ACHARYA NARENDRA DEV COLLEGE

UNIVERSITY OF DELHI

Teaching Assistantship Proposal

Physical Sciences

(2022-23)

Prime Minister Research Fellow

Department of Chemistry

IIT DELHI

Semester 1, Course plan (Total time: 60 hours)

Course Objective

1. Essential Research related software and search engine- **15 hrs**
    - ChemDraw
    - Origin
    - Scifinder
    - Basic of Gaussian
    - Application of these softwares in MS Office

2. How to plan any General Reaction (Organic and Inorganic)- **15 hrs**
    - Searching for appropriate literature
    - Calculation in ChemDraw
    - Reaction setup
    - Apparatus Required
    - Putting the reaction
    - Checking the progress of reaction by TLC
    - Workup
    - Column (Flash+Mannual)
    - Rota Evaporation
    - High vacuum
    - Characterization

3. Electrochemistry (Theory + Practical Experience)- **10 hrs**

4. General Text book Name Reaction and their Practical Experiment (Synthesis)- **20 hrs**
    A. Aldol Reaction
    B. Grignard Reaction
    C. Wittig Reaction
    D. Photochemical Reaction

Assessment Plan

1. **Quizzes**

One quiz will be conducted (post-mid semester) to test conceptual understanding of the students.

2. Hands on

Short and simple hand on test for software related skill development.

3. Assignment

Students would submit a term paper (not more than 2 pages) on any topic related to the course content and give oral presentation (max 5 minutes) on it.

4. Mid Semester Exam

An assessment to evaluate the student's understanding of the course (theory only).

5. End Semester Exam

A comprehensive assessment for the students to indicate their understanding of the course and practical skill.

Reading Recommendation

Reading materials including relevant chapters from various books and research articles will be shared along with the presentations during the course.

Talk 1: Why to do Research?

The first official engagement between the 5 PMR Fellows and the students will be a formal presentation. The primary reason for doing so is to encourage an increasing number of students to join us in this effort, which will assist them in learning moreabout scientific research. This presentation will focus primarily on informing students about research career prospects.

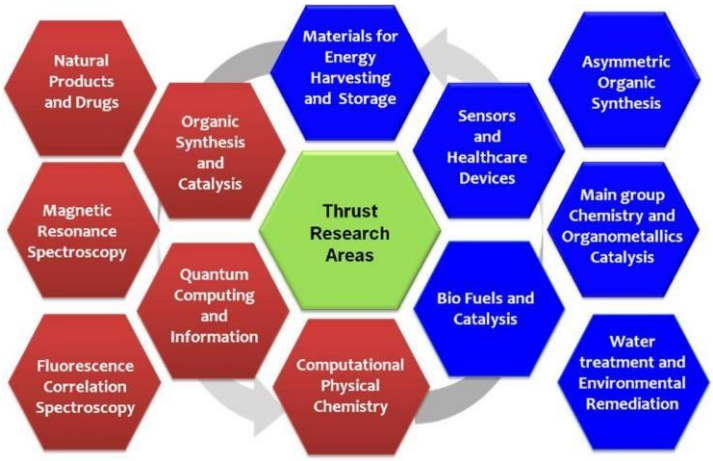
There are three main purposes of research:

1. **Exploratory:** Exploratory research is the first research to be conducted around a problem that has not yet been clearly defined. Exploration research therefore aims to gain a better understanding of the exact nature of the problem and not to provide a conclusive answer to the problem itself. This enables us to conduct more in-depth research later on.

2. **Descriptive:** Descriptive research expands knowledge of a research problem or phenomenon by describing it according to its characteristics and population. Descriptive research focuses on the 'how' and 'what', but not onthe 'why'.

3. **Explanatory:** Explanatory research, also referred to as casual research, isconducted to determine how variables interact, i.e., to identify cause-and- effect relationships. Explanatory research deals with the 'why' of research questions and is therefore often based on experiments.

Area of Research in chemistry for the students:



Talk 2: What we will teach you?

1. Essential Research related software and search engine:
    - ChemDraw
    - Origin
    - Scifinder
    - Basic of Gaussian
    - Application of these software in MS Office.

2. How to plan any General Reaction: (Organic and Inorganic)
    - Searching for the appropriate literature.
    - Calculation in ChemDraw.
    - Reaction Setup.
    - Apparatus Require
    - Putting the Reaction.
    - Checking the progress of reaction by TLC.
    - Workup
    - Column (flash + manual)
    - Rota Evaporation.
    - High Vacuum
    - Characterization

3. Electrochemistry (Theory + practical Experience)
4. General text book Name Reaction and their practical experiment (synthesis).
    1. Aldol Condensation.
    2. Grignard Reaction.
    3. Wittig Reaction.
    4. Photochemical Reaction.

Essential Research related software and search engine:

1. ChemDraw:

ChemDraw is a molecule editor first developed in 1985 by David A. Evans and Stewart Rubenstein (later by the cheminformatics company CambridgeSoft). The company was sold to PerkinElmer in the year 2011. ChemDraw, along with Chem3D and ChemFinder, is part of the ChemOffice suite of programs and is available for Macintosh and Microsoft Windows.

Feature of ChemDraw:

- Chemical structure to name conversion
- Chemical name to structure conversion
- NMR spectrum simulation (^{1}H and ^{13}C)
- Mass spectrum simulation
- Structure cleanup
- An extensive collection of templates, including style templates for mostmajor chemical journals.
- Export to SVG
- Export to PDF (Mac Version only).

2. Origin:

Origin is a computer program for scientific/research based graphing and data analysis. Graphing can be done in form of 2D/3D plot types in Origin. Data analyses in Origin include statistics, signal processing, curve fitting and peak analysis. The plotted data can be exportedin form of various image file formats such as JPEG, GIF, EPS, TIFF, etc. It allows the various mathematical operations on raw data.

3. Scifinder:

SciFinder, produced by Chemical Abstracts Service (CAS), is the most comprehensive database for the chemical literature, searchable by topic, author, substances by name or CAS Registry Number, OR use the editor to draw chemical structures, substructures, or reactions. It is a core research tool for chemistry, biochemistry, chemical engineering, materials science, nanotechnology, physics, environmental science and other science and engineering disciplines.

4. Gaussian:

Gaussian /ˈɡaʊsiən/ is a general purpose computational chemistry software package initially released in 1970 by John Pople and his research group at Carnegie Mellon University as Gaussian 70. It has been continuously updated since then. The name originates from Pople's

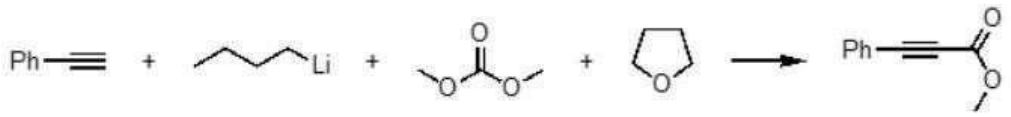
use of Gaussian orbitals to speed up molecular electronic structure calculations as opposed to using Slater-type orbitals, a choice made to improve performance on the limited computing capacities of then-current computer hardware for Hartree–Fock calculations. The current version of the program is Gaussian 16. Originally available through the Quantum Chemistry Program Exchange, it was later licensed out of Carnegie Mellon University, and since 1987 has been developed and licensed by Gaussian, Inc.

How to plan any General Reaction: (Organic and Inorganic)

Literature Survey: Before doing any reaction, someone should do lots of literature surveys. As it can give you the information about what is an appropriate condition for your reaction. We generally use a search engine like Sci-finder, reaxys and so on.

Necessary things: Someone should check the availabilities of required chemicals (it is better to check once the condition of the chemicals) and required glassware.

Chem-Draw Stoichiometric table: in Chem-Draw we can make a stoichiometric table with respect to the limiting reagents. We can estimate the required equivalent, mass, and volume.



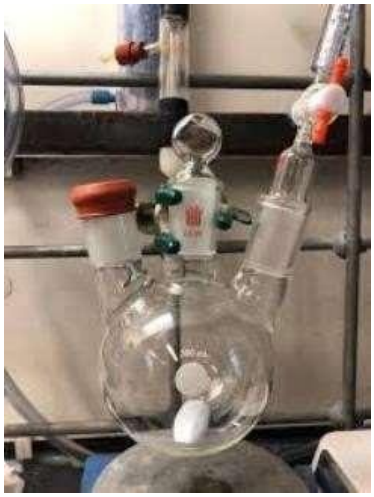
Reactants					*Products*	
Formula	C_8H_6	C_4H_9Li	$C_3H_6O_3$	C_4H_8O	Formula	$C_{10}H_8O_2$
MW	102.14	64.06	90.08	72.11	MW	160.17
Limiting?	***Yes***	No	No	No	Equivalents	
Equivalents		***1.20***	***2.00***		%Completion	
Sample Mass	***1.00g***	752.60mg	1.76g	705.99mg	Expected Mass	1.57g
%Weight					Expected Moles	9.79mmol
Molarity		***1.60M***		***300.00mM***	Measured Mass	
Density					Purity	
Volume		7.34mL		32.64mL	Product Mass	
Reactant Moles	9.79mmol	11.75mmol	19.58mmol	9.79mmol	Product Moles	
Reactant Mass	1.00g	752.60mg	1.76g	705.99mg	%Yield	

Glassware:

Before the reaction:

For solvent: Steelhead condenser, reflux condenser, tubing, Argon balloon system, Mantle setup.

For the cooling system: arrange the Low-temperature bath at -78 C / liquid N_2 in acetone



Typical inert reaction set up

For the reaction:

Round bottom flask: 100 ml (B19)
Magnetic bead (suitablefor 100 ml)
Septa (B19)
Syringe and needles: 10ml (for BuLi), 20 ml (for Solvent), 5 ml (for reagentaddition)
Argon balloon systems: 2 (two balloons + two balloon adapters) Spatula, weighing balance, pipettes.

Monitoring the reaction:

TLC chamber, petri dish, TLC plate, capillary, forceps, solvents (Ethyl acetate andhexane), Iodine, PMA and Alc. KMnO4 stains, heat gun.

Running the TLC

Quenching the reaction:

Aq. NH4Cl

For work up:

Ethyl acetate, distilled water, separating funnel (B24, 100 ml), Stopper (B24), Conicalflasks (250 ml, 100 ml), stand with clamp, sodium sulphate, funnel, cotton.

Reaction Work-Up

For solvent evaporation:

100 ml RB, Funnel, rota joint, rota.

For column chromatography:

Column, Dropper, Dropper teat, cotton, Ethyl acetate, hexane, test tubes, test tubestand, sodium sulfate, TLC plate, capillary, TLC chamber.

Column Chromatography

Evaporation of solvent collected from column:

250 ml RB, Funnel, rota joint.

To remove the trace amount of solvent

High vacuum pump, balloon joint, argon balloon, liq. N2, trap.

Analysis through NMR:

NMR tube, CDCl3, Dropper

Storing the compound:

15 ml Vial, dropper.

Electrochemistry (Theory + practical Experience):

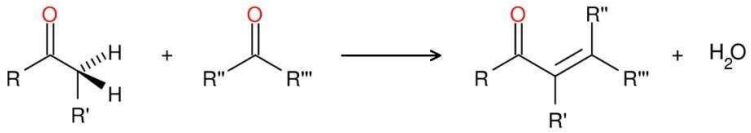
Fig: The cell setup

- To understand the basic electrochemistry operating behind cell operation and water splitting.
- To understand the need for water splitting
- To acknowledge the energetics and mechanism of various components of water splitting.

General text book Name Reaction and their practical experiment (synthesis).

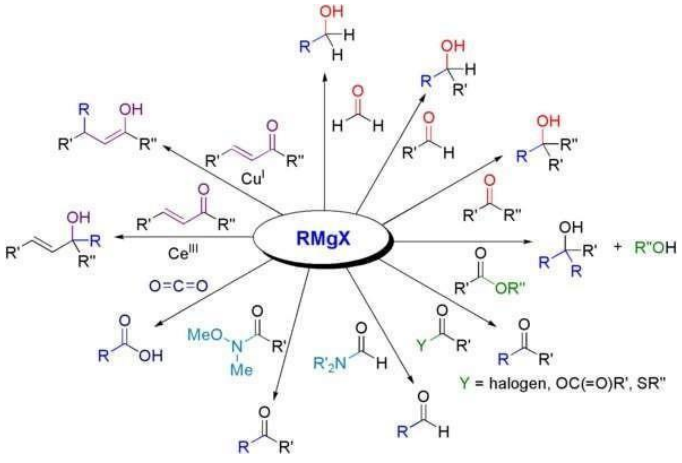
1. **Aldol Condensation:**

   An aldol condensation is a condensation reaction in organic chemistry in which an enol or an enolate ion reacts with a carbonyl compound to form a β- hydroxyaldehyde or β-hydroxyketone (an aldol reaction), followed by dehydration to give a conjugated enone.



2. **Grignard Reaction:**

Grignard reagents (RMgX) are commonly used for organic synthesis. However, these highly reactive compounds are supplied in flammable solvents, which cause extra complexity in their transport. Herein we note that Grignard reagents with linear alkyl chains can be trapped and stabilized by the macrocyclic host pillar arene while retaining their reactivity. Reactions that form carbon-carbon bonds are among the most beneficial to the synthetic organic chemist. In 1912, Victor Grignard was awarded the Nobel Prize in Chemistry for his discovery of a new sequence of reactions resulting in the creation of a carbon-carbon bond. Grignard synthesis involves the preparation of an organomagnesium reagent through the reaction of an alkyl bromide with magnesium metal.



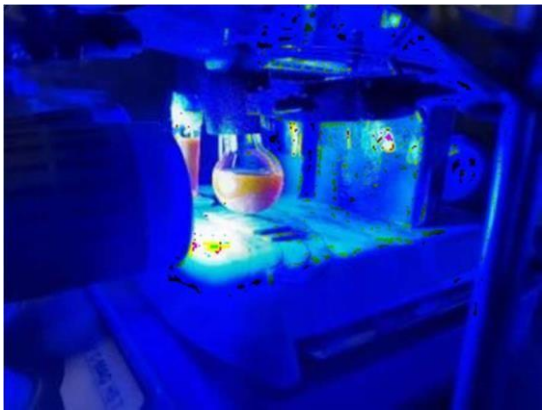
The Grignard reaction is an organic reaction used to produce a variety of products through the reaction of an organomagnesium compound, also known as anelectrophilic "Grignard reagent," followed by an acidic reaction. The Grignard reagent is formed by the reaction of an alkyl or aryl halide with magnesium metal via a radical mechanism.

3. **Wittig Reaction:**

Wittig reaction is used to introduce a methylene group using methylenetriphenylphosphorane ($Ph_3P=CH_2$). Using this reagent, even a sterically hindered ketone such as camphor can be converted to its methylene derivative.

4. Photochemical Reaction:

In recent years, photo redox catalysis has come to the forefront in organic chemistry as a powerful strategy for the activation of small molecules. In a general sense, these approaches rely on the ability of metal complexes and organic dyes to convert visible light into chemical energy for generating reactive intermediates.



In this module we would like to explore:

- The basic principles of photochemistry.
- Understanding why photochemistry is an emerging field of research.
- Relating photocatalysis to sustainability and green chemistry.
- Introducing various metal and organic dye catalysts that can harness lightenergy.
- Designing photochemical strategies for organic synthesis.
- Reviewing scientific papers for hands-on understanding.

Course schedule:

Unit	Topic	Name of Student	No. of Hours
1	Chemdraw	Daksh and Ritu	2
1	Chemdraw	Vishal and Vaishali	2
1	Origin	Anubha and Shubhangi	2
1	Scifinder	Abhijeet and Arindam	2
1	Gaussian	Vikas and Raju	2
1	Gaussian	Vikas and Raju	2
1	Application in MS office	Daksh and Ritu	2
1	Application in MS office	Vishal and Vaishali	2
2	How to plan any General Reaction (Organic and Inorganic)	Abhijeet and Arindam	2
2	How to plan any General Reaction (Organic and Inorganic)	Vikas and Raju	2
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3	Electrochemistry (Theory + Practical Experience)	Anubha and Shubhangi	2
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4	General Text book Name Reaction and their Practical Experiment (Synthesis)	Daksh and Ritu	2
4	General Text book Name Reaction and their Practical Experiment (Synthesis)	Vikas and Raju	2
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