergoes **enzymatic degradation** in biological environments. Studies (both **in vivo** and **in vitro**) show that degradation is influenced by factors like **pH**, which helps predict in vivo performance.
Enzymes like **proteinase K** and **pronase** can hydrolyze PLA, although **crystalline regions resist enzyme penetration**. Initially, degradation is minimal, but over time **pores and cracks** develop, increasing the surface area for further enzymatic action.

Conclusion

As we come to the end of this presentation, I want to leave you with a broader perspective on what bioplastics truly represent. They are not just another class of materials—they are a reflection of our collective urgency to rethink the way we produce, consume, and discard. In a world grappling with the environmental toll of petroleum-based plastics, bioplastics offer us a tangible step toward a more sustainable future.

While challenges remain in production, scalability, and waste management, continued research and collaboration can unlock their full potential. As students, it's our duty to drive this transition, ensuring that innovation always aligns with ecological responsibility.

THANK YOU!!

Acknowledgment:

We would like to take this opportunity to express my sincere gratitude to all those who have supported and encouraged this presentation. First and foremost, we extend our heartfelt thanks to our college, Teacher-in-charge sir and Vice-Principal Sir for providing us with the platform and resources to pursue academic exploration and scientific discussions.

We are deeply grateful to our respected Head of the Department, Dr. Kalyan Kumar Mondal, whose guidance, encouragement continue to inspire us in our academic journey. We also thank all our professors, whose dedication to teaching and guidance constantly motivates us to aim higher. Our thanks also go to the Internal Quality Assurance Cell (IQAC) for their support in promoting academic excellence and quality initiatives within our institution.

A special word of appreciation to the non-teaching staff of our department, whose tireless efforts behind the scenes ensure that everything runs smoothly and efficiently. Lastly, we extend our warmest thanks to all of our batchmates, juniors and seniors who are present today – your participation and interest make endeavors like these truly meaningful.

Thank you all once again for being part of this academic occasion.

References

1. **Mehta R., Kumar V., Bhunia H., Upadhyay S.N., Synthesis of poly(lactic acid): A review, J. Macromol. Sci., Polym. Rev. , 2005**
2. **Doi Y., Steinbüchel A., Biopolymers, Applications and Commercial Products – Polyesters III , Wiley-VCH, Weiheim – Germany , 2002**
3. **Ajioka M. , Enomoto K. , Suzuki K. , Yamaguchi A. , The basic properties of poly lactic acid produced by the direct condensation polymerisation of lactic acid , J. Environ. Polym. Degrad. , 3 (8), 1995**
4. **Kricheldorf H.R., Sumbel M., Polymerization of l, l -lactide with tin(II) and tin(IV) halogenides , Eur. Polym. J. , 25 (6) , 1989**
5. **Hakkarainen M., Karlsson S., Albertsson A.C., Rapid (bio)degradation of polylactide by mixed culture of compost micro-organisms low molecular weight products and matrix changes, Polymer, 41, 2000**
6. **Tormala P. , Vasenius J., Vainionpaa S. , Laiho J., Pohjonen T., Rokkanen P., Ultra-high-strength absorbable self-reinforced polyglycolide (SR-PGA) composite rods for internal fixation of bone fractures: In vitro and in vivo study, J. Biomed. Mater. Res., 25, 1991**
7. **S. Farah, etal., Physical and mechanical properties of PLA, and their functions in wide spread applications —A comprehensive review, Adv. Drug Deliv. Rev. (2016)**
8. **E. Castro-Aguirre, F. Iñiguez-Franco, H.Samsudin, X. Fang, R.Aurasa, Poly(lactic acid)—Mass production, processing, industrial applications, and end of life, Adv. Drug Deliv. Rev. (2016)**

Link to the Presentation: **Beyond Petroleum: The Science and Scope of Bioplastics**

OR Scan the QR code to see the Presentation

Scan me!

Kinetically Controlled Product vs Thermodynamically Controlled Products

Ankita Roy, Debashmita Adhikary, Amrick Maity

Semester II

Abstract

Chemical reactions often yield more than one possible product, depending on the reaction conditions. The concepts of kinetic and thermodynamic control help explain why different products form under different circumstances. A kinetically controlled product is favored when a reaction proceeds rapidly under mild conditions, forming the product with the lowest activation energy. In contrast, a thermodynamically controlled product is favored at higher temperatures or longer reaction times, where equilibrium allows the formation of the most stable product.

This presentation explores the fundamental differences between kinetic and thermodynamic control, including reaction energy profiles, activation barriers, and reaction reversibility. Real-world examples and experimental illustrations are used to highlight how reaction conditions influence product distribution. Understanding these concepts is essential in organic synthesis, drug design, and industrial chemistry, where product selectivity is critical.

Introduction

Kinetics – How quickly a product forms. **Thermodynamics** – How stable a product is in the long run.

Many reactions give two products: **A → B + C**

Which one would be the major product?

This issue is settled by the fact that whether the given reaction is reversible under the given condition or not. The product that is formed faster than the other is the **KINETICALLY CONTROLLED PRODUCT (KCP)** and it is the major product in an irreversible, kinetically–controlled reaction.

The product that is more stable of the two is the **THERMODYNAMICALLY CONTROLLED PRODUCT (TCP)** and it is the major product in a reversible, thermodynamically- controlled reaction.

When are reactions irreversible?

When the reaction temperature is deliberately kept low, and the reaction is done very rapidly so that the backward reaction does not get a chance to happen.

When are reactions reversible?

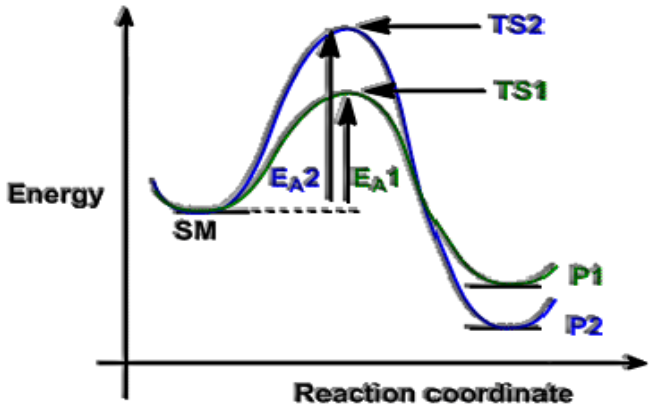
If temperature is increased so that both the forward and the backward reactions get faster and equilibrium is reached. If we allow the reaction to go on for a very long time, since every reaction can become reversible if proper amount of time is given to reach equilibrium

If the reaction is irreversible

TS-P1 is lower in energy than TS-P2, so the former is accessed at a faster rate. Reaction under kinetic control. P1 is the KCP. When the reactions are irreversible, KCP is the major product, i.e., P1 is the major product.

If the reaction is reversible

P2 is more stable than P1, and should dominate the equilibrium Reaction under thermodynamic control. P2 is the TCP. When the reactions are reversible, TCP is the major product, i.e., P2 is the major product.



Kinetic vs Thermodynamic Control: The Difference

Feature	Kinetic control	Thermodynamic control
Definition	Product that forms fastest	Most stable product
Activation energy	Lower	Higher
Reaction conditions	Low temp, short time	Higher temp, long time
Reversibility	Usually irreversible	Reversible
Product Stability	Less stable	More stable
Selectivity	Based on rate	Based on stability

Reaction Coordinate Diagram

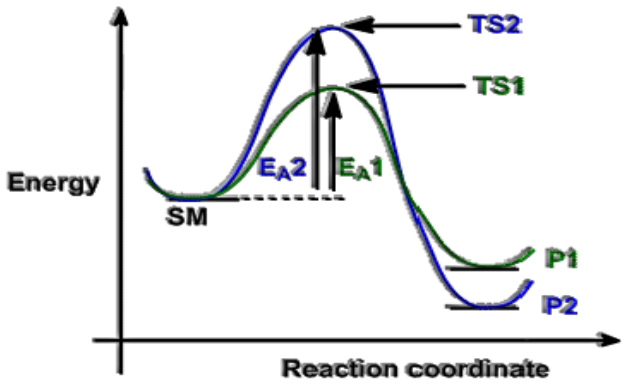


Diagram showing: Two products:

i. Kinetic: lower activation energy

ii. Thermodynamic: higher activation energy

The low temperature favors kinetics while the high temperature favors thermodynamics

Example 1 – Addition of HBr to 1,3-butadiene

Reaction: 1,3-butadiene + HBr → 1,2-addition product or 1,4-addition product

Important steps during the Reaction:

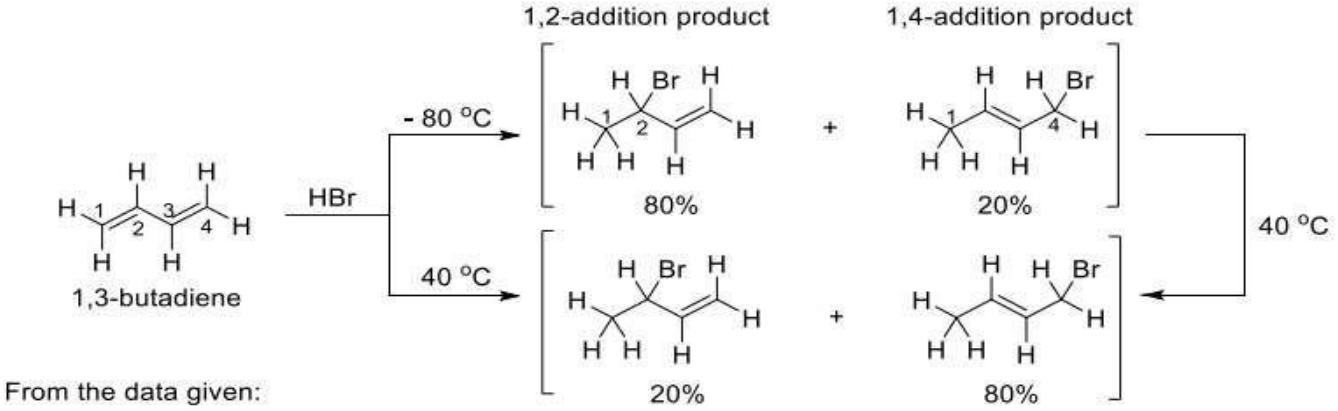
- Protonation forms allylic carbocation.
- Br^- (bromide) attacks at C2 or C4.

Products:

- 1,2-addition (KCP)
- 1,4-addition (TCP)

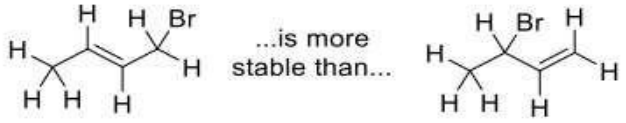
Low Temp (~0°C) favors 1,2-addition product i.e. the KCP
High Temp (~40°C): favors 1,4-addition product i.e. the TCP

Case study in KCP and TCP: 1,2- and 1,4-addition of hydrogen bromide to a conjugated diene

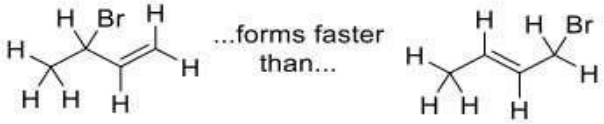


From the data given:

a) 1,4-addition product is the TCP, which means

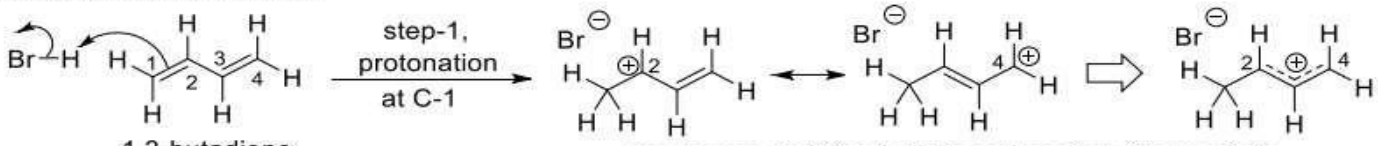


b) 1,2-addition product is the KCP, which means



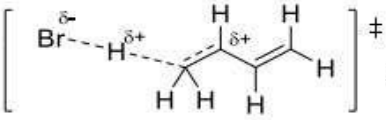
c) Once the reaction is done at low temp. and the product mixture is obtained in a certain ratio in favour of the 1,2-addition product (KCP), increasing the temp. changes the ratio in favour of the 1,4-addition product (TCP) - the 1,2-addition product converts to 1,4-addition product at higher temp.

Mechanism of HBr addition:



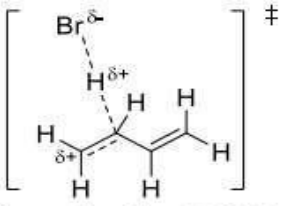
Step-1 is the RDS. It is regioselective. Protonation occurs at C-1 and not at C-2.

Resonance-stabilized allylic carbocation is formed selectively and not the alternative prim. carbocation that does not have such allylic stabilization.



TS for protonation @ C-1; e-deficiency on *sec*. C

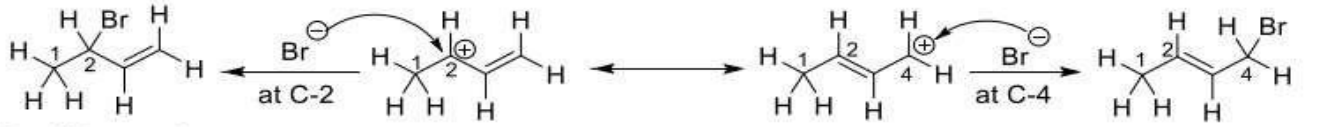
...is more stable than...



TS for protonation @ C-2; e-deficiency on *prim*. C

As protonation is an endothermic reaction, the TSs follow the respective carbocation intermediates (Hammond postulate).

Step-2 is the nucleophilic capture of the allylic cation by bromide either @ C-2 or @ C-4:



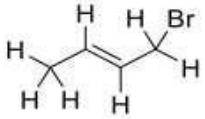
1,2-addition product

1,4-addition product

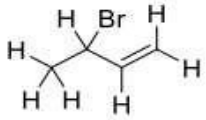
Why is the 1,4-addition product more stable than the 1,2-addition product?

As more substituted alkenes are more stable than isomeric, less substituted alkenes, the 1,4-addition product is more stable than the 1,2-addition product.

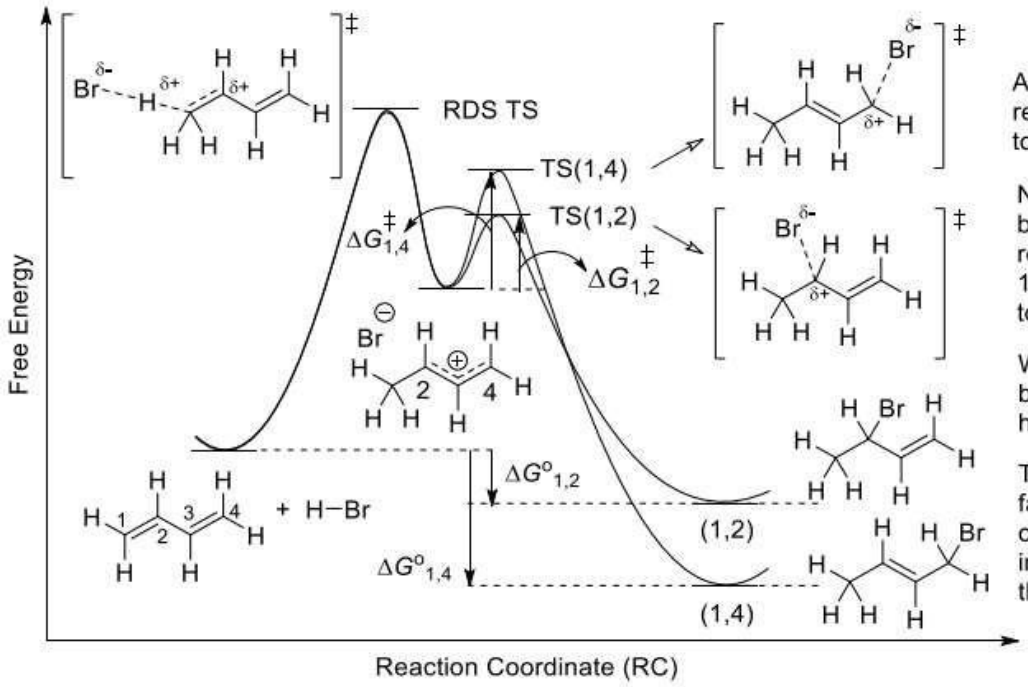
1,4-addition product is the TCP.



1,4-addition product disubstituted alkene, 5 hyperconjugative Hs



1,2-addition product monosubstituted alkene, only 1 hyperconjugative H



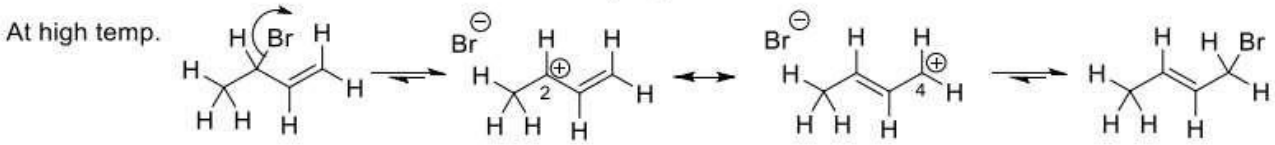
$\Delta G^{\ddagger}_{1,4} > \Delta G^{\ddagger}_{1,2}$

At low temp., the reverse reactions do not take place to any appreciable extent.

Note the large activation barriers for the backward reaction (conversion of the 1,2- and the 1,4-product to the allylic cation).

When temp. is raised, the backward reactions start happening.

The 1,2 product still forms faster, but at this temp. it can also get converted into the 1,4-product in the following way:



So, essentially now there is an eqm. between the 1,2- and 1,4-product.

As the latter is more stable, it accumulates and dominates the product mixture under this condition.

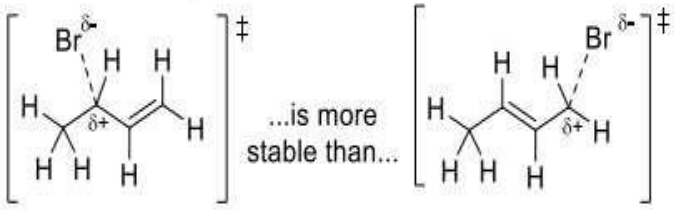
TCP is the major product.

Why does the 1,2-addition product form faster than 1,4-addition product?

Any discrimination must arise in the step-2, as step-1 is common for both products.

To understand the kinetic preference for 1,2-product, we must look at the two TSs for the respective step-2.

Step-2 is exothermic (as the carbocation intermediate is being quenched here), the TSs mimic the carbocation more than they do the products.



TS(1,2)

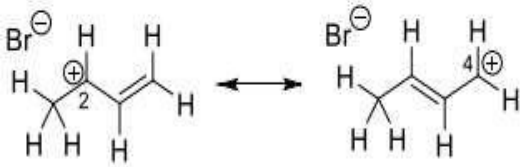
δ+ on *sec.* carbon

TS(1,4)

δ+ on *prim.* carbon

TS(1,2) is thus accessed by the allylic carbocation int. at a rate faster than the same int. accesses TS(1,4), leading to faster formation of the 1,2-addition product.

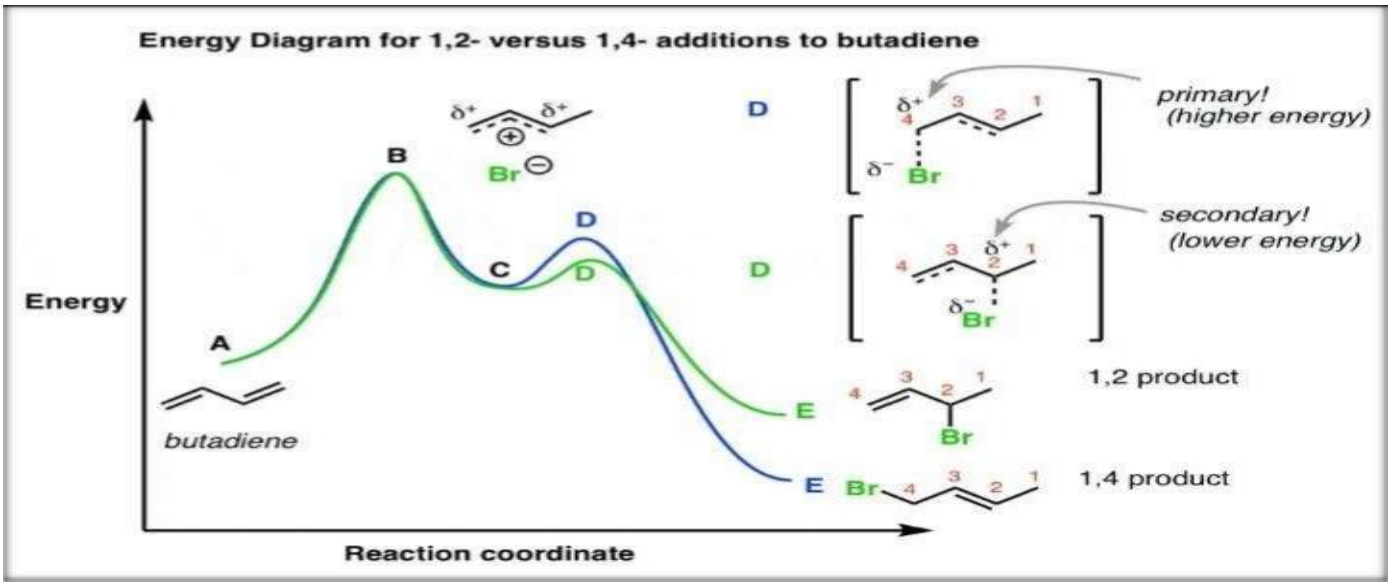
Secondly, as the carbocation generates by protonating the C-1 with HBr, bromide remains in close proximity to C-2 than it is for C-4; this *proximity effect* favours 1,2-addition:



Br^- closer to C^+(C2) Br^- away from C^+(C4)

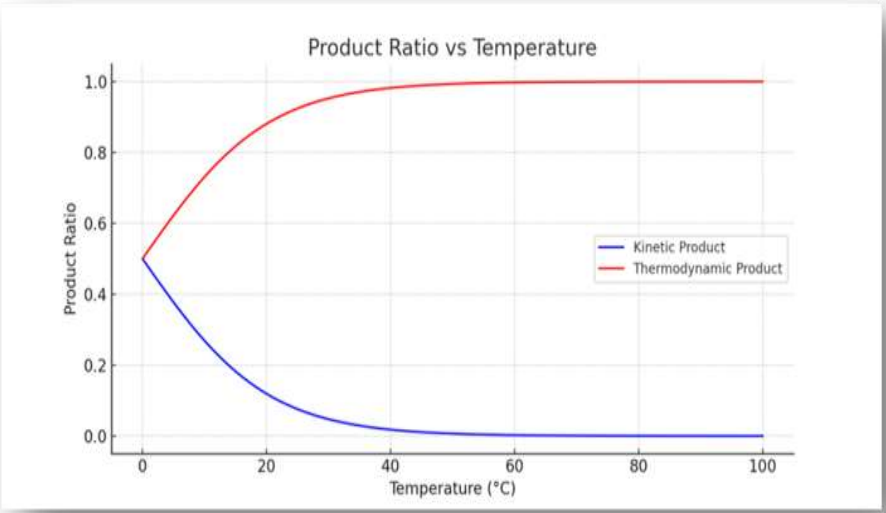
Br^- has to *travel a lot more* to reach C-4, so attack at C-2 is more favoured, leading to faster formation of 1,2-addition product.

Energy profile diagram for the Addition of HBr to 1,3-butadiene



Reversibility and Temperature Effects

- Low temp: insufficient energy for rearrangement → kinetic product
- High temp: allows equilibrium → thermodynamic product
- Graph: Product ratio vs temperature:
- Low T: kinetic dominates
- High T: thermodynamic dominates



Example 2 – Enolate Formation

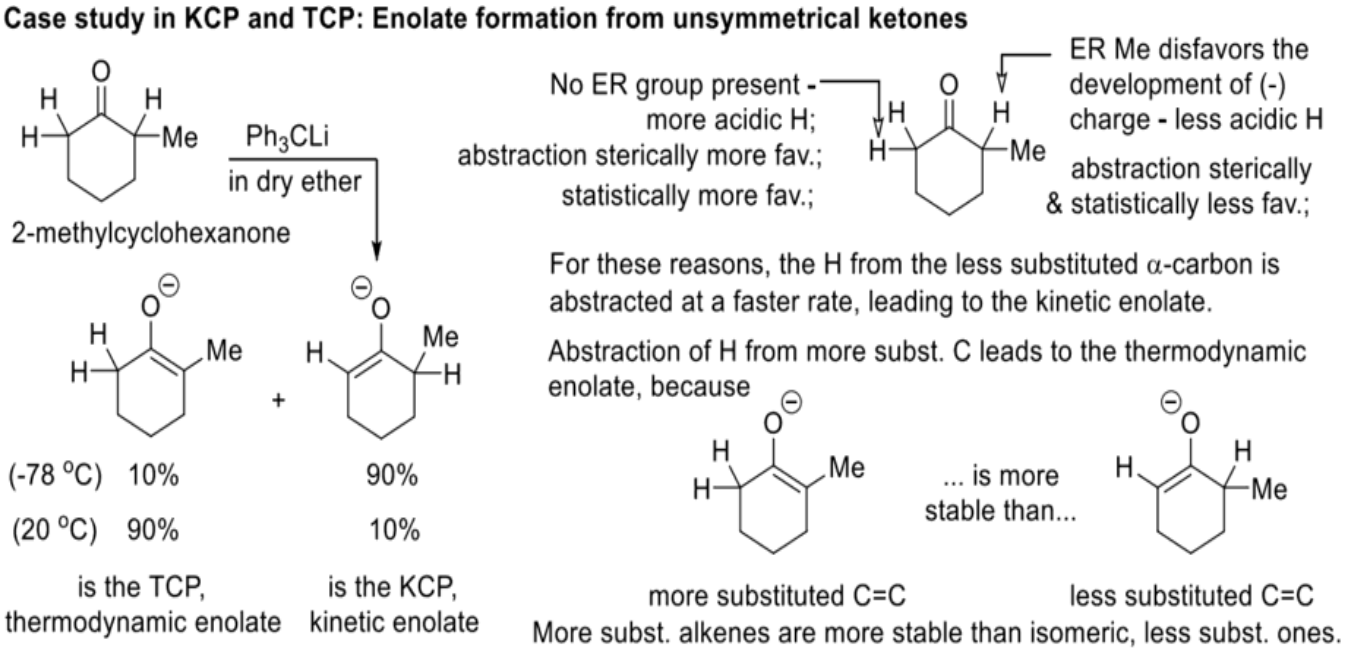
- Substrate: Acetone (or ketones)
- Kinetic Enolate:

  i. We use bulky base (like Ph_3CLi) at temperature around -78°C
  ii. Results in less substituted enolate and it forms faster.

- Thermodynamic Enolate:

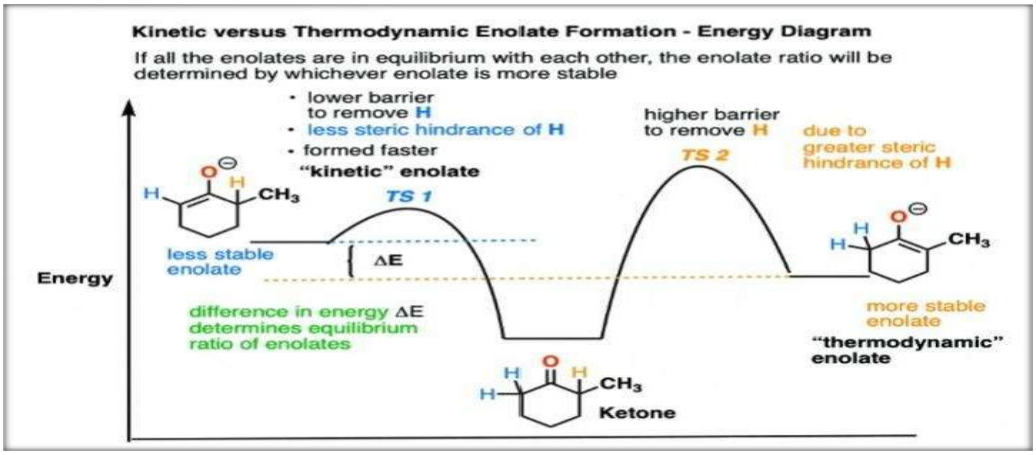
  i. We use weaker base (like NaOEt) and carry out the reaction at room temperature
  ii. Results in more substituted enolate, though it forms slower but it's stable.

Mechanism of Enolate formation from unsymmetrical Ketone



Kin. enolate promoted by: bulky base, lower temp., no excess ketone, non-protic solvent (irreversible conditions)
Thermo. enolate promoted by: small base, high temp., excess ketone, protic solvent (reversibility promoted).

Energy diagram for formation of Enolate from unsymmetrical Ketone



Key Concepts Recap

- Kinetic Control:
  i. Product depends on rate, low activation energy
  ii. Low temp, short reaction time

- Thermodynamic Control:
  i. Product is more stable
  ii. High temp, longer time

Real-World Applications

- Pharmaceuticals: stable or active isomer control
- Organic synthesis: regio-/stereoselective pathways
- Materials chemistry: material properties
- Catalysis: tuning for kinetic/thermodynamic selectivity

Summary Table

Parameter	Kinetic product	Thermodynamic product
Rate	Forms faster	Forms slower
Activation energy	Lower	Higher
Stability	Less stable	More stable
Conditions	Cold, short time	Warm, long time
Reversibility	Irreversible	Reversible
Selectivity	Pathway speed	Product energy

THANK YOU!!

Acknowledgment

We would like to express my sincere gratitude to **Kaushik Basu sir** for his guidance and support throughout the preparation of this presentation. We also extend our appreciation to the **Department of Chemistry and St Paul's Cathedral Mission College,** for providing access to academic resources and a learning environment that fostered curiosity and critical thinking.

References

a) **Organic Chemistry Lifesaver 2: Kalyan Kumar Mandal & Kaushik Basu.**
b) **https://www.masterorganicchemistry.com**
c) **https://www.chem.ucalgary.ca**
d) **https://chem.libretexts.org/**

Link to presentation: **Kinetically Controlled Product vs Thermodynamically Controlled Products**

OR Scan the QR code to see the presentation

Scan me!

The Manhattan Project

Subho Haldar, Aishani Chanda, Mrinmoyee Giri, A B Masud

Semester II

Abstract

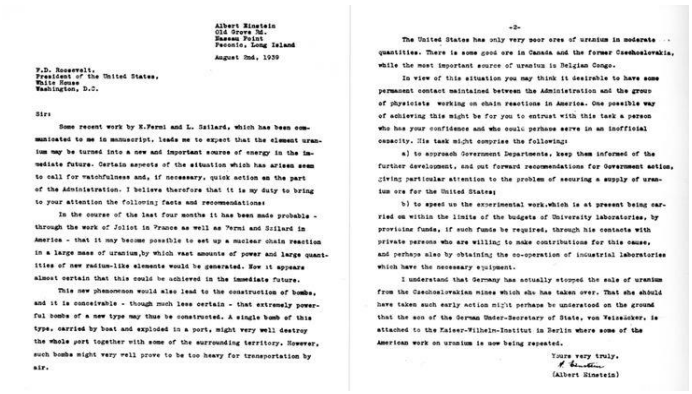
The Manhattan Project was a secret World War II research initiative led by the United States, with support from the United Kingdom and Canada, to develop the first nuclear weapons. Initiated in 1942 and directed by General Leslie Groves and physicist J. Robert Oppenheimer, the project resulted in the successful detonation of the first atomic bomb in July 1945. This led to the bombings of Hiroshima and Nagasaki, contributing to the end of the war. The project marked the beginning of the nuclear age, raising lasting scientific, political, and ethical implications.

Introduction

The Manhattan Project was one of the most significant and secretive scientific undertakings of the 20th century. Initiated during World War II, it was driven by the fear that Nazi Germany might develop nuclear weapons first. Officially launched in 1942 by the United States government, with crucial contributions from British and Canadian scientists, the project brought together leading minds in physics, engineering, and chemistry. Under the leadership of General Leslie R. Groves and Dr. J. Robert Oppenheimer, the program led to the development of the world's first atomic bombs. This breakthrough not only played a critical role in ending the war but also introduced nuclear weapons to global geopolitics, fundamentally altering international relations and ethical perspectives on science and warfare.

1. Historical Background: The Scientific Origins and Global Alarm:

In the midst of the Second World War, as global conflict intensified and the future of nations hung in the balance, a covert scientific mission was launched under utmost secrecy. This mission—codenamed the Manhattan Project—would become one of the most ambitious and consequential undertakings in modern history. It was conceived in response to a growing and terrifying possibility: that Nazi Germany, under Adolf Hitler, might weaponize the newly discovered process of nuclear fission.



Albert Einstein
Old Grove Rd.
Nassau Point
Peconic, Long Island

August 2nd, 1939

F.D. Roosevelt,
President of the United States,
White House
Washington, D.C.

Sir:

Some recent work by E.Fermi and L. Szilard, which has been communicated to me in manuscript, leads me to expect that the element uranium may be turned into a new and important source of energy in the immediate future. Certain aspects of the situation which has arisen seem to call for watchfulness and, if necessary, quick action on the part of the Administration. I believe therefore that it is my duty to bring to your attention the following facts and recommendations:

In the course of the last four months it has been made probable - through the work of Joliot in France as well as Fermi and Szilard in America - that it may become possible to set up a nuclear chain reaction in a large mass of uranium,by which vast amounts of power and large quantities of new radium-like elements would be generated. Now it appears almost certain that this could be achieved in the immediate future.

This new phenomenon would also lead to the construction of bombs, and it is conceivable - though much less certain - that extremely powerful bombs of a new type may thus be constructed. A single bomb of this type, carried by boat and exploded in a port, might very well destroy the whole port together with some of the surrounding territory. However, such bombs might very well prove to be too heavy for transportation by air.

-2-

The United States has only very poor ores of uranium in moderate quantities. There is some good ore in Canada and the former Czechoslovakia, while the most important source of uranium is Belgian Congo.

In view of this situation you may think it desirable to have some permanent contact maintained between the Administration and the group of physicists working on chain reactions in America. One possible way of achieving this might be for you to entrust with this task a person who has your confidence and who could perhaps serve in an unofficial capacity. His task might comprise the following:

a) to approach Government Departments, keep them informed of the further development, and put forward recommendations for Government action, giving particular attention to the problem of securing a supply of uranium ore for the United States;

b) to speed up the experimental work,which is at present being carried on within the limits of the budgets of University laboratories, by providing funds, if such funds be required, through his contacts with private persons who are willing to make contributions for this cause, and perhaps also by obtaining the co-operation of industrial laboratories which have the necessary equipment.

I understand that Germany has actually stopped the sale of uranium from the Czechoslovakian mines which she has taken over. That she should have taken such early action might perhaps be understood on the ground that the son of the German Under-Secretary of State, von Weizsäcker, is attached to the Kaiser-Wilhelm-Institut in Berlin where some of the American work on uranium is now being repeated.

Yours very truly,
(Albert Einstein)

In 1938, German scientists Otto Hahn and Fritz Strassmann succeeded in

splitting the uranium atom, a breakthrough later interpreted by Lise Meitner and Otto Frisch. This discovery revealed that nuclear fission could release a tremendous amount of energy—enough to create a weapon far more destructive than anything the world had seen before. The potential military use of this discovery deeply alarmed physicists worldwide, especially those who had fled fascist regimes in Europe.

One of them, Leo Szilard, recognized the danger of falling behind. In 1939, he drafted a letter—co-signed by Albert Einstein and delivered to U.S. President Franklin D. Roosevelt—warning that Nazi Germany might already be attempting to build an atomic bomb. This now-famous Einstein–Szilard letter urged the United States to begin its own nuclear research. Though quiet in tone, the letter sparked one of the loudest scientific responses in history, leading to the formation of the Advisory Committee on Uranium and, eventually, the full-scale Manhattan Project.

2. Role of Chemistry in Manhattan Project

The Manhattan Project was not born on battlefields or in political chambers, but in hidden laboratories and isolated desert testing grounds. It brought together some of the world's brightest scientists in a race against time, driven by a single goal: to build a weapon capable of ending the war through unprecedented power.

Albert Einstein(L) and Leo Szilard(R)

While physics laid the theoretical groundwork for nuclear fission—the process by which atoms are split to release energy—it was chemistry that transformed that theory into reality. Chemists played a vital role in the practical development of the bomb, beginning with the separation and purification of uranium-235 from natural uranium through complex and highly precise chemical techniques. The discovery and isolation of plutonium-239, a synthetic element with even greater explosive potential, required innovative chemical reactions and large-sca

Beyond material refinement, chemistry was essential in the design of explosive lenses, the handling of initiators, and the stability of components under extreme conditions. The work of chemists ensured that the weapon functioned as intended—not just as a concept, but as a devastating force.

Without chemistry, the ideas of physics would have remained equations on paper. It was chemistry that gave the atomic bomb form, function, and firepower—reshaping not only the outcome of the war but also the trajectory of science, ethics, and international relations in the decades to follow.

3. From Theory to Trinity: The Manhattan Project Timeline (1938–1945):

The story of the Manhattan Project began in 1938 with the discovery of nuclear fission—a breakthrough that transformed scientific curiosity into a global concern. As the realization of

atomic energy's destructive potential spread, particularly after German advancements in uranium research, scientists feared the possibility of Nazi Germany developing nuclear weapons first.

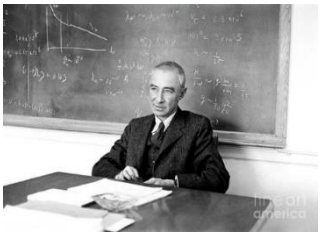
By 1940, research intensified on both sides of the Atlantic. In Britain, early work on plutonium highlighted its explosive potential. In the U.S., physicists like Enrico Fermi and John Wheeler confirmed that uranium-235 could sustain a chain reaction—paving the way for weapon development. These findings led to the Einstein–Szilard letter in 1939, which urged President Roosevelt to act. The letter triggered a shift in U.S. policy, ultimately leading to the formation of the National Defense Research Committee (NDRC) and the Office of Scientific Research and Development (OSRD).

As scientific urgency grew, elite universities such as Columbia, Chicago, and Berkeley became key research hubs, operating under high secrecy. The once theoretical discussions on fission now focused on uranium enrichment, reactor design, and the synthesis of plutonium. By the end of 1941, the United States had officially entered a scientific and military race to harness atomic power before its enemies.
In 1942, the Manhattan Project took formal shape under the U.S. Army Corps of Engineers. General Leslie Groves assumed command, and physicist J. Robert Oppenheimer was appointed scientific director. The transition from academic theory to industrial-scale production began. Facilities were established at Oak Ridge, Hanford, and Los Alamos, and the nation's scientific community was mobilized on an unprecedented scale.

A critical milestone came on December 2, 1942, when Enrico Fermi's team achieved the world's first controlled, self-sustaining nuclear chain reaction at the University of Chicago. This historic success marked the moment atomic energy moved beyond theory—confirming that a functional bomb was not only possible but imminent.

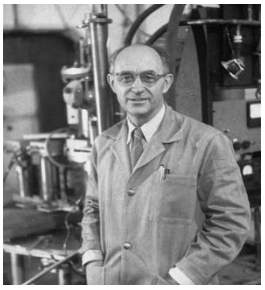
Leading Scientists and Contributors of the Manhattan Project:

Behind the immense technical achievement of the Manhattan Project stood a team of extraordinary scientists, engineers, and visionaries drawn from across the globe. United by urgency and guided by scientific ambition, they laid the foundation for one of the most consequential innovations in modern history.



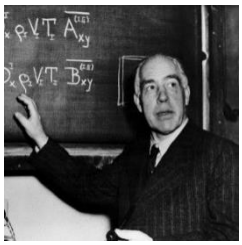
J. Robert Oppenheimer
Scientific Director of the Manhattan Project. Oppenheimer oversaw all research activities at Los Alamos Laboratory and coordinated efforts between theoretical physicists and experimental teams. He was known for his intellectual brilliance and leadership under pressure.

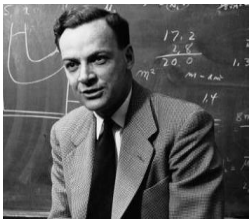
General Leslie Groves
Military head of the Manhattan Project. Groves managed logistics, funding, security, and construction. He appointed Oppenheimer and made critical administrative decisions, ensuring the project's swift progress.



Enrico Fermi
An Italian-American physicist who achieved the first controlled, self-sustaining nuclear chain reaction (Chicago Pile-1). His work on neutron moderation and reactor design was foundational to both weapon and energy applications.

Niels Bohr
A Nobel Prize-winning Danish physicist who contributed to the understanding of nuclear fission and advised the Los Alamos team. He emphasized the need for international cooperation in atomic research, foreseeing the long-term implications of nuclear power.



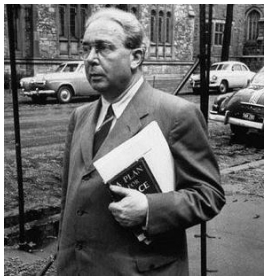


Richard Feynman
A young and highly energetic theoretical physicist. He worked on the mathematical modeling of bomb assembly and safety measures. Known for simplifying complex problems and boosting morale at Los Alamos.

Ernest Lawrence
Inventor of the cyclotron and a pioneer in electromagnetic isotope separation. Lawrence's lab developed crucial technology for enriching uranium at the Oak Ridge facility.

Glenn T. Seaborg
Chemist who co-discovered plutonium and led efforts to isolate plutonium-239. His radiochemical methods were key to producing the core material used in the "Fat Man" bomb.

George Kistiakowsky
An expert in explosives who perfected the implosion method used in the plutonium bomb. He helped design the explosive lenses critical for symmetrical compression in "Fat Man."



Leo Szilard
One of the first to realize the potential for a nuclear chain reaction. He co-authored the Einstein–Szilard letter and worked on reactor physics and isotope separation at the University of Chicago.

Hans Bethe

Head of the Theoretical Division at Los Alamos. Bethe led calculations for bomb design, including energy yield, neutron behavior, and detonation sequences.

Edward Teller
A theoretical physicist who contributed to the plutonium bomb but later became more focused on developing the hydrogen bomb. He also worked on explosive shockwave theory.

Klaus Fuchs

A German-born physicist who made substantial technical contributions at Los Alamos. Later revealed as a Soviet spy, Fuchs leaked atomic secrets that helped accelerate the USSR's nuclear program.

Chemistry and Physics: The Scientific Core of the Manhattan Project:

At the heart of the Manhattan Project lay two fundamental scientific disciplines—physics and chemistry—each playing a distinct yet deeply interconnected role in the creation of the atomic bomb. While physics provided the theoretical framework, chemistry made it operationally possible.

Physics: The Theory of Fission

The foundation of the atomic bomb rested on nuclear fission—the process in which a heavy atomic nucleus (such as uranium-235 or plutonium-239) splits into smaller nuclei, releasing an immense amount of energy. This process also emits neutrons, which can trigger further fission in a chain reaction. The concept of a self-sustaining chain reaction was crucial to weapon design.

Physicists like Leo Szilard, Enrico Fermi, and Hans Bethe studied neutron behavior, calculated critical mass, and modeled reaction rates. Their theoretical predictions guided bomb design, energy output estimates, and detonation mechanisms. Understanding the difference between fast and slow neutrons, and how materials moderated or reflected them, became essential in optimizing bomb performance.

Chemistry: From Raw Elements to Reality

While physics laid the theoretical foundation for nuclear fission, it was chemistry that turned theory into weaponry. The development of atomic bombs required the separation, purification, and manipulation of fissile materials—tasks deeply rooted in complex chemical processes. Chemists played a central role in enriching uranium-235 from natural uranium, a technically demanding task achieved through methods such as gaseous diffusion and electromagnetic separation. Simultaneously, the production of plutonium-239—an element not found in nature in usable quantities—required the transformation of uranium-238 in nuclear reactors, followed by intricate radiochemical separation techniques to extract the plutonium from spent fuel.

Beyond materials processing, chemistry was vital to several other aspects of bomb construction. Chemists developed the explosive lenses used in the implosion design of Fat Man, ensuring symmetrical compression of the plutonium core to achieve supercriticality. They also designed initiators to inject neutrons at precisely the right moment to trigger the chain reaction, and they addressed critical challenges related to the stability, handling, and performance of materials under extreme pressure, temperature, and radiation. In essence, while physics provided the blueprint, it was chemistry that brought the bomb into existence—bridging theory and reality with precision, innovation, and an unprecedented scale of scientific coordination.

Scientific Rationale behind the Bomb Designs: The Physics and Chemistry of Catastrophe:

The Manhattan Project produced two fundamentally different atomic bomb designs — “Little Boy” (uranium-based) and “Fat Man” (plutonium-based). Though both relied on the principle of nuclear fission, the differences in fissile materials and their behavior under neutron bombardment required distinct engineering and scientific approaches. Understanding the rationale behind each design reveals the interplay between nuclear physics, materials science, and precise explosive engineering.

Plutonium-239 and **the Fat Man Bomb**

1. Production of Plutonium-239:

The production of Plutonium-239 was one of the Manhattan Project’s most complex scientific achievements, representing a landmark in the field of applied nuclear chemistry. Unlike Uranium-235, Plutonium-239 does not occur naturally in usable quantities. Instead, it had to be artificially synthesized from Uranium-238, a fertile but non-fissile isotope that cannot sustain a chain reaction on its own.

This transformation involved a carefully orchestrated sequence of nuclear reactions inside specially designed nuclear reactors, most notably the B-Reactor at the Hanford Site in Washington:

1. Neutron capture: Uranium-238 absorbs a neutron, forming Uranium-239

U-238 + n → U-239

2. First beta decay (half-life ~23.5 minutes) U-239 decays to Neptunium-239

U-239 → Np-239 + β^- + anti-neutrino

3. Second beta decay (half-life ~2.36 days) Np-239 decays to Plutonium-239

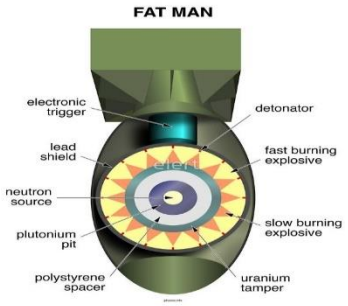
Np-239 → Pu-239 + β^- + anti-neutrino

The resulting Plutonium-239 is a fissile material capable of sustaining a rapid nuclear chain reaction, making it suitable for weaponization. Once produced in the reactor, Pu-239 had to be chemically separated from intensely radioactive spent fuel and residual uranium. This was accomplished using the bismuth phosphate process, a pioneering radiochemical method based on selective precipitation. In this technique, plutonium was precipitated out of aqueous solution as a solid compound using bismuth phosphate, while unwanted uranium and fission products remained dissolved. The precipitate was then redissolved and reprecipitated in successive cycles to achieve higher purity.

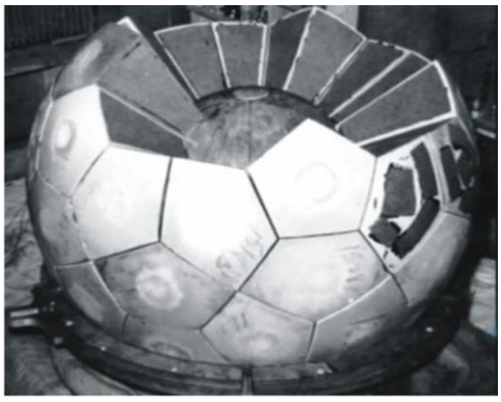
This multi-step sequence—from neutron bombardment to radiochemical isolation—was a monumental collaboration between nuclear physics and chemical engineering. It exemplified the indispensable role of chemistry in the Manhattan Project, bridging the gap between theoretical nuclear science and real-world weapon development.

2. Implosion Design and Engineering:

The Fat Man bomb used a spherical implosion mechanism to achieve supercriticality in a plutonium core:

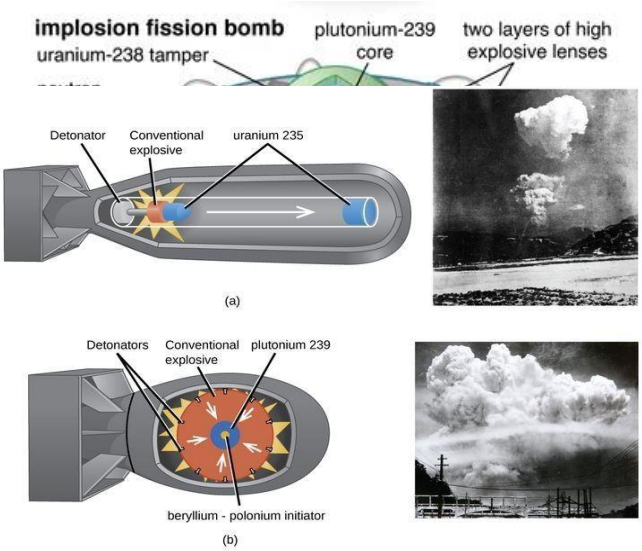


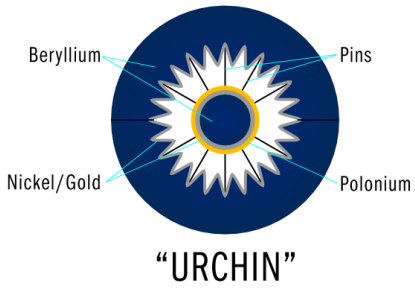
Plutonium Core: At the heart of the Fat Man bomb was a sub-critical plutonium-239 core, weighing approximately 6.19 kg. This core was carefully engineered to remain below critical mass under normal conditions, ensuring safety during assembly and transport. Upon detonation, the core was rapidly compressed into a supercritical state using symmetrical shockwaves generated by explosive lenses. To enhance the efficiency of the chain reaction, the core was surrounded by a layer of uranium-238, which acted as both a neutron reflector and a tamper—slowing expansion and reflecting escaping neutrons back into the core. This compact design ensured maximum neutron economy, energy yield, and structural stability at the moment of detonation.



Explosive Lenses: To achieve the rapid and symmetrical compression needed for criticality, 32 precisely shaped explosive lenses were arranged spherically around the plutonium core. These lenses consisted of fast and slow explosives—commonly RDX and TNT—strategically layered to manipulate detonation wave speeds. Their configuration focused the blast inward, generating a uniform spherical shockwave. This ensured the core's dense and even compression, which was essential to reaching supercriticality. The successful use of explosive lensing was a remarkable feat of chemical and mechanical precision.

Neutron Reflector: Encasing the plutonium core was a shell of uranium-238, functioning as a neutron reflector. During fission, many neutrons escape the core; the reflector bounced some of these neutrons back into the plutonium, thereby increasing the probability of further fission events. This reflection not only amplified the chain reaction but also enhanced the weapon's efficiency. Additionally, the dense uranium layer acted as a tamper, delaying the expansion of the core to allow more complete fission before disassembly.





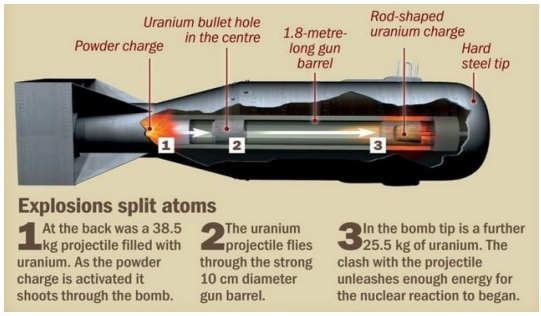
Initiation Device – "Urchin": At the core's center was a neutron initiator called Urchin, designed to release neutrons at the exact moment of maximum compression. This device contained polonium-210, an alpha emitter, and beryllium, which emits neutrons when bombarded with alpha particles. During implosion, the two elements were forced together, triggering an (α, n) reaction that produced a burst of neutrons. This precise timing initiated the chain reaction within the supercritical core, ensuring full explosive efficiency. The urchin's intricate design resembled a spiked metallic sphere—hence its nickname.

This design avoided premature detonation—an issue with plutonium due to spontaneous neutron emission—and ensured the bomb's efficiency.

3. Physical Specifications and Detonation

- Length: 3.3 m
- Diameter: 1.5 m

- Weight: 4,600 kg.
- Explosion Altitude: ~1,650 feet over Nagasaki.
- Blast Yield: ~21 kilotons of TNT.
- Core Temperature: Over 100 million °C.
- Mushroom Cloud: Reached ~18 km height.
- Casualties: ~40,000–75,000 instantly; ~100,000+ by end of 1945



Uranium-235 and **The Little Boy Bomb**

1. Uranium Enrichment and Properties:-

Natural uranium is composed mostly of U-238 with only ~0.7% U-235, the fissile isotope. U-235 cannot be chemically separated from U-238; instead, isotope separation techniques were used:

- Gaseous Diffusion (K-25 Plant, Oak Ridge)
- Electromagnetic Separation (Y-12 Plant, using calutrons)
- Thermal Diffusion (S-50 Plant)

These processes enriched uranium to weapons-grade levels. The uranium used was sourced from the Shinkolobwe Mine (Belgian Congo), Colorado, Utah, New Mexico, and Eldorado Mine (Canada)

2. Gun-Type Design:-

Design Principle: Two subcritical masses of U-235 were fired together using a gun-like barrel to form a supercritical mass.
Initiator: A neutron initiator injected neutrons at the moment of contact to start the chain reaction.

Components:

- 38.4 kg of U-235 total (two masses: 25.6 kg and projectile portion)
- Tungsten-carbide disk accelerated at ~300 m/s
- Smokeless propellant ignited by barometric-triggered detonation

Tempering: U-238 used as a tamper to reflect neutrons and hold the core together longer during explosion.

3. Physical Specifications and Detonation

- Length: ~3 meters (10 feet)
- Weight: 4,400 kg.
- Explosion Altitude: ~1,900 feet over Hiroshima.
- Blast Yield: ~15 kilotons of TNT.
- Core Temperature: ~100 million °C; Ground Temp: ~4,000 °C.
- Fireball Diameter: ~300 meters.
- Casualties: 70,000–80,000 instantly; ~190,000+ by end of 1945

Testing, Deployment, and the Global Impact of the Manhattan Project:

The final phase of the Manhattan Project marked not only a technological triumph but also the beginning of a new era in human history. With the successful development and testing of nuclear weapons, followed by their deployment in warfare, the consequences were both immediate and far-reaching — spanning human, environmental, political, and ethical dimensions.

Testing: The Trinity Experiment: On July 16, 1945, the world witnessed the first-ever detonation of a nuclear device, codenamed "Trinity," in the New Mexico desert. The test involved a plutonium-239 implosion-type bomb — the same design later used in "Fat Man." The explosion released energy equivalent to about 21 kilotons of TNT, producing a blinding flash, a powerful shockwave, and a mushroom cloud that rose over 12 kilometers into the sky. This unprecedented demonstration confirmed the devastating potential of nuclear weapons and ushered in the atomic age.

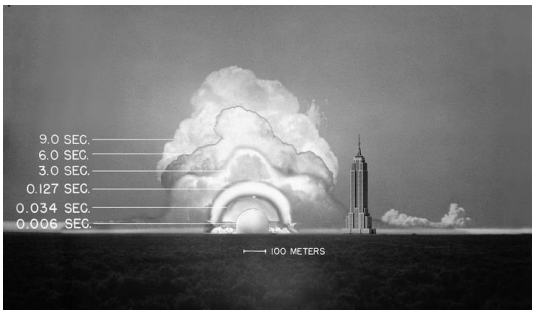
Deployment: Hiroshima and Nagasaki

Hiroshima – The First Use in Warfare

On August 6, 1945, the U.S. dropped the first uranium-based atomic bomb, codenamed Little Boy, on the Japanese city of Hiroshima. The bomb mechanism was a gun-type design using uranium-235. The weapon detonated approximately 1,900 feet above the city. Hiroshima was devastated, marking the first use of nuclear weapons in war.

Nagasaki – The Second Detonation

Just three days later, on August 9, 1945, a second bomb, codenamed Fat Man, was dropped on Nagasaki. This bomb used plutonium-239 and an implosion design. Although its design was more complex, it was more powerful and efficient than the Hiroshima bomb.



Strategic Impact and Immediate Aftermath

The bombings caused massive destruction and loss of life and are believed to have contributed directly to Japan's decision to

surrender on August 15, 1945. These events effectively ended World War II. The devastation also launched the world into the atomic age, raising global awareness of the catastrophic potential of nuclear warfare.

The deployment of atomic weapons during World War II thus marked not just a military victory, but a turning point in history—reshaping geopolitics, science, ethics, and humanity's relationship with its own technological capabilities.

Aftermath, Political Implications, and Reflections:

The Manhattan Project did more than develop a weapon — it reshaped the course of history and redefined the role of science in society. The immediate aftermath was devastating: Hiroshima and Nagasaki bore the brunt of unimaginable destruction, with over 100,000 people killed instantly and many more suffering from radiation sickness, long-term illnesses, and generational trauma. It was the first — and only — time in human history that nuclear weapons were used in war.

Politically, this event marked the dawn of the nuclear era. The United States, having demonstrated its technological supremacy, entered into a prolonged Cold War with the Soviet Union. The nuclear arms race that followed ushered in decades of global tension, deterrence policies, and fears of mutual destruction — all rooted in the technology that had first been proven successful in a desert test.

We respectfully acknowledge the indispensable role of physics, especially in the understanding of nuclear fission, chain reactions, and the energy-mass relationship. However, it was chemistry that made the Manhattan Project possible in practice. The isolation and purification of fissile materials like Plutonium-239 and Uranium-235, the complex separation techniques, the materials chemistry of initiators like polonium-210 and beryllium, and the explosive lens systems were all remarkable chemical triumphs. The transformation from theoretical physics to real-world weaponization was, fundamentally, a chemical challenge solved by chemists.

Yet, even among the project's creators, there was a growing sense of moral conflict. The project's scientific director, J. Robert Oppenheimer, famously quoted the Bhagavad Gita upon witnessing the first nuclear test:

"**Now I am become Death, the destroyer of worlds.**"

This haunting realization reflected the internal turmoil many scientists faced. After the war, Oppenheimer strongly opposed the development of the hydrogen bomb and became a vocal advocate for international arms control. He later led efforts to regulate nuclear weapons, a stance that led to his political isolation during the Red Scare era.

The Manhattan Project was both a pinnacle of scientific collaboration and a cautionary tale. As chemistry students, we do not celebrate the destruction it caused — rather, we reflect on the scientific ingenuity it required and the ethical responsibilities it revealed. It teaches us that the

power unlocked by chemistry is profound, and with such power comes the duty to use science for the progress and preservation of humanity, not its harm.

Conclusion

The Manhattan Project was more than a wartime operation—it was a defining moment where science, politics, and ethics collided. It demonstrated how deeply scientific discovery, particularly in chemistry, could influence the course of history. From isotope separation to high-explosive designs, chemistry turned theoretical physics into a powerful, world-changing reality.

As chemistry students, our journey through this project is not just about understanding formulas or reactions—it's about recognizing science's potential to shape society. The Manhattan Project reminds us that with great discovery comes great responsibility. What we choose to create with our knowledge defines not just our success, but our legacy.

THANK YOU!!

ACKNOWLEDGEMENT

We would like to thank our college to help our department organize this kind of event by allowing us to access books, articles and internet present in the campus as well as providing a comfortable place to deliver our talk. Secondly, we would like thank our departmental head and professors for their sincere guidance and help, without them this seminar would not be a success. I would also thank our non-teaching staff and our seniors for their constant support.

SOURCES

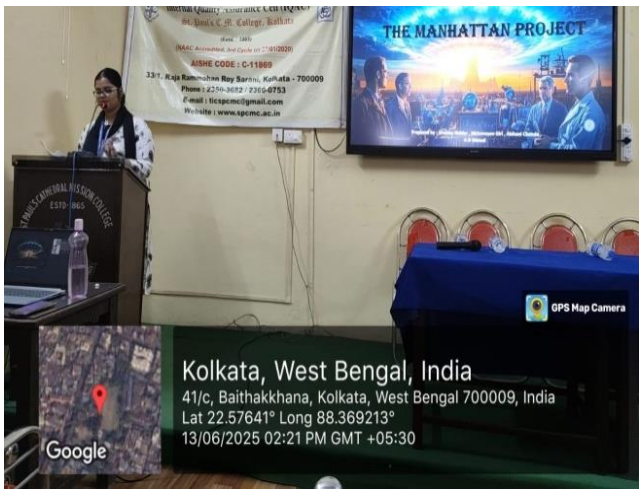
1. https://en.wikipedia.org/wiki/Manhattan_Project
2. https://www.britannica.com/event/Manhattan-Project
3. https://chem.libretexts.org/Courses/Furman_University/CHM101%3A_Chemistry_and_Global_Awareness_(Gordon)/06%3A_Nuclear_Weapons-_Fission_and_Fusion/6.03%3A_The_Manhattan_Project_-_Labs_and_Fuel

4. https://www.atomicarchive.com/resources/documents/manhattan-project/index.html
5. https://chatgpt.com/c/6853f99f-3ccc-8010-87bf-e2cd57a60d61

Link to Presentation: **The Manhattan Project**

OR Scan the QR code to see the presentation

Scan me!



Estimation of Zn (II) by using Complexometric Titration

Praymanjita Das, Koyena Bhattacharjee

Semester IV

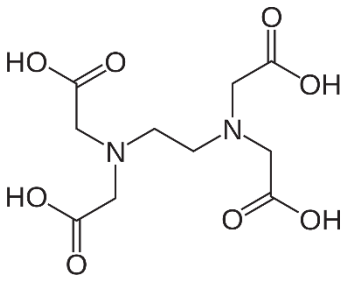
Abstract

Complexometric titrations with EDTA have traditionally been performed in undergraduate analytical chemistry courses to determine the concentration of zinc ions present in a given mixture. This titration is carried out specifically in an acidic medium, since the Zn-EDTA complex is stable at pH ~5. So it can be concluded that practical EDTA titrations can also be performed at low pH (as traditional Complexometric titrations are carried out at higher pH). In addition, it widens the window of possible metal ions for complexometric titration affords the possibility of analyzing real world products, such as brass and steel.

Introduction

Now the question arises, **what is complexometric titration?**

It is a type of volumetric analysis that involves the formation of a complex (a coordination compound) between a metal ion in solution and a chelating agent (a substance that can bind to the metal ion through multiple sites).



Key Features

i. We use complextometry to determine the concentration of metal ions in given solution or a given mixture.
ii. We most commonly use Ethylene-diamine-tetraacetic acid (EDTA) as the chelating or complexing agent as it is a hexadentate ligand and forms stable complexes with the metal ion. Moreover use of EDTA is preferred over any other chelating agent because it is commonly found (easy to prepare) and has a high stabilization constant with almost every major metal ion.

iii. As the indicator, a special dye ERICHROME BLACK T is used, it is also an chelating agent but has a low value of stabilization constant with all metal ions, it signal the end point by changing color when all metal ions have reacted with the chelating agent.
iv. The titration often requires a buffer solution to maintain an appropriate pH since complex formation is pH-dependent.

Types of Complexometric Titration

Complexometric titrations are categorized based on how the titration is carried out and the types of reactions involved. Here are the main types of complexometric titrations:

1. Direct Titration

- Description: The metal ion solution is directly titrated with a standard solution of a complexing agent like EDTA.
- Used when: The metal forms a stable complex directly with EDTA without requiring masking agents or prior treatment.
- Example: Titrating a solution of Ca^{2+} with EDTA using Eriochrome Black T as the indicator at a basic medium.

2. Back Titration

- Description: A known excess of EDTA is added to the metal ion solution. The excess (unreacted) EDTA is then titrated with a standard solution of another metal ion (like Mg^{2+} or Zn^{2+}).
- Used when: The metal-EDTA complex forms slowly and the metal ion precipitates or interferes with direct titration.
- Example: Determination of aluminum or lead.

3. Replacement Titration

- Description: The metal ion being analyzed displaces another metal ion from its EDTA complex. The released metal ion is then titrated with EDTA.
- Used when: The metal ion of interest doesn't form a suitable complex with EDTA for direct titration.
- Example: Determination of mercury (Hg^{2+}) by displacing Mg^{2+} from Mg-EDTA.

4. Indirect Titration

- Description: The analyte doesn't react directly with EDTA but can be converted into a form that does.
- Used for: Anions or substances that don’t form direct complexes with EDTA.
- Example: Determination of sulfate ions by precipitating them as $BaSO_4$, then titrating the remaining Ba^{2+} with EDTA.

DIRECT COMPLEXOMETRIC TITRATION OF ZINC

Complexometric titration of zinc typically involves using EDTA as the titrant. EDTA forms stable, colorless 1:1 complexes with most metal ions, including Zn^{2+}.

Q: Why is zinc preferred?

Zinc is often preferred over other elements in Complexometric titrations for several key reasons:

a. Ease of Formation of Complexes:

Zinc forms stable complexes with common complexing agents (e.g., EDTA). The stability constant for the zinc-EDTA complex is high, making it easier to determine the endpoint of a titration. Zinc ions tend to form more stable and easily measurable complexes.

b. Control of pH:

Zinc can form stable complexes with EDTA in a relatively neutral pH range (typically around pH 5-7), which is convenient for titration. This range allows for better control over the reaction conditions.

c. Reaction Selectivity:

Zinc has a relatively high selectivity for complexing agents like EDTA. It is less likely to be interfered with by other metal ions in a sample compared to magnesium and aluminum, which makes it a preferred choice in many cases.

d. Availability and Common Usage:

Zinc is widely used in a variety of Complexometric titrations, especially in the analysis of alloys, electroplating, and water treatment, making it a standard metal for such analyses.

e. Titration Endpoint Detection:

Zinc generally provides a sharper and more distinct endpoint when titrated with complexing agents like EDTA. The color change of the indicator (e.g., Eriochrome Black T) is usually more evident for zinc, which helps in obtaining accurate results.

Q: What Is The Importance Of EDTA?

Metal Ion Detection: EDTA is used to detect metal ions (e.g., Ca^{2+}, Mg^{2+}, Zn^{2+}, Fe^{3+}) in a solution. It forms 1:1 complexes with most metal ions regardless of their charge:

a. **Stable Complex Formation:** The complexes formed are very stable due to multiple bonds between EDTA and the metal ion. This prevents the metal ion from reacting with other substances in the solution, improving titration accuracy.
b. **Sharp Endpoint with Indicators:** Indicators like Eriochrome Black T (EBT) are used, which change color when the metal ion is completely complexed by EDTA. At the beginning, the indicator forms a weak complex with the metal ion (e.g., a red color). As EDTA is added, it displaces the indicator and forms a stronger complex, changing the color (e.g., from red to blue).

Q: What are the reagents used in Complexometric titration?

1. **EDTA Solution (Titrant):** It is used in the form of disodium EDTA di-hydrate ($Na_2H_2Y \cdot 2H_2O$), usually ~0.02 M or 0.05 M.
   Function: Chelates Zn^{2+} to form a 1:1 stable complex

2. **Zinc Ion Solution (Analyte):** Source-$ZnSO_4$ or any soluble zinc salt.
   Function: The sample containing zinc ions to be analyzed.

3. **pH Buffer Solution:** Usually ammonia-ammonium chloride buffer (NH_3-NH_4Cl), pH ~10
   Function: Ensures optimal conditions for EDTA to bind Zn^{2+} effectively and for the indicator to work properly.

4. **Indicator:** Eriochrome Black T (EBT)
   Function: Forms a weak complex with Zn^{2+} (red or wine-red color). When all Zn^{2+} is complexed by EDTA, the free indicator changes color (e.g., to blue or yellow-orange depending on the indicator).

5. **Masking Agents (if interfering ions are present)**
   Example: Potassium cyanide (KCN) can be used to mask interfering ions like Cu^{2+} or Ni^{2+} by forming stable complexes that do not react with EDTA.

6. **Distilled Water:** Used for dilution and preparation of standard and sample solutions.

Q: What is the role of buffer solution?

Ammonia-Ammonium Chloride (NH_3/NH_4Cl) buffer is typically used in this titration. In the Complexometric titration of zinc, a buffer solution plays a crucial role in maintaining a constant pH, which is essential for accurate and reliable titration results. Here's a detailed breakdown of its role:

1) **Maintains optimal pH for Complex Formation**: The titration of zinc typically uses EDTA as the titrant. EDTA forms stable complexes with metal ions like Zn^{2+}, but this reaction is highly pH-dependent. For zinc, the complex with EDTA is most stable around pH 10. A buffer solution (commonly an ammonia-ammonium chloride buffer) is used to maintain this pH.

2) **Prevents Precipitation of Metal Hydroxides:** At higher pH values, zinc ions may start forming $Zn(OH)_2$ precipitate. The buffer keeps the pH in a range that prevents precipitation, ensuring zinc stays in solution for complexation.

3) **Ensures Accurate Endpoint Detection:** The endpoint is often detected using a metal ion indicator like Eriochrome Black T, which changes color when all zinc ions have complexed with EDTA. The indicator also works best at a specific pH (~10), and the buffer ensures the conditions are suitable for a sharp and clear color change.

Q: What is the role of indicator?

1) Acts as a Metal Ion Indicator: EBT is a dye that can form a weak complex with metal ions such as Zn^{2+}. When it binds to zinc ions, it forms a wine-red colored complex.

2) Signals the Endpoint: During the titration, EDTA is added to the solution containing zinc and EBT. EDTA has a stronger affinity for Zn^{2+} than EBT does. As EDTA is added, it displaces EBT from the Zn–EBT complex and forms a stable Zn–EDTA complex. Once all Zn^{2+} ions are complexed with EDTA, EBT is free in solution, and its color changes from wine red to blue — this signals the endpoint of the titration.

3) Depends on pH: EBT works effectively around pH 10, which is why a buffer is used to maintain the pH during titration.

Q: What is the role of distilled water?

1) **Solvent for Reagents and Samples:** Distilled water is used to dissolve the zinc salt sample, EDTA solution, and buffer. It provides a neutral, non-reactive medium that does not interfere with the titration.
2) **Prevents Contamination:** Tap water contains metal ions (like Ca^{2+}, Mg^{2+}, Fe^{3+}, etc.) that can interfere by reacting with EDTA or the indicator. Using distilled water ensures no unwanted metal ions are introduced, which could otherwise lead to inaccurate results.

3) **Used for Rinsing:** Distilled water is used to rinse beakers, burettes, pipettes, and conical flasks before use. This removes any residual substances or ions that might skew the titration results.
4) **Dilution and Mixing:** During the titration, distilled water may be added to the flask to ensure proper mixing and to make the color change of the indicator more visible. It helps to maintain an appropriate volume for efficient stirring and endpoint detection.

Q: What is the role of masking agents?

1. **Prevents Interference from Other Metal Ions:** In real samples (e.g., alloys, water, and biological fluids), other metal ions such as Fe^{3+}, Cu^{2+}, Al^{3+}, Ca^{2+}, etc., may be present along with Zn^{2+}. These metals also form stable complexes with EDTA. A masking agent chemically binds to these interfering ions to form stable, non-reactive complexes, so they no longer react with EDTA.
2. **Ensures Selective Titration of Zinc:** By "hiding" the other metals, the titration proceeds with only zinc ions reacting with EDTA, ensuring accurate determination of zinc content.

DETAILED STEP BY STEP PROCEDURE

 Step 1:

- Rinse and Prepare Apparatus
- Rinse the burette with EDTA solution.
- Rinse the pipette with zinc solution.
- Rinse the conical flask and beakers with distilled water.

 Step 2:

- Fill Burette
- Fill the burette with standard EDTA solution.
- Remove air bubbles and record the initial volume.

 Step 3:

- Pipette Zinc Solution
- Use a 25 mL pipette to transfer the zinc ion solution into a clean conical flask.

 Step 4:

- Add Buffer Solution
- Add about 10 mL of ammonia–ammonium chloride buffer to the flask.
- This maintains the pH around 10, which is ideal for Zn–EDTA complexation.

 Step 5:

- Add Indicator
- Add 2–3 drops of Eriochrome Black T (EBT).
- The solution should turn wine red, indicating the presence of uncomplexed Zn^{2+} ions.

 Step 6:

- Titrate with EDTA
- Titrate by slowly adding EDTA from the burette while swirling the flask continuously.
- Near the endpoint, the red color will begin to fade.

 Step 7:

- Detect Endpoint
- The endpoint is reached when the color changes from wine red to clear blue.
- This indicates all Zn^{2+} ions have formed complexes with EDTA, freeing the indicator.

 Step 8:

- Record Final Reading
- Record the final burette reading.
- Subtract to find the volume of EDTA used.

 Step 9:

- Repeat for Accuracy
- Repeat the titration 2–3 times until you obtain concordant readings (values within ±0.1 mL).

Q: What are the advantages?

1. **High Selectivity and Accuracy:**
   EDTA forms a 1:1 stable complex with Zn^{2+}, allowing for precise and accurate quantification. Minimal side reactions when pH and conditions are properly controlled.
2. **Clear Endpoint Detection:**
   Indicators like Eriochrome Black T (EBT) give a sharp color change (wine red → blue) at the endpoint. Easy to detect by eye, especially with a white background.
3. **Simple and Fast Procedure:**
   Requires basic lab equipment (burette, pipette, conical flask). Titration can be performed quickly and repeated easily for consistency.
4. **Wide Applicability:**
   Can be used to analyze zinc in alloys, plating baths, water samples, and biological fluids. Versatile method for quality control and environmental monitoring.
5. **No Need for Expensive Equipment:**

Unlike spectrophotometry or atomic absorption, this method does not require specialized instruments, making it cost-effective.

6. **Can Be Used in Mixed Metal Solutions:**
   With proper use of masking agents, EDTA titration can selectively determine zinc even in the presence of other metals (e.g., Cu^{2+}, Fe^{3+}).
7. **Reproducible Results**
   When standardized solutions and proper pH buffering are used, results are highly reproducible across trials.
8. **Quantitative Determination**
   Provides a direct way to calculate the exact amount or concentration of Zn^{2+} in a sample.

Q: What can be the scope of ERRORS in the estimation?

1. **Incorrect pH (Buffer Error)**
   Cause: Improper buffering or use of an incorrect buffer.
   Effect: At low pH, EDTA may not fully complex with Zn^{2+}; at high pH, $Zn(OH)_2$ may precipitate.
   Result: Underestimation or overestimation of zinc concentration.

2. **Endpoint Detection Error**
   Cause: Misjudging the color change of Eriochrome Black T (wine red → blue).
   Effect: Over-titration or under-titration.
   Result: Inaccurate zinc concentration, especially if the color change is subtle or delayed.

3. **Interference from Other Metal Ions**
   Cause: Other metal ions (e.g., Cu^{2+}, Fe^{3+}) also react with EDTA.
   Effect: More EDTA is consumed than expected.
   Result: Overestimation of zinc unless proper masking agents are used.

4. **Contaminated or Impure Reagents**
   Cause: Impure EDTA, buffer, or indicator solutions.
   Effect: May contain trace metals or affect the pH.
   Result: Unreliable titration results.

5. **Use of Tap Water Instead of Distilled Water**
   Cause: Tap water contains Ca^{2+}, Mg^{2+}, and other metal ions
   Effect: EDTA reacts with these ions.
   Result: Overestimation of zinc concentration.

6. **Air Bubbles in Burette**

Cause: Not properly removing air bubbles during burette setup.
Effect: Less EDTA is actually delivered than measured.
Result: Underestimation of zinc.

7. **Parallax Error When Reading Volumes**
   Cause: Eye not level with the meniscus when reading burette or pipette.
   Effect: Misreading volumes.
   Result: Inaccurate calculations of concentration.

8. **Indicator Decomposition or Wrong Amount**
   Cause: Using old or degraded Eriochrome Black T or adding too much/little.
   Effect: Poor or unclear color change
   Result: Unclear endpoint, leading to errors.

Conclusion

Complexometric estimation of zinc, typically using EDTA (ethylenediaminetetraacetic acid) titration, allows for the quantitative determination of zinc concentration in a sample. The method relies on the formation of a stable zinc-EDTA complex, with the endpoint of the titration indicated by a color change of a suitable metallochromic indicator. This technique is valuable for assessing zinc levels in various materials, including pharmaceuticals, alloys, and ores. This is applicable for-

- **Quality Control:** Complexometric titration is used to determine zinc content in pharmaceuticals, food products, and fertilizers.
- **Material Analysis:** It is used to determine zinc content in alloys like brass and in zinc ores.
- **Environmental Monitoring:** It can be used to assess zinc levels in environmental samples.

THANK YOU!!

ACKNOWLEDGEMENT

We would like to thank our college to help our department organize this kind of event by allowing us to access books, articles and internet present in the campus as well as providing a comfortable place to deliver our talk. Secondly, we would like thank our departmental head and professors for their sincere guidance and help, without them this seminar would not be a success. I would also thank our non-teaching staff and our juniors for their constant support.

Source: VOGEL'S Textbook of Quantitative Chemical Analysis, 6e, Mendham J., Denney R. C., Bassett J., Jeffery G. H.

Link to Presentation: **Estimation of Zn (II) by using Complexometric Titration**

OR

Scan this QR to see the presentation

Scan me!

Magic Bullets or Delusional Potion: How do they work?

Shramana De, Kazi Mohammed Hameem, Momtaj Mondal

Semester II

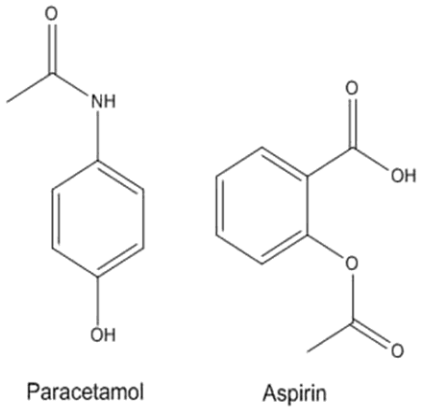
Abstract

The study of drugs and their interactions with the human body is a foundational aspect of pharmaceutical and medical sciences. This paper explores the fundamental chemistry behind drugs, focusing on their classification, molecular interactions, and pharmacological behavior. It begins by defining what constitutes a drug and categorizing them based on source, chemical structure, pharmacological effects, and therapeutic use. This paper encompasses two critical areas: **pharmacokinetics**, which examines the absorption, distribution, metabolism, and excretion (ADME) of drugs; and **pharmacodynamics**, which investigates the biochemical and physiological effects of drugs and their mechanisms of action, especially drug–receptor interactions, analyzed using models such as the lock-and-key model. Key drug examples—aspirin, paracetamol, morphine, heroin, penicillin, caffeine, and ibuprofen—are examined in terms of their structure, synthesis, pharmacokinetics, and clinical use. Special emphasis is placed on drug kinetics and thermodynamics, highlighting how dosage, binding affinity, metabolism, and elimination impact drug efficacy. This paper highlights the various roles of drugs in our everyday lives.

Introduction

What are Drugs?

A drug is a chemical substance that, when introduced into a living system, produces a biological effect. It is a bioactive organic molecule designed to produce a therapeutic effect. In chemistry and pharmacology, a drug is typically defined as:



A bioactive compound used to diagnose, treat, prevent, or alleviate symptoms of diseases by interacting with biological systems at the molecular level. Drugs can act by:

i. Binding to receptors or enzymes
ii. Altering biochemical pathways

iii. Modulating physiological responses

Classification of Drugs:

1. Classification Based on Origin-

- Natural Drugs: Derived from natural sources like plants, animals, or microbes
  Examples: Morphine (from poppy), Quinine (from cinchona bark)
- Semi-synthetic Drugs: Chemically modified versions of natural drugs
  Examples: Heroin (from morphine), Amoxicillin (from penicillin)
- Synthetic Drugs: Fully manufactured in laboratories using chemical processes
  Examples: Aspirin, Paracetamol

2. Classification Based on Action (Therapeutic Use)-

- Analgesics – pain relievers (e.g., ibuprofen)
- Antibiotics – fight bacterial infections (e.g., penicillin)
- Antipyretics – reduce fever (e.g., paracetamol)
- Antacids – neutralize stomach acid (e.g., magnesium hydroxide)
- Antidepressants – treat depression (e.g., fluoxetine)

3. Classification Based on Target System-

- CNS Drugs – affect the central nervous system (e.g., diazepam)
- Cardiovascular Drugs – regulate heart and blood pressure (e.g., atenolol)
- Respiratory Drugs – treat asthma or allergies (e.g., salbutamol)

4. Classification Based on Chemical Structure-

- Alkaloids – nitrogen-containing (e.g., morphine, atropine)
- Steroids – four-ring structure (e.g., cortisol, testosterone)
- Peptides – short chains of amino acids (e.g., insulin)
- Heterocycles – rings with carbon and other atoms (e.g., caffeine)

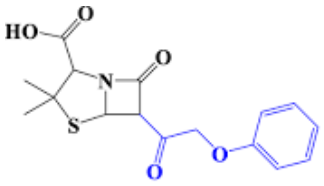
5. Classification Based on Mode of Action-

- Receptor Agonists – mimic natural ligands (e.g., salbutamol)
- Receptor Antagonists – block receptors (e.g., propranolol)

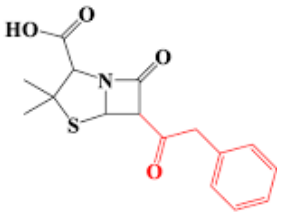
- Enzyme Inhibitors – inhibit enzymes (e.g., aspirin inhibits COX enzymes)

Some Common Drugs:

1. Penicillin



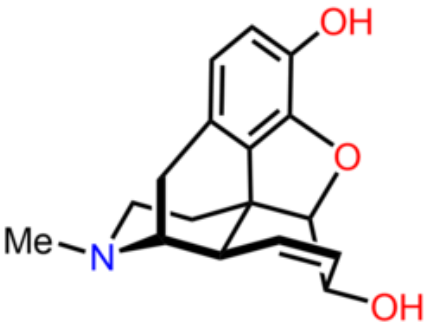
Penicillin V



Penicillin G

- Chemical Name: Benzylpenicillin (Penicillin G) ($C_{16}H_{18}N_2O_4S$)
- Drug Class: Antibiotic, specifically, β-lactam antibiotic
- Discovery: Discovered by Alexander Fleming in 1928 from the mould *Penicillium notatum*. The first true antibiotic used widely in medicine.
- Effective Against: Mostly Gram-positive bacteria (e.g., Streptococcus, Staphylococcus) and some Gram-negative bacteria.

- Types of Penicillin:
  - Natural: Penicillin G, Penicillin V
  - Semi-synthetic: Amoxicillin, Ampicillin, Methicillin (broader spectrum or β-lactamase resistant)



- Pharmacokinetics:
  - Usually administered by injection (Penicillin G) or orally (Penicillin V).
  - Excreted rapidly via the kidneys.
  - Short half-life; often dosed multiple times per day.

2. Morphine

- Chemical Name: Morphine sulphate or Morphine hydrochloride
- Chemical formula: $C_{17}H_{19}NO_3$
- Drug Class: Opioid analgesic (narcotic), a natural alkaloid from the opium poppy (*Papaver omniferum*). It increases dopamine levels (euphoria)

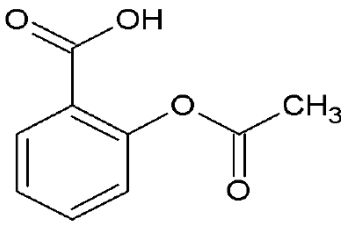
- Uses:
  - Severe acute and chronic pain (e.g., post-surgical, cancer-related)
  - Myocardial infarction (relieves pain and anxiety)
  - Palliative care (improves comfort in terminal illness)

- Some side effects are:
  - Drowsiness, dizziness, nausea, vomiting
  - Constipation

- Respiratory depression (dose-dependent and life-threatening in overdose)
- Physical dependence and addiction with prolonged use

- Tolerance and Dependence:
  - Long-term use leads to tolerance (increased dose needed)
  - Physical and psychological dependence are common
  - Withdrawal symptoms include anxiety, sweating, muscle pain, and nausea

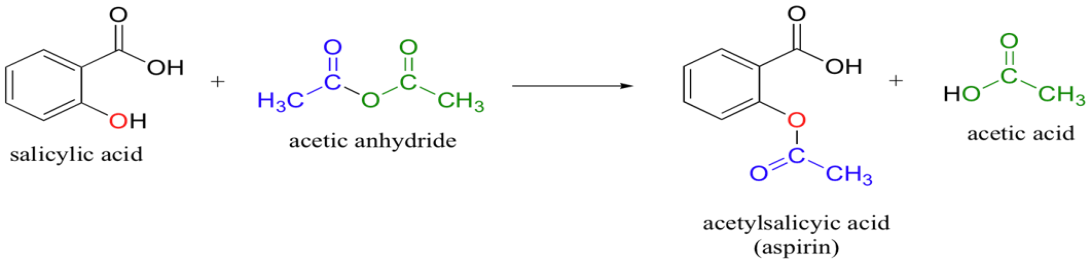
- Pharmacokinetics:
  - Administered orally, intravenously, or via injection.
  - Undergoes first-pass metabolism in the liver.
  - Active metabolite: morphine-6-glucuronide (also analgesic).
  - Excreted mainly via the kidneys.



3. Aspirin

- Chemical Name: Acetylsalicylic acid ($C_9H_8O_4$)
- Origin: Originally derived from salicin, a natural compound found in willow bark.
- Class: Analgesic (pain reliever), Antipyretic (fever reducer), Anti-inflammatory, Antiplatelet agent (prevents blood clots)

- Synthesis of Aspirin:



- Uses:
  - Mild to moderate pain (headache, muscle ache, arthritis)
  - Fever
  - Prevention of heart attack and stroke
  - Anti-inflammatory treatment for conditions like rheumatoid arthritis

- Some side effects are:
  - Gastric irritation, ulcers
  - Risk of bleeding (especially gastrointestinal)
  - Allergic reactions

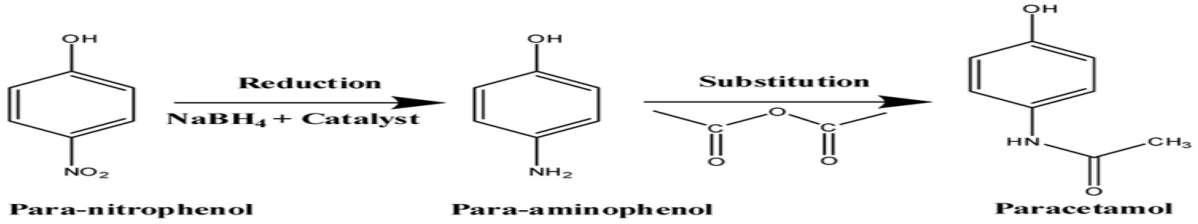
- Pharmacokinetics:
  - Absorbed in the stomach and small intestine

- Hydrolysis to salicylic acid in the liver
- Excreted in urine

4. Heroin

- Chemical Name: Diacetylmorphine (C21H23NO5)
- Drug Class: Semi-synthetic opioid, Derived from morphine (by acetylation)
- Origin: First synthesized in 1874 from morphine. Originally marketed by Bayer as a cough suppressant before its addictive potential was realized
- Effects:
  - Powerful painkiller
  - Euphoric "rush" followed by drowsiness and slowed breathing
  - Suppression of physical and emotional pain
  - High potential for addiction and dependence
  - Respiratory depression (major cause of overdose deaths)
  - Risk of infectious diseases (e.g., HIV, hepatitis) when injected with shared needles

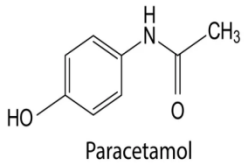
- Chemistry Note: Heroin is more potent and fast-acting than morphine, It is a prodrug, it becomes active only after metabolic conversion.
- Some side effects are:



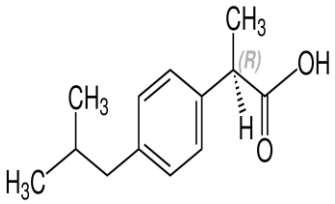
  - High potential for addiction and dependence
  - Respiratory depression (major cause of overdose deaths)
  - Risk of infectious diseases (e.g., HIV, hepatitis) when injected with shared needles

5. Paracetamol

- Chemical Name: N-acetyl-p-aminophenol (C8H9NO2)
- Class: Analgesic (pain reliever), Antipyretic (fever reducer), Not classified as an anti-inflammatory (minimal anti-inflammatory action)
- Synthesis of Paracetamol:



- Uses:
  - Relief of mild to moderate pain (headache, toothache, muscle pain)
  - Reduces fever
  - Often used in children due to fewer side effects compared to aspirin



- Some side effects are:
  - High doses can lead to liver damage (hepatotoxicity)
  - Metabolized in the liver; toxic metabolite (NAPQI) is detoxified by glutathione.
- Pharmacokinetics:
  - Rapid absorption from the gastrointestinal tract
  - Peak plasma concentration within 30–60 minutes
  - Metabolized in the liver via conjugation and oxidation pathways
  - Excreted mainly in urine

6. Ibuprofen

- Chemical Name: (±)-2-(4-isobutylphenyl) propanoic acid
- Drug Class: Nonsteroidal Anti-Inflammatory Drug (NSAID), Analgesic, antipyretic, and anti-inflammatory
- Mechanism of Action:
  - Inhibits cyclooxygenase enzymes (COX-1 and COX-2)
  - Reduces synthesis of prostaglandins that mediate inflammation, pain, and fever
- Therapeutic Uses:
  - Relief of mild to moderate pain (e.g., headache, menstrual cramps, muscle pain)
  - Fever reduction
  - Treatment of inflammatory conditions like arthritis and osteoarthritis
- Side Effects:
  - Gastric irritation, nausea
  - Risk of gastrointestinal ulcers or bleeding (especially at high doses or long-term use)
  - May affect kidney function (especially in dehydrated individuals)
  - Rare allergic reactions
- Advantages:
  - More GI-tolerable than aspirin (especially in short-term use)
  - Available over the counter (OTC) in many countries
- Pharmacokinetics:
  - Rapid oral absorption
  - Peak plasma concentration in 1–2 hours
  - Metabolized in the liver and excreted by kidneys
  - Half-life: ~2 hours

7. Caffeine

- Chemical Name: 1,3,7-Trimethylxanthine
- Drug Class: Central nervous system (CNS) stimulant, belongs to the methyl xanthine group
- Natural Source: Found in coffee beans, tea leaves, and cacao, guarana, and kola nuts.
- The most widely consumed psychoactive substance in the world.
- Effects:
  - Increased alertness and wakefulness
  - Reduced fatigue
  - Improved concentration and physical performance (in moderate doses)
  - Insomnia, anxiety, restlessness
  - Increased heart rate (tachycardia), blood pressure
  - Diuresis (increased urination)

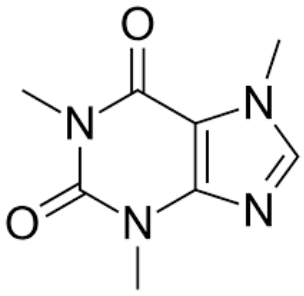
- Side effects:
  - Insomnia, anxiety, restlessness
  - Increased heart rate (tachycardia), blood pressure
  - Diuresis (increased urination)
  - Physical dependence and withdrawal (headache, irritability, fatigue)

- Pharmacokinetics:
  - Rapidly absorbed in the stomach and small intestine
  - Peak blood levels in 30–60 minutes
  - Metabolized in the liver by cytochrome P450 enzymes
  - Half-life: 3–5 hours (varies with age, liver function, pregnancy)

History and Discovery of Drugs

Ancient Times

- *Observation and Natural Remedies:* Early humans likely discovered the therapeutic properties of various plants and animals through observation and trial and error.
- *Traditional Practices:* Indigenous knowledge and herbal remedies played a crucial role in healing for centuries. Examples: Alcohol was used in ancient Egypt (3500 BCE), cannabis in ancient China (3000 BCE), and opium poppies in what is now Switzerland (2500 BCE).



The Rise of Modern Drug

- *19th Century*: The development of synthetic chemistry and the discovery of active ingredients from natural sources paved the way for modern drug discovery.
- *Early 20th Century*: The era of antibiotics began with the discovery of penicillin. Advances in technology, including molecular modeling, combinatorial chemistry, and high-throughput screening, have revolutionized the field of drug discovery.

- *Recombinant DNA Technology*: Enabled the development of drugs targeting proteins and biological processes.
- *Omics Revolution*: The use of genomic and proteomic data has further advanced drug discovery.

Structure Activity Relationships (SAR)

Structure determines function!

It was presented by Crum-Brown and Fraser in 1865. It examines the connection between a drug's chemical structure and its biological activity. It helps scientists understand how structural changes in a molecule affect its ability to interact with a target and elicit a desired biological response. Determining structural and functional relationships helps medicinal chemists synthesize new drugs and pharmaceutical agents.

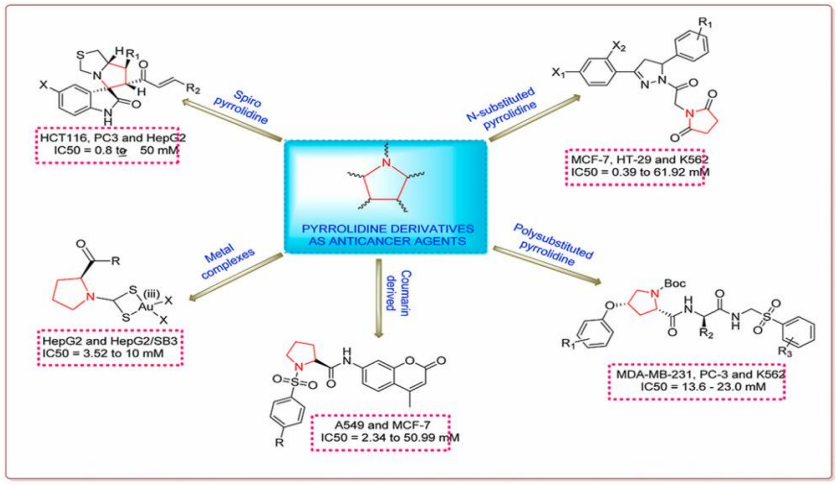


Fig: *Analysis of Pyrrolidine Derivatives as Anticancer Agents using SAR*

Pharmacodynamics

Pharmacodynamics is the study of the biochemical and physiologic effects of drugs (especially pharmaceutical drugs). The effects can include those manifested within animals, microorganisms, or combinations of organisms.

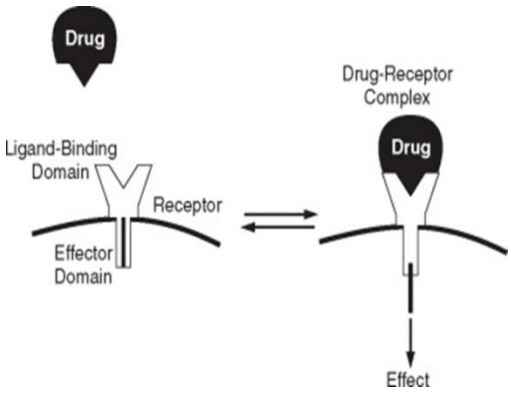
***Drug–Receptor Interactions**:*

Drug–receptor interaction refers to the binding of a drug (ligand) to a specific biological receptor (usually a protein) to initiate a biochemical or physiological response.

- Receptor: A protein molecule that receives chemical signals from outside a cell. Examples: G-protein-coupled receptors, ion channels, enzyme-linked receptors.
- Drug/Ligand: Binds to a receptor to activate (agonist) or block (antagonist) its action. Can be natural (like neurotransmitters or hormones) or synthetic (drugs).

***Types of Ligands**:*

- Agonist: Activates the receptor to produce a biological response. Example: Morphine (opioid receptor agonist)
- Antagonist: Binds to the receptor but blocks activation. Example: Naloxone (blocks opioid receptors)
- Partial Agonist: Activates the receptor but produces a weaker response.
- Inverse Agonist: Produces the opposite effect to that of an agonist.



Drug–Receptor Binding Mechanism

Lock-and-Key Model

The Lock and Key hypothesis explains how drugs interact with their target molecules in the body, much like a key fits into a specific lock. This hypothesis highlights the high specificity of drug-target interactions.

At the molecular level, several factors contribute to the interaction between the drug and receptor, controlling the strength, duration, and type of the drug-receptor interaction. Together, these factors dictate the strength with which the drug forms a complex with its receptor, also known as the *affinity*. These factors are:

- ✓ Size and shape of the drug molecule
- ✓ Types, number, and spatial arrangement of drug binding sites (stereochemistry)

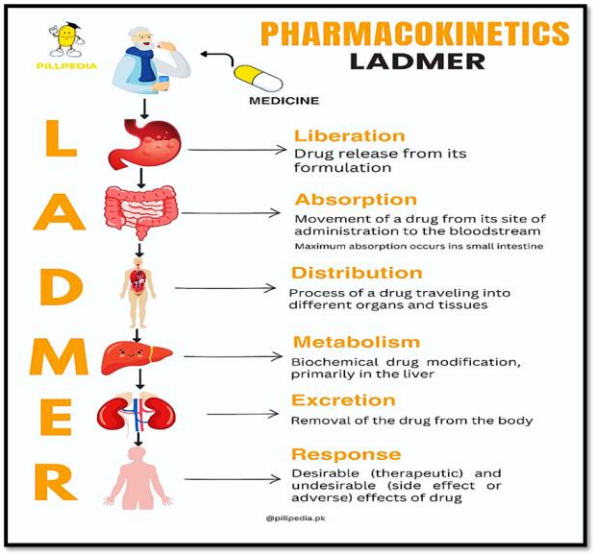
Intermolecular forces present between the drug and binding sites:

- ✓ *Van der Waals forces* - weak bonds and transient, reversible effects
- ✓ *Hydrogen bonds* - intermediate bonds and transient, reversible effects
- ✓ *Covalent bonds* - strong bonds and long-lasting or irreversible effects

Pharmacokinetics

Pharmacokinetics refers to the body's interaction with drugs and how a drug moves through the body over time. It involves four main processes:

- ➢ Absorption
- ➢ Distribution
- ➢ Metabolism (Biotransformation)
- ➢ Drug excretion



1. Absorption

The process by which a drug enters the bloodstream from its site of administration. Absorption affects the speed and concentration at which a drug reaches its desired location of action.

Factors affecting absorption:

a) *Route of administration*: There are many possible methods of drug administration, including oral, intravenous, intramuscular, intrathecal, subcutaneous, buccal, rectal, vaginal, ocular, optic, inhaled, nebulized, and transdermal. Each administration method has its absorption characteristics, advantages, and disadvantages.
b) *Solubility*: Drugs with high solubility are generally absorbed more quickly than those with low solubility.
c) *Gastrointestinal pH and pK_a of drugs*: The amount of drug that exists in un-ionized form and ionized form is a function of pK_a of the drug and the pH of the fluid at the absorption site, and it can be determined by the Henderson-Hasselbach equation:
d) *Effective surface area of absorption (e.g., small intestine > stomach) and particle size*: The smaller the particle size, the greater the surface area, thus the greater the rate of absorption.

2. Distribution

The dispersion of a drug throughout the body fluids and tissues. Distribution is based on the biochemical properties as well as the physiology of the individual taking that medication. The goal of the distribution is to achieve effective drug concentration. To be effective, a medication must reach its designated destination, described by the volume of distribution, and not be protein-bound.

- *Volume of distribution (Vd):* A theoretical volume that relates the total amount of drug in the body to its concentration in the bloodstream. Vd is defined as the total amount of drug in the body divided by its concentration in plasma.
- *Plasma protein binding*: Protein-bound drugs (drugs that are bound to circulating proteins, usually albumin) are pharmacologically inactive; only the unbound drugs can act on target sites in the tissues, elicit a biologic response and be available to the processes of elimination.

3. Metabolism (Biotransformation):

Metabolism refers to the processing of drugs by the body into subsequent compounds. This is often used to convert the drug into more water-soluble substances for excretion. The metabolic processes convert the inactive drug into a more hydrophilic metabolite, and allow it to be excreted in the urine or bile through two phases, where Phase I reactions generally modify substances into polar metabolites by oxidation, reduction, etc., allowing Phase II conjugation reactions to occur.

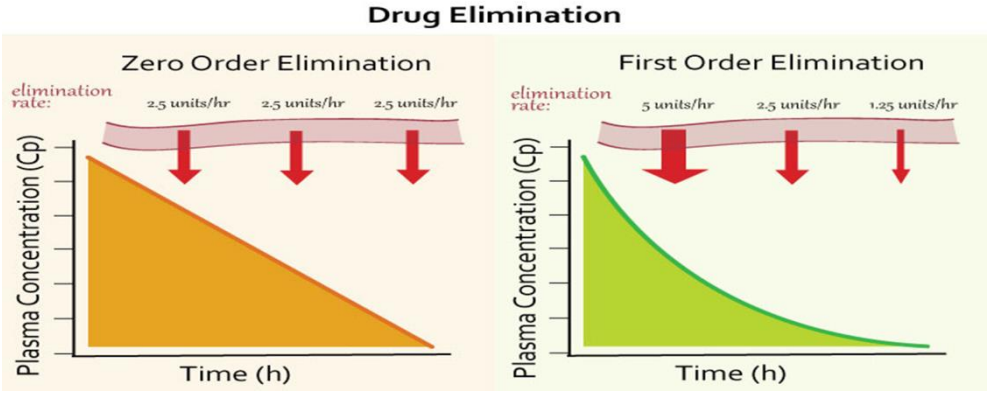
4. Drug excretion

Excretion is the process by which the drug is eliminated from the body. The kidneys most commonly conduct excretion, but for certain drugs, it may be via the lungs, skin, or gastrointestinal tract.

PARAMETERS	DESCRIPTION
Dose	Amount of drug administered.
Dose interval	Time interval between drug dose administrations
Absorption Half-life	The time required for 50% of a given dose of drug to be absorbed into the systemic circulation (t1⁄2=ln2/ka)
Absorption rate constant	The rate at which a drug enters the body through oral and other extravascular routes.
Elimination half-life	The time required for the concentration of the drug to reach half of its original value.
Bioavailability	Refers to the fraction of an administered drug that reaches the systemic circulation
Clearance	The volume of plasma cleared of the drug per unit time.

Drug Kinetics

This is the graphical manifestation of metabolism and excretion and depicts a medication's half-life. The two major forms of drug kinetics are described by zero-order and first-order kinetics. Zero-order kinetics show a constant rate of metabolism or elimination independent of the concentration of a drug (E.g., alcohol and phenytoin elimination). In contrast, first-order kinetics relies on the proportion of the plasma concentration of the drug.



Lethal or Lifesaver:

1. **Therapeutic Role**

- Treat diseases by targeting specific biological pathways
- Antibiotics kill or inhibit bacterial growth (e.g., penicillin)
- Antivirals slow viral replication
- Anticancer drugs inhibit tumor growth (e.g., cisplatin)

2. **Preventive Role**

- Prevent the onset of diseases
- Vaccines stimulate immunity (e.g., mRNA COVID-19 vaccines)
- Prophylactic drugs (e.g., malaria prophylaxis)

3. **Diagnostic Use**

- Aid in identifying diseases
- Radiopharmaceuticals (e.g., Technetium-99 used in scans)
- Glucose tolerance test agents

4. **Palliative Role**

- Relieve symptoms without curing the disease
- Analgesics relieve pain (e.g., morphine in cancer patients)
- Anti-inflammatory drugs reduce swelling and discomfort

5. **Restorative and Supportive Role**

- Help in recovery or maintaining normal physiological functions
- Hormone replacement therapy (e.g., insulin in diabetes)
- Nutritional supplements and electrolyte therapy

6. **Increases life expectancy and quality of life**

- Reduces healthcare costs through disease control
- Drives pharmaceutical innovation and industry growth

7. **Research and Technological Advancement**

- Drugs serve as tools to understand biochemical pathways
- Help in developing new diagnostic and therapeutic strategies

8. **Detrimental Role**

- Harmful to organs and systems in your body, such as your throat, stomach, lungs, liver, pancreas, heart, brain, and nervous system.
- Cancer (such as lung cancer from inhaling drugs).

- Infectious disease, from sharing the injecting equipment, and increased incidence of risk-taking behaviors.
- Acne or skin lesions, if the drug you are taking causes you to pick or scratch at your skin.
- Needle marks and collapsed veins, if you inject regularly.
- Male pattern hair growth in women, such as facial hair.
- Jaw and teeth issues due to clenching and grinding your teeth, tooth cavities, and gum disease.
- Mood swings and erratic behaviors.
- Addiction
- Psychosis (losing touch with reality).
- Accidental overdose.
- Higher risk of mental illness, depression, suicide, and death.
- Substances manufactured in home labs may contain bacteria, dangerous chemicals, and other unsafe substances. Even one dose may cause an overdose that leads to brain damage or death.

Conclusion

The chemistry of drugs forms a crucial bridge between molecular science and human health. Understanding drug classification, synthesis, and mechanisms of action equips us to develop more targeted, effective, and safer medications. The study of how drugs interact with biological receptors illustrates the precision required in drug design. Examples like aspirin and ibuprofen demonstrate how small structural changes can significantly influence therapeutic use and side effects, while compounds like morphine and heroin highlight the balance between medical benefit and potential for abuse. In essence, drug chemistry not only shapes the pharmaceutical industry but also plays a vital role in modern medicine and public health. Ongoing research and responsible use will continue to expand the benefits of pharmacological science for future generations.

THANK YOU!!

ACKNOWLEDGEMENT

We would like to convey our heartfelt gratitude to our professors for their tremendous support and guidance throughout this project. We also extend our sincere thanks to my friends, whose help and encouragement made this work possible. The completion of the project would not have been possible without their help and insights.

References:

1. Wikipedia
2. Pharmacokinetics by Sean Grogan; Charles V. Preuss
3. Drug Distribution within the Body *by Jennifer Le.*
4. Factors affecting drug absorption (presentation) by Suryakant Verma
5. PHARMACOKINETICS (presentation) by MERLYN A.
6. 2011, Applied Pharmacology by Stan K. Bardal BSc (Pharm), Douglas S. Martin
7. DRUG RECEPTOR INTERACTIONS (presentation) by TATHAGATA PRADHAN
8. Atkins, P., & de Paula, J. (2014). **Atkins' Physical Chemistry** (10th Ed.). Oxford University Press.
9. Foye, W. O., Lemke, T. L., & Williams, D. A. (2012). **Foye's Principles of Medicinal Chemistry** (7th ed.). Lippincott Williams & Wilkins.

Link to presentation: **Magic Bullets or Delusional Potion: How do they work?**

OR Scan the QR code to see the presentation

Scan me!

Explaining Wittig Reaction and Johnson-Corey-Chaykovsky Reaction

Swastika Acharyya, Arpita Mondal, Mukhesh Kumar Sah

Semester IV

Abstract

This article is all about explaining the Wittig reaction that includes synthesis of alkene from haloalkanes and carbonyl compounds via a stable ylide formation. Along with few other modifications of this technique and their mechanisms. The second part includes Johnson-Corey-Chaykovsky reaction which explores the technique of synthesizing methylsulphonium ylides and epoxide like products. Finally, concluding with a note of difference between the two mentioned rections.

Introduction

George Wittig (16 June, 1897 -26 August 1987) was a German chemist who reported a method for synthesis of alkenes from aldehydes and Ketone) using compounds called Phosphonium ylides in the Wittig Reaction. He shared the Nobel Prize in chemistry with Herbert C. Brown in 1979 mainly for developing the Wittig Reaction. Wittig's contributions also include the preparation of phenyllithium and the discovery of the 1, 2-wittig rearrangement and the 2, 3-wittig rearrangement. He died on 26 August in 1987 in Germany.

Elias James Corey (born July 12, 1928) is an American organic chemist. In 1990, he won the Nobel Prize in Chemistry "for his development of the theory and methodology of organic synthesis", specifically retrosynthetic analysis. Among numerous honours, Corey was awarded the National Medal of Science in 1988, the Nobel Prize in Chemistry in 1990, and the American Chemical Society's greatest honour, the Priestley Medal, in 2004.

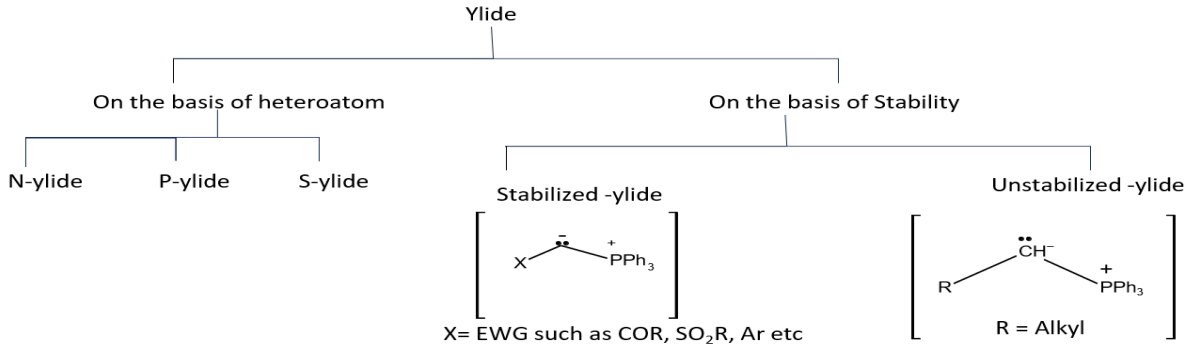
Michael Chaykovsky, (1935-May 10, 2014) he was a postdoctoral fellow at Harvard University, working with Professor E. J. Corey, recipient of the Nobel Prize in Chemistry. Their collaboration, published as the Corey-Chaykovsky Reaction, broke new ground in the existing knowledge of

organic chemistry. It continues to be used in many high-profile applications and is recognized as a powerful transformative tool in organic synthesis. He received numerous awards and accolades for his work and extensive publications. Dr. Chaykovsky was a gifted scientist who collaborated with colleagues around the world.

Wittig Reaction

Formation of alkene from carbonyl compound:

Classification of ylide

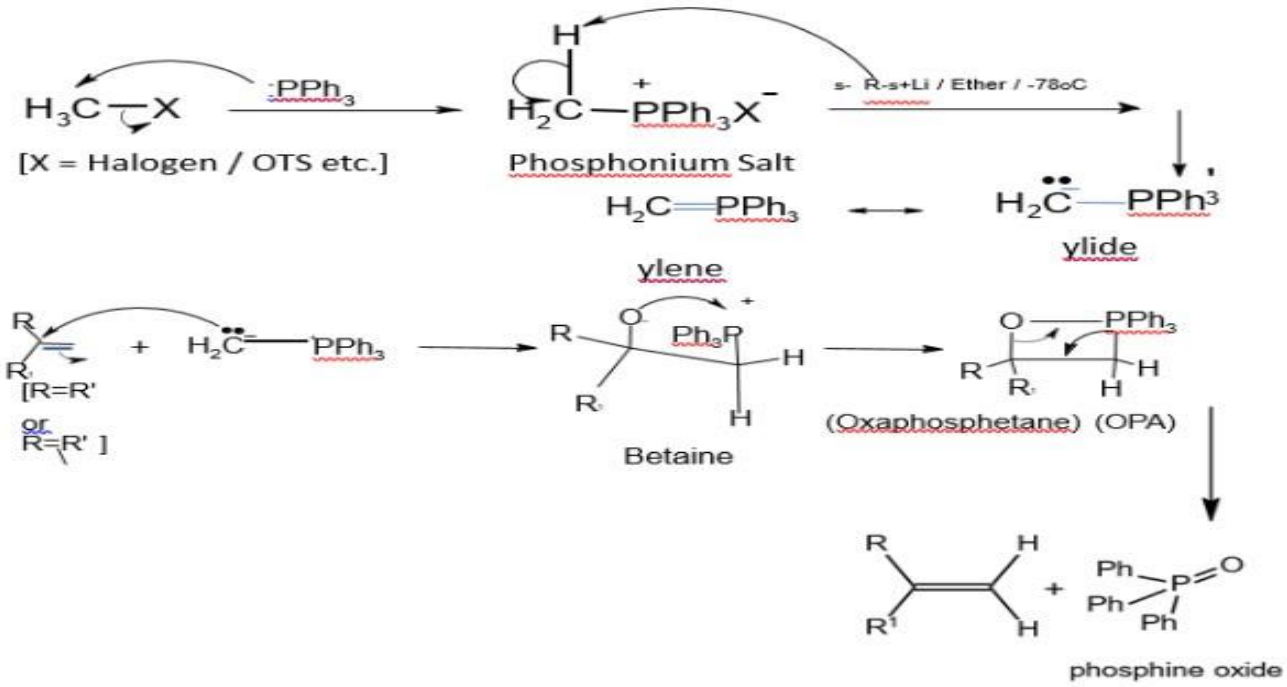


Definition of Ylides:

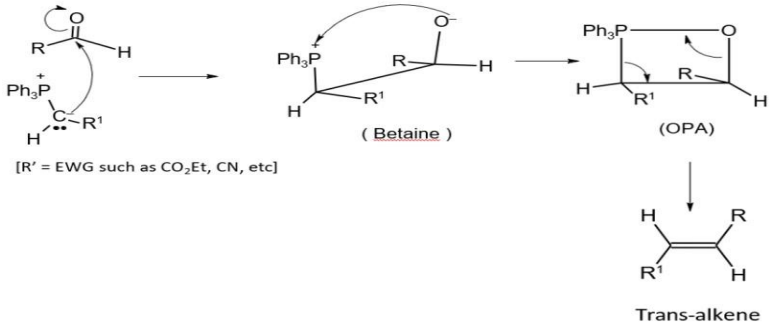
An organic species that contain negative charge over electro positive **C** atom and positive charge over heteroatom such as (N, P, S); such species are called ylide of that heteroatom and hence they are electrically neutral.

- Wittig reaction is a Stereoselective reaction.The Stereochemistry of the Alkene produced depends on the nature of the Ylides.
- From ***Stabilized P-ylide***, we get ***trans-alkene*** as a major product.
- From ***Unstabilized P-ylide***, we always get ***cis-alkene*** as a major product.

Preparation of Phosphonium Ylide:



Preparation of trans alkene using stabilized phosphorus ylide:



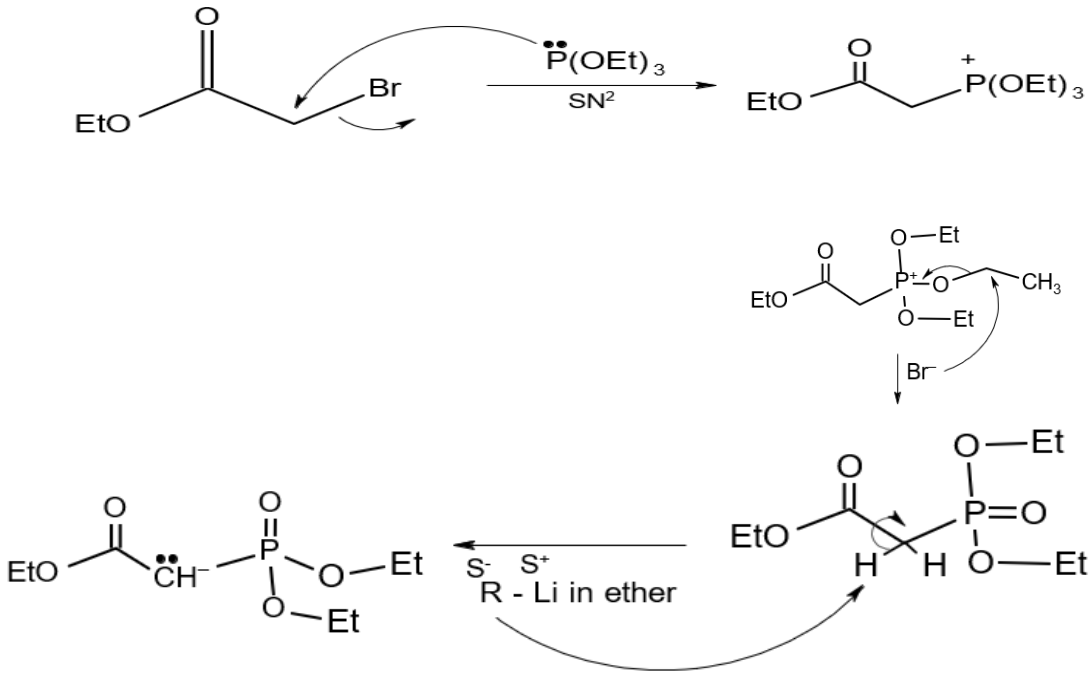
MODIFICATION

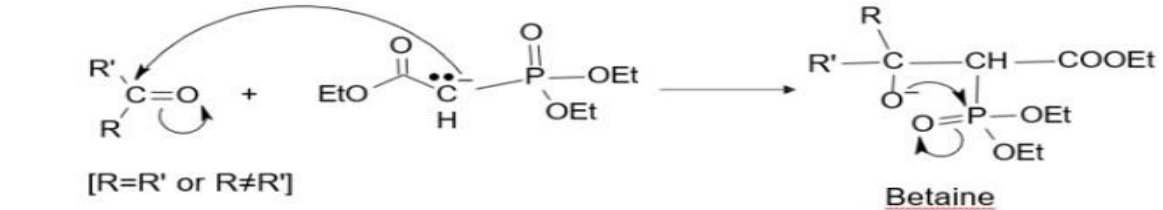
Horner- Wordsworth-Emmons Modification

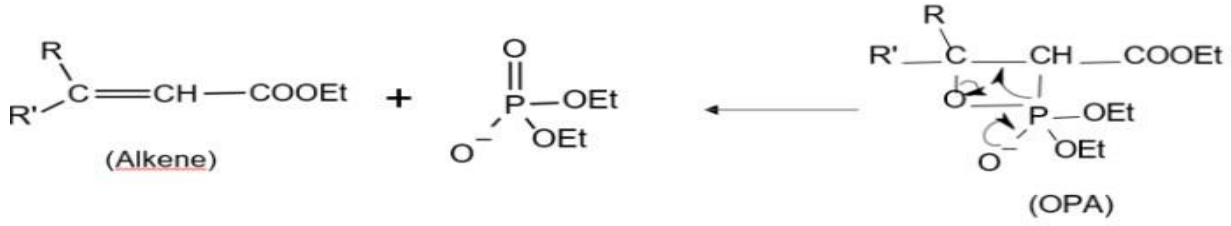
Stabilized p-ylides are generally less reactive so, olefination of the sterically hindered ketone using stabilized P-ylides give poor yield of the final product. Thus, modification is needed.

Reagent: P (OEt)$_3$

Formation of ylide:

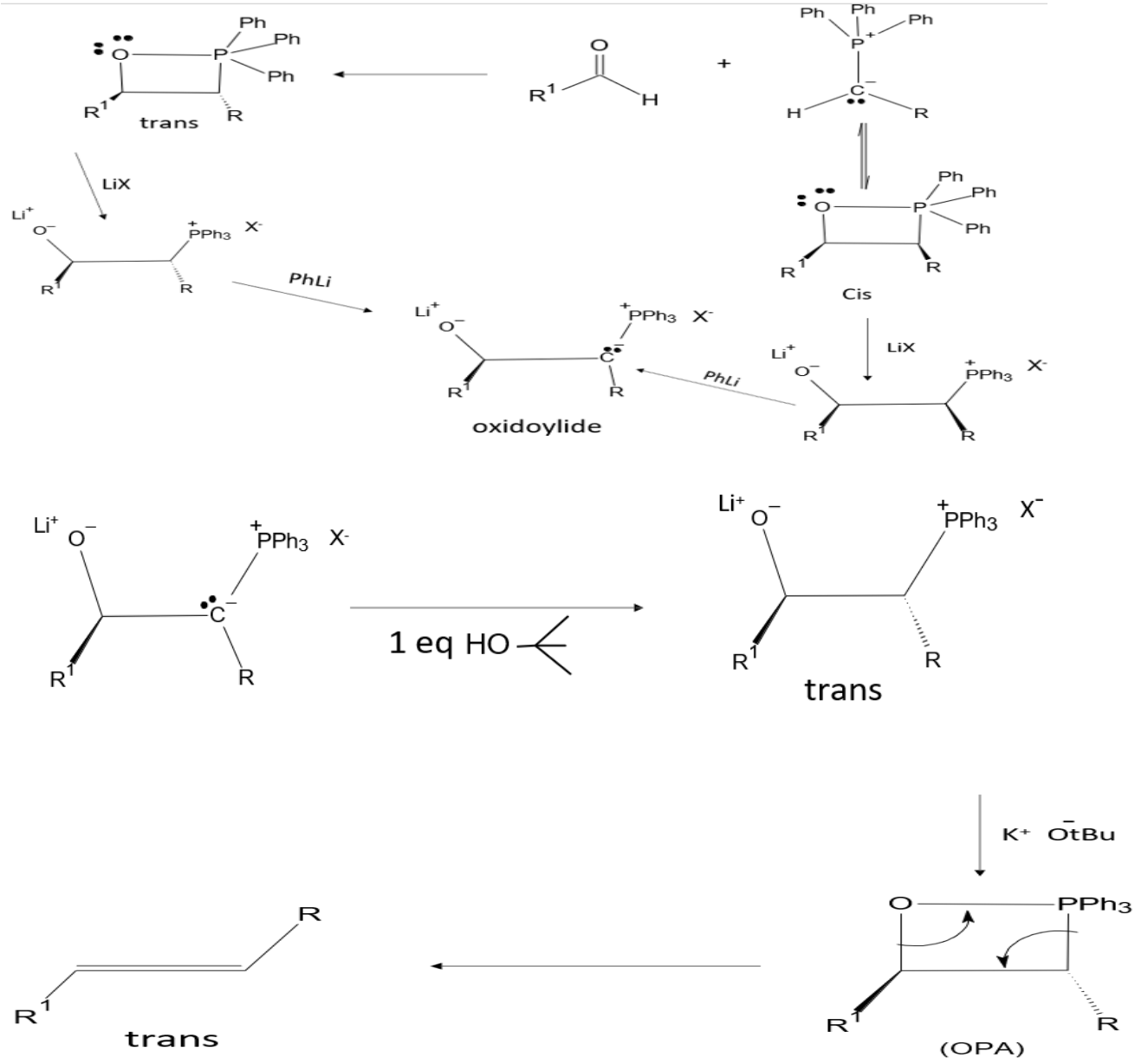






Schlosser Modification

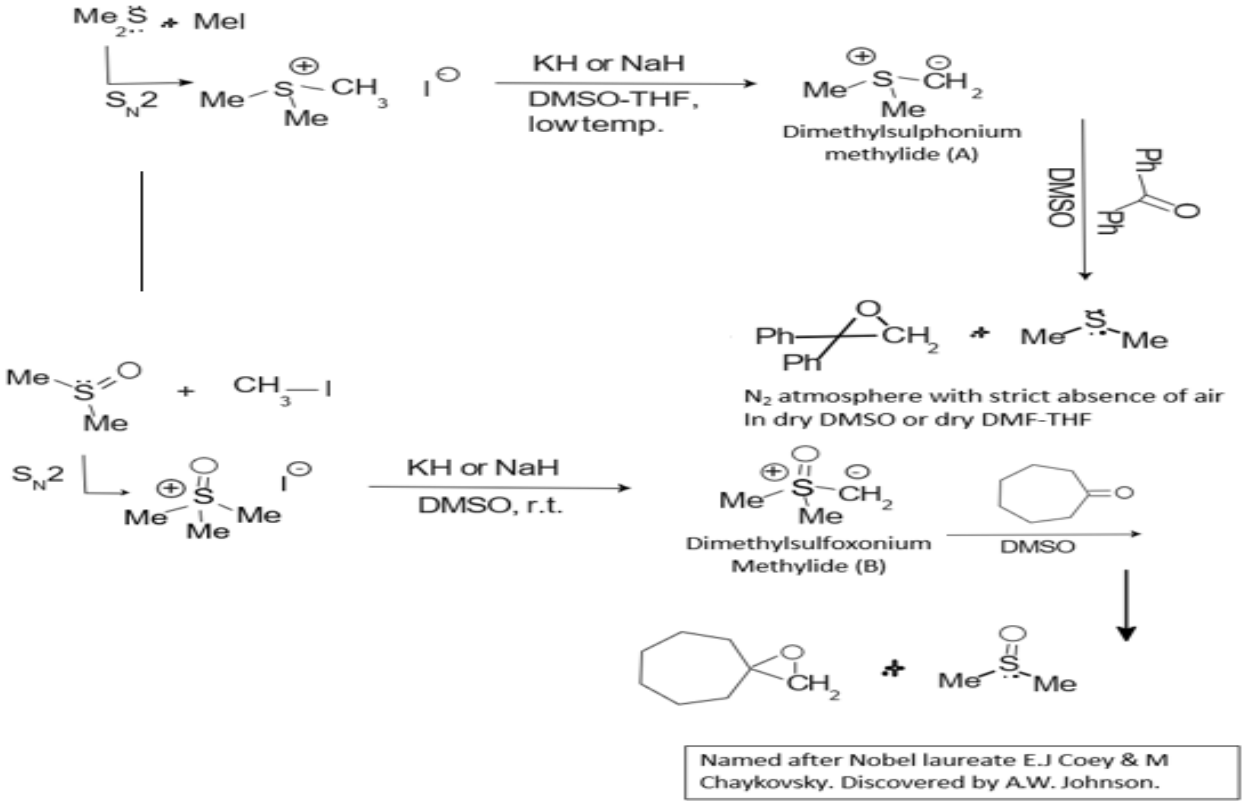
It allows the selective formation of E-alkene through the use of excess Li- salts during Addition step of the Ylide and the subsequent deprotonation /protonation step in Wittig Reaction.



Johnson-Corey-Chaykovsky Reaction

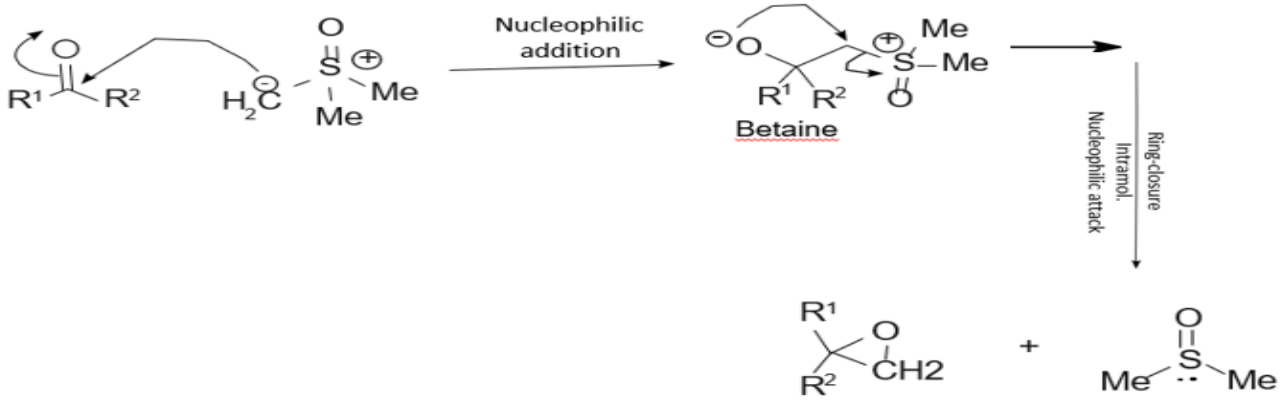
Reaction with ylides

The synthesis of monosubstituted or geminally disubstituted epoxides from aldehydes or ketones with sulfur ylides such as dimethylsulfonium methylide (A) or dimethylsulfoxonium methylide

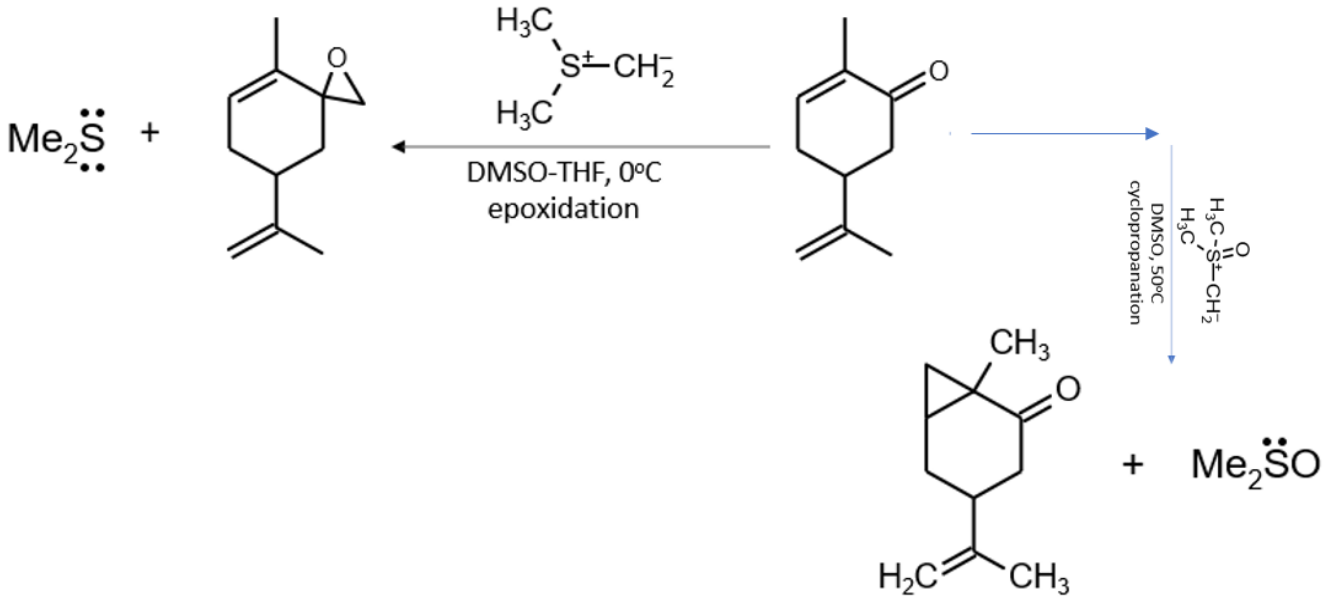


(B).

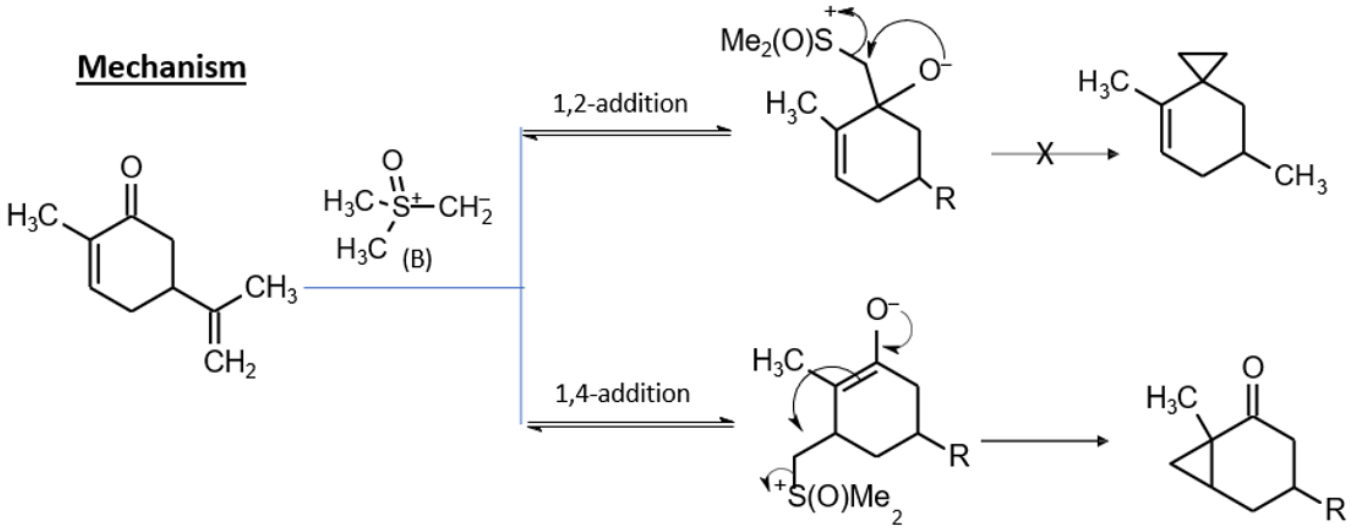
Mechanism



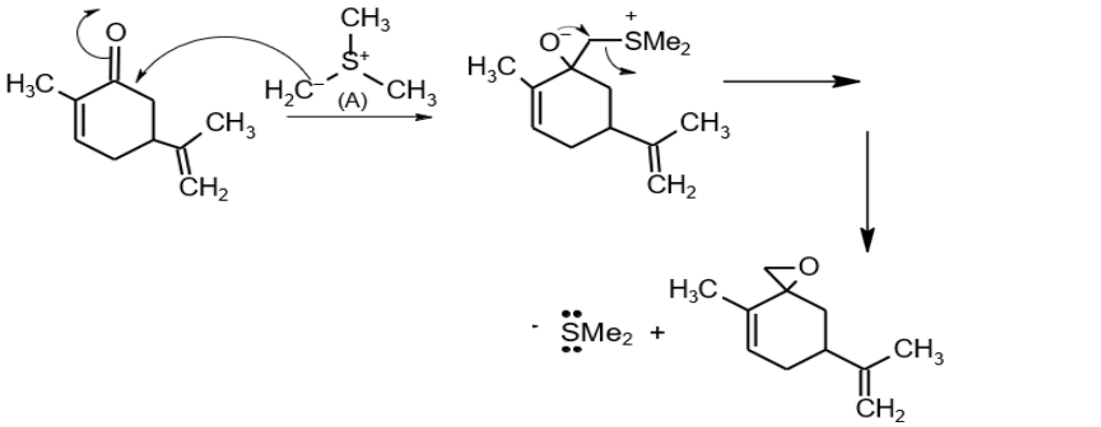
Dimethylsulfonium methylide (A) and dimethylsulfoxonium methylide (B) behave differently



when reacting with α, β-unsaturated carbonyl compounds. The former gives epoxide while the latter leads to cyclopropanation.



With A, the reaction is under kinetic control and 1,2-addition followed by ring closure leads to epoxide; with B, which is a more stable S-ylide, the reaction is reversible & under thermodynamic control - leading to 1,4- addition and eventual cyclopropanation.



Kinetically-controlled 1,2-addition of non-stabilized S-ylide; not reversible only epoxidation is seen.

Epoxidation with dimethylsulfonium methylide (A) proceeds in the following way

Conclusion

Difference Between Wittig & Johnson–Corey–Chaykovsky Reaction

1. ***Oxaphosphetane (OPA)*** formation is energetically more favourable than ***Oxathietane (OTA)*** formation as a P-O bond is than a S-O bond consequently the strain associated with the 4-membered ring is too much for S-ylides, but can be compensated by the stronger P- O bond in case of P-ylides. Hence, betaine int. are preferred for S-ylides while OPA int. are favoured for the P-ylides. The lack of OTA int. for S-ylides mean no olefination can take place with it.

2. Even if betaine int. is involved for P-ylides , the epoxides formation is unfavourable in comparison to the traditional Wittig reaction outcome i.e. olefination because ---

    a) PR_3 is a poorer leaving group than SR_2.
    b) The C-P bond is stronger than the C-S bond.

ACKNOWLEDGEMENT

We would like to thank our college to help our department organize this kind of event by allowing us to access books, articles and internet present in the campus as well as providing a comfortable place to deliver our talk. Secondly, we would like thank our departmental head and professors for their sincere guidance and help, without them this seminar would not be a success. I would also thank our non-teaching staff and our juniors for their constant support.

Source:

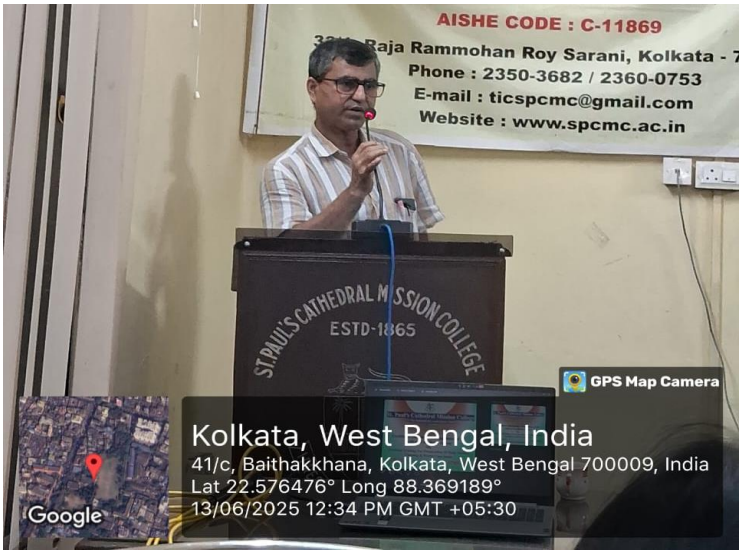
1. **Organic Chemistry Lifesaver, Vol-4, 1e, Mandal K K., Basu K.**
2. **A Guidebook to Mechanisms in Organic Chemistry, Skyes Peter, 6e.**

Link to presentation: [Explaining Wittig Reaction and Johnson-Corey-Chaykovsky Reaction]

OR Scan the QR code to see the presentation

Scan me!

Moments from the Seminar

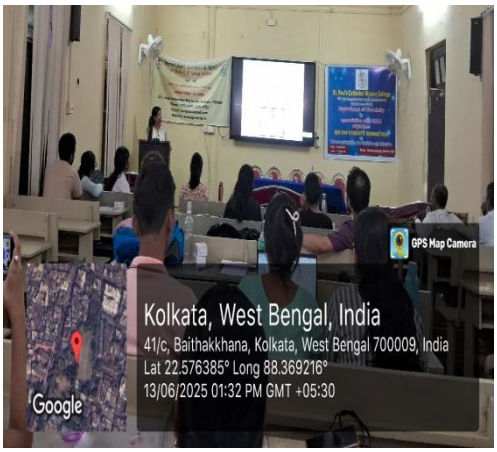



GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.57647° Long 88.369238°
13/06/2025 03:55 PM GMT +05:30
Google


GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576475° Long 88.369217°
13/06/2025 02:13 PM GMT +05:30
Google

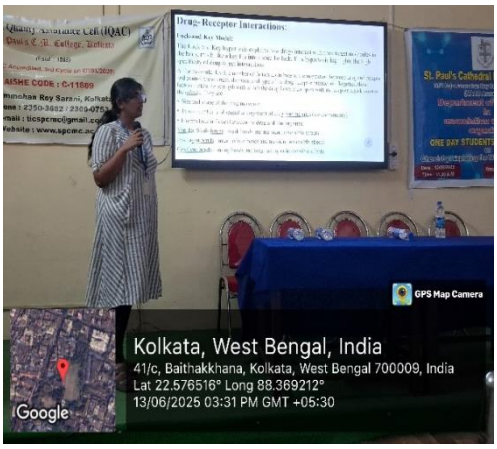

COMPLEXOMETRIC
TITRATION OF ZINC
GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576434° Long 88.369229°
13/06/2025 02:57 PM GMT +05:30
Google


GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576434° Long 88.369193°
13/06/2025 12:56 PM GMT +05:30
Google


GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576385° Long 88.369216°
13/06/2025 01:32 PM GMT +05:30
Google

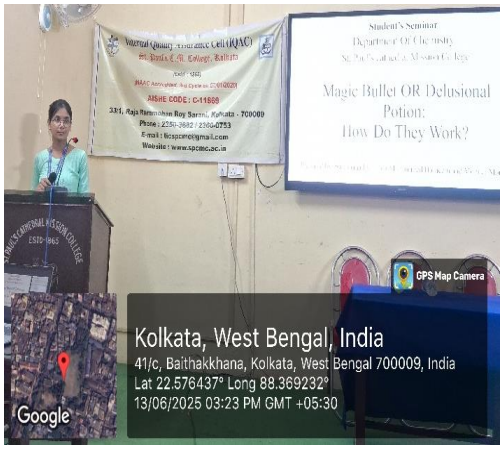

GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576432° Long 88.369225°
13/06/2025 03:00 PM GMT +05:30
Google


Kolkata - 700009
GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576479° Long 88.369245°
13/06/2025 01:50 PM GMT +05:30
Google


Drug-Receptor Interactions:
GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576516° Long 88.369212°
13/06/2025 03:31 PM GMT +05:30
Google


GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576478° Long 88.369231°
13/06/2025 02:08 PM GMT +05:30
Google


St. Paul's C. M. College, Kolkata
AISHE CODE : C-11869
Phone : 2350-3682 / 2360-0753
E-mail : ticspcmc@gmail.com
Website : www.spcmc.ac.in
ST PAUL'S CATHEDRAL MISSION COLLEGE
ESTD·1865
GPS Map Camer
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576474° Long 88.36922°
13/06/2025 02:46 PM GMT +05:30
Google


Student's Seminar
Department Of Chemistry
Magic Bullet OR Delusional
Potion:
How Do They Work?
GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576437° Long 88.369232°
13/06/2025 03:23 PM GMT +05:30
Google


GPS Map Camera
Kolkata, West Bengal, India
41/c, Baithakkhana, Kolkata, West Bengal 700009, India
Lat 22.576501° Long 88.369202°
13/06/2025 03:30 PM GMT +05:30
Google