Syllabus Summer School in Organic Chemistry for US Students (June – August) – UCD School of Chemistry

Module 1 (week 1-4)

Week 1 – Prof. P. Evans

Content: Revision of fundamental concepts about the structures, reactivity and importance of organic compounds, including covalent and polar covalent bonding, reactivity of organic compounds with a focus on nucleophilicity and electrophilicity, organic acids and bases, and the valence bond model for bonding in carbon compounds containing single bonds. Acyclic alkanes, structure and nomenclature, conformational analysis, nomenclature, physical properties, chemical reactivity, combustion and heat of combustion, free radical halogenation and radical chain mechanisms.

Recommended reading in McMurry (edition 9): chapters 1, 2, 3

Week 2 – Prof. M. Casey

Content: Cycloalkanes from cyclopropanes to large rings, including sources of strain, and conformational analysis of six-membered rings. Amines, including bonding, basicity, base strength, alkylation and overalkylation, and other preparative methods. Common functional groups. Alcohols, including bonding, acidity and basicity, conversion into haloalkanes, oxidation, conversion into ethers, and preparative methods.

Recommended reading in McMurry (edition 9): chapters 4, 6, 11

Week 3 – Prof. D. Gilheany

Content: This week's topics are the interlinked areas of alcohols, alkyl halides, stereochemistry and reaction mechanisms. An overview of the types of organic chemical reactions and their operational description will set the scene for the description of the synthesis and reactivity of alcohols and alkyl halides, their interconversions, which will also cover the concept of competing substitution and elimination reactions. Then there will then be a digression to introduce the topic of stereochemistry, which will include a brief history of molecular chirality, the basics of enantiomers vs. diastereomers, how they are distinguished and why they are important. Finally, we will return to the alkyl halides to study in detail the mechanisms of nucleophilic substitution, in which stereochemical considerations are crucial.

Recommended reading in McMurry (edition 9): chapters 5, 10, 11, 17

Week 4 – Prof. M. Rubini

Content: Compounds containing carbon-carbon multiple bonds (alkenes and alkynes) are very versatile. The material covered in this week is associated with an introduction to the structure and chemistries of these types of compounds. In more detail: the bonding present in alkenes and alkynes will be explained using the valence bond model. Positional and geometrical isomerism will be discussed along with the systematic IUPAC methods for naming these compounds. In terms of reactions, building upon the material covered in Week 3, main methods for the synthesis of alkenes (and alkynes) will be reviewed. Then the main classes of alkene (and alkyne) addition reactions will be looked at in detail. Accompanying this discussion will be the use of curved arrows/reaction mechanisms to provide understanding of the process and to explain aspects of selectivity. Some of the reactions covered will feature in the laboratory section of the course.

Recommended reading in McMurry (edition 9): chapters 7, 8, 9

Labs

There will be 10 lab afternoons (typically 3 h sessions) during this module. The focus is on familiarising the students with key techniques utilised in Organic Chemistry, such as liquid-liquid extraction, distillation, solvent evaporation and (re)crystallisation in case of solid products. The lab experiments will be based on important chemical transformations that the students will encounter in the lectures. The students will additionally be using boiling and melting points to assist in confirming product identity and purity. The last lab in each week will be assessed by the demonstrators allowing the students to familiarise themselves with the relevant technique while gaining confidence in applying this. The students will work individually and write lab reports for each experiment, which will be evaluated by demonstrators in order to provide immediate feedback to the students.

Module 2 (week 5-8)

Week 5 – Prof. M. Baumann: **Structure Determination in Organic Chemistry**

Content: This week's topic is the use of spectroscopic techniques used in organic chemistry to determine the structure of molecules and will focus on mass spectrometry, infrared spectroscopy, UV-Vis spectroscopy and NMR spectroscopy (^{1}H, ^{13}C, DEPT). For each technique the underlying principles as well as multiple examples and problems will be presented and discussed. These techniques will also feature throughout the labs of module 2 where the students will run their own spectroscopic experiments and practice analysis and interpretation of the resulting data.

Recommended reading in McMurry (edition 9): chapters 12, 13, 14

Week 6 – Prof. M. Baumann: **Carbonyl Chemistry (Carbonyl Additions and Condensation Reactions)**

Content: This set of lectures will introduce the important topic of carbonyl chemistry and will further acquaint the students with the creation of relevant reaction mechanisms. First, the reactivity of the carbonyl group will be discussed as well as various relevant nucleophilic addition reactions involving aldehydes and ketones. Subsequently, acyl substitution reactions on different acid derivatives will be highlighted (carboxylic acids, acid chlorides, anhydrides, amides, esters). Next, carbonyl α-substitution reactions including condensation reactions will be discussed (aldol additions and condensations). This section will also showcase various examples of target molecules that can be generated by exploiting carbonyl chemistry.

Recommended reading in McMurry (edition 9): chapters 19, 20, 21, 22, 23

Week 7 – Prof. D. Gilheany

Content: The topic of this week focuses on aromatic compounds with particular emphasis on the structure and reactivity of benzene. First, the structure and anomalous reactivity of benzene will be discussed to highlight the differences in reactivity between compounds containing double bonds and aromatic rings. Criteria for aromaticity will be explained and examples will be discussed. Subsequently, the reaction mechanism for the electrophilic aromatic substitution on the benzene ring (halogenation, nitration, sulfonation, Friedel-Crafts alkylation and acylation) will be presented. Next, the effects of substituents on reactivity and orientation of the substituted benzene ring will be introduced. Finally, the mechanism of the nucleophilic aromatic substitution reaction will be discussed. The variety of reactions at benzylic sites (radical substitutions, nucleophilic substitution, oxidation of toluene, reduction reactions) will be also presented.

Recommended reading in McMurry (edition 9): chapters 15, 16

Week 8 – Prof. E. McGarrigle

In this final set of lectures, we will take a closer look at nitrogen containing molecules such as amines, heterocycles, related naturally occurring biomolecules (nucleic acids, peptides, alkaloids) and simple examples of drugs. A short overview of the prevalence of other naturally occurring structures such as carbohydrates and lipids will be included. This week will discuss and highlight the relevance of all previously encountered concepts (bonding, pKa, structure, reactivity vs. property etc.) and several examples will demonstrate how these are interlinked.

Recommended reading in McMurry (edition 9): chapters 24-28

Labs

The structure of the labs will be analogous to those in the first lab; there will be 10 lab afternoons in this module and for the first 8 the students will work individually on experiments that focus on preparing a target compound, whose synthesis will exploit a number of techniques the students have encountered. Additionally, there will be a mini-project during the last 2 labs where the students work in small teams and design their own set of experiments to test a number of hypotheses they previously established. Each group will write an assessed report that presents the idea, the execution and the conclusions of the experiments undertaken. Throughout this second module, the students will use spectroscopic data to link with their experiments, which in the second half they will be able to acquire themselves (MS, IR, UV, NMR).

Standard Conversion Grade Scale*

40% Pass (70% = A-)

Grades	Lower %	Upper %
A+	≥90	100
A	≥80	<90
A-	≥70	<80
B+	≥66.67	<70
B	≥63.33	<66.67
B-	≥60	<63.33
C+	≥56.67	<60
C	≥53.33	<56.67
C-	≥50	<53.33
D+	≥46.67	<50
D	≥43.33	<46.67
D-	≥40	<43.33
E+	≥36.67	<40
E	≥33.33	<36.67
E-	≥30	<33.33
F+	≥26.67	<30
F	≥23.33	<26.67
F-	≥20	<23.33
G+	≥16.67	<20
G	≥13.33	<16.67
G-	≥0.01	<13.33
NM	0	<0.01
ABS	No work was submitted by the student or the student was absent from assessment	