University College Dublin – School of Chemistry

Organic Chemistry for Scientists and Engineers (*OChem 1 + 2*)

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Aims: The principal aim of this summer course is to provide each student with a firm understanding of the key concepts prevalent in organic chemistry and the resulting properties of organic molecules. These will be presented based on standard U.S. text books and will be complemented by specific examples of compounds present in important drug molecules and natural products. As such the course initially introduces key concepts such as molecular structure, chemical bonding and orbital interactions. The resulting properties of molecules are then introduced on key compound classes such as alkanes, alkenes and alkynes that later will be complemented by aromatic rings and functional groups such as alcohols, carbonyls and amines. Furthermore, the crucial properties that explain the reactivity of organic molecules and enable a detailed understanding through distinct reaction mechanisms will be highlighted throughout the course. Finally, these concepts will be applied towards the planned synthesis of target molecules in combination with suitable structure determination methods.

Duration: This summer course will take place over 2 consecutive 4-week periods.

Objectives and Learning Outcomes: By the end of this course each student will have acquired an understanding of the following concepts and principles that determine the importance of organic chemistry in modern society.

- Describe the nature of chemical bonding present in organic molecules.
- Explain the reasons for acidic or basic properties of molecules.
- Analyse the structure of alkanes and cycloalkanes and rationally name these compounds.
- Explain the reactivity of organic molecules based on orbital considerations.
- Describe organic reaction pathways through curved arrow mechanisms.
- Account for the properties of alkenes and alkynes based on their structure.
- Describe and account for substitution and elimination reactions of organohalides.
- Understand and apply key structure determination methods for organic compounds.
- Understand the importance of aromatic compounds based on benzene.
- Understand the effect of key functional groups on the properties of organic molecules.

Reading list:

- McMurry, *Organic Chemistry*, 8th Edition;
- McMurry, *Study Guide and Solutions Manual for McMurry's Organic Chemistry*, 8th Edition;
- Any molecular model kit.

Tentative Lecture Schedule:

Week/Lecture number	Topic	Reading Assignment
W 1, **L** 1-8	Structure, Bonding, Orbitals, Acids and Bases	Chapter 1,2
W 2, **L** 9-16	(Cyclo)Alkanes, Alkenes and Alkynes	Chapters 3-5, 7-9
W 3, **L** 17-24	Organic Reactions and Their Mechanisms	Chapter 6
W 4, **L** 25-32	Organohalides: Substitution and Elimination	Chapters 10,11
	Mid Exam Chapters 1 – 11;	
W 5, **L** 33-40	Structure Determination: NMR, IR, MS, UV	Chapters 12,13,14
W 6, **L** 41-48	Benzene, Aromatic Chemistry; Alcohols and Ethers	Chapters 15-18
W 7, **L** 49-56	Carbonyls: α-substitution and condensation reactions	Chapters 19-23
W 8, **L** 57-64	Functional Groups: Amines, Heterocycles, Drugs	Chapters 24, 26
	Final Exam All Chapters.	

Teaching Methods:

Regarding teaching and learning methods, a combination of lecture-based teaching, continuous assessment, laboratory-based practical experimentation and self-study will be used. Key concepts and tools will be presented in lectures, while regular practical laboratories and tutorial sessions, as well as informal self-study sessions, will enable the students to apply this knowledge to solve problems relevant to chemistry. In detail:

1. Lectures
   There are 8 lectures per week scheduled for 1 hour each.
2. Homework / Problem Solving
   One set of problems will be handed out each week, which must be submitted for marking.
3. Workshops
   There are several 2-hour workshops each week devoted to problem solving.
4. Laboratories
   There are three 3-hour laboratory afternoons each week in which new experiments will be performed. The students will typically work individually.
5. Independent Study
   In addition, each of the 2 modules (weeks 1-4 and 5-8) will require a minimum of 40 hours independent study.

Suggested Laboratory Experiments:

Module 1:

1. **Acids and bases.**

This practical demonstrates the very important technique of titration and how knowing the standardized molarity of one solution can be used to determine an unknown. You will also learn to use indicators.

2. **Separation of mixtures:**

purification, recrystallisation and identification of an organic compound using melting points. Students use differing solubilities of organic and inorganic materials to separate these. They then identify the organic component in a mixture using melting points as a guide

3. **Understanding molecular structures**

Using a molecular kit the students will build 3D models of several organic molecules. This will include the generation of chiral molecules and the relative relationship between chiral centres within the structure.

4. **Separation of a mixture of hydrocarbons by distillation**

Students will be provided by a mixture of different alkanes/alkenes and separate these by distillation. GC-MS will be used to identify the individual fractions and assess their purity.

5. **Preparation of paracetamol**

Students prepare paracetamol from the reaction between 4 aminophenol and acetic anhydride. The techniques include hot filtrations and recrystallizations. They also determine a product yield

6. **Addition Reaction of an Alkene with Bromine:**

Addition of bromine to stilbene, recrystallization, melting point determination, percentage yield calculation.

7. **Preparation of banana oil**

Fischer esterification reaction between acetic acid and isopentyl alcohol in the presence of an acid catalyst. Setting up a reaction to safely heat using a condenser and concept of distillation for the purification of volatile reaction products.

8. **Substitution Reaction of an Alcohol:**

Conversion of tert-butanol into tert-butyl chloride using HCl, extraction, distillation, percentage yield calculation.

9. **Nucleophilic Addition to a Ketone**

Sodium borohydride reduction of benzophenone, thin layer chromatography

10. **Alcohols and Carbohydrates**

Oxidation of primary, secondary and tertiary alcohols using chromic acid, Fehling's test of fructose and glucose, acid hydrolysis of sucrose and change of optical rotation

Module 2:

11. **Structure determination:**

Based on 1H-/13C-NMR, IR, MS data provided the structure of an unknown organic molecule will be determined.

12. **Preparation of an Amide**

Reaction of 3,4,5-trimethoxybenzoyl chloride with morpholine in a Schotten-Baumann reaction. Isolation and purification of the resultant amide by recrystallization.

13. **Preparation Triphenylmethanol via a Grignard Reaction**

Two-step reaction protocol. Synthesis of phenylmagnesium bromide from bromobenzene and magnesium metal. Subsequent conversion of ethyl benzoate to triphenylmethanol by its reaction with 2 equiv. of PhMgBr. Purification and recrystallization are to be performed.

14. **Nitration of acetanilide**

Electrophilic aromatic substitution reaction of acetanilide to form para-nitroacetanilide. Purification and recrystallization.

15. **Methanolysis of 1,2-dichloro- 4-nitrobenzene**

Nucleophilic aromatic substitution reaction of 1,2-dichloro- 4-nitrobenzene using sodium methoxide to generate 2-chloro- 4-nitroanisole. Its purification by extraction and recrystallization.

16. **Heterocyclic chemistry**

A substituted pyrazole will be synthesised based on a Paal-Knorr cyclocondensation reaction.

17. **Preparation of caprolactam**

Two-step formation of caprolactam via conversion of cyclohexanone to cyclohexanone oxime with hydroxylamine. Then the Beckmann rearrangement of this oxime with concentrated sulfuric acid to generate caprolactam the precursor to Nylon 6.

18. **Synthesis of a protected monosaccharide**

This experiment will show the selective protection of methyl α-D-glucopyranoside at the 4 and 6 hydroxyl positions with benzaldehyde dimethyl acetal under acid catalysis. The reaction is followed by TLC and yield and melting point for the product will be determined.

19. **Protection of an amino acid**

The amino group of L-alanine undergoes Boc-protection using Boc-anhydride and basic conditions. Students will work with pH meters in the work up of the reaction and solubility of the product in aqueous or organic layer will be investigated. TLC will be used to verify the purity of the product. Yield will be calculated.

20. **Peptide synthesis**

N-Boc-L-alanine is reacted with glycine ethyl ester in the presence of a carbodiimide coupling reagent to promote peptide synthesis. TLC is used to monitor the reaction. Students are provided with a MS spectrum of the product and are asked to analyze the fragmentation pattern. Yield will be calculated.

Assessment:

The assessment of this course will be aided by means of problem sets/tutorials/workshops, laboratory reports, problem sets as well as a mid-exam and a final exam as outlined below:

Type	Due Date	Weighting
Problem set/tutorials/workshops	weekly	15%
Laboratory (reports)	weekly	25%
Mid-exam	mid-point	10%
Final exam	end-point	50%