

KOT 222 – Organic Chemistry II

- Course Objectives:**
- 1) To introduce the chemistry of alcohols and ethers.
 - 2) To study the chemistry of functional groups.
 - 3) To learn the chemistry of aromatic compounds and their reactions.
 - 4) To become familiar with the spectroscopic methods of structure determinations.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
1. Structure and Synthesis of Alcohols	<ul style="list-style-type: none">• Structure, classification, nomenclature and physical properties of alcohols• Nomenclature of phenols• Acidity of alcohols and phenols• Synthesis of alcohols• Thiols	3	<ul style="list-style-type: none">• Draw and name alcohols, phenols, diols and thiols.• Predict the relative boiling points, acidities and solubilities of alcohols.• Show how to convert alkenes, alkyl halides and carbonyl compounds to alcohols.• Predict the alcohol products of hydration, hydroboration and hydroxylation of alkenes.• Use Grignard and organolithium reagents effectively for the synthesis of primary, secondary and tertiary alcohols with the required carbon skeletons.• Propose synthesis and oxidation products of simple thiols.
2. Reactions of Alcohols	<ul style="list-style-type: none">• Oxidation of alcohols• Alcohols as nucleophiles and electrophiles• Reduction, dehydration and esterification of alcohols• Reactions of alcohols with hydrohalic acids, phosphorus halides and thionyl chloride• Reactions of alkoxides	3	<ul style="list-style-type: none">• Identify whether oxidation or reduction is needed to interconvert alkanes, alcohols, aldehydes, ketones and acids, and identify reagents that will accomplish the conversion.• Predict the products of the reactions of alcohols with (a) oxidizing and reducing reagents, (b) carboxylic acids and acid chlorides, (c) dehydrating agents (H_2SO_4 and H_3PO_4), (d) inorganic acids and (e) sodium, potassium, and sodium hydride.• Predict the products of the reactions of alkoxide ions.• Use knowledge of alcohol and diol reactions to propose mechanisms and products of similar reactions the student has never seen before.• Show how to convert an alcohol to a related compound with a different functional group.• Predict the products of pinacol rearrangement and periodate cleavage of glycols.• Use retrosynthetic synthesis to propose effective single-step and multistep syntheses of compounds using alcohols as intermediates.

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3. Infrared Spectroscopy and Mass Spectrometry	<ul style="list-style-type: none"> • The electromagnetic spectrum • IR-active and IR-inactive vibrations • IR of hydrocarbons characteristic absorptions of alcohols, amines, carbonyl compounds, C-N bonds • Interpreting IR spectra • Mass spectrometry • Determination of molecular formula by MS • Fragmentation patterns in MS 	3	<ul style="list-style-type: none"> • Identify the reliable characteristic peaks of a given IR spectrum. • Explain why some characteristic peaks are usually strong or weak and why some may be absent. • Predict the stretching frequencies of common functional groups. • Identify functional groups from IR spectra. • Identify conjugated and strained C=O bonds along with conjugated and aromatic C=C bonds from their absorptions and IR spectra. • Determine molecular weights from mass spectra. • Use mass spectra to recognize the presence of Br, Cl, I, N and S atoms, if possible. • Predict the major ions from fragmentation of alkanes, alkenes and alcohols. • Use fragmentation pattern to determine whether a proposed structure is consistent with the mass spectrum.
4. Nuclear Magnetic Resonance Spectroscopy	<ul style="list-style-type: none"> • Theory of NMR • The chemical shift, number and intensity of signals. Spin-spin splitting • Interpretation of proton NMR spectra • Carbon-13 NMR spectra and their interpretation 	6	<ul style="list-style-type: none"> • Determine which protons are equivalent and which are nonequivalent; predict the number of signals and their approximate chemical shifts of a given structure. • Suggest types of protons based on signals and chemical shifts. • Use the integral trace to determine the relative numbers of different types of protons. • Predict which protons in a structure will be magnetically coupled and predict the number of peaks and approximate coupling constants of their multiplets. • Use proton spin-spin splitting patterns to determine the structure of alkyl and other groups. • Draw the NMR spectrum of a given compound. • Predict the approximate chemical shifts of carbon atoms in a given compound. Suggest types of carbons based on the chemical shifts of ¹³C absorptions.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
			<ul style="list-style-type: none"> • Use the off-resonance decoupled or DEPT ¹³C spectrum to determine the number of hydrogens bonded to a given carbon. • Combine the chemical shifts, integrals and spin-spin splitting patterns in the NMR spectrum with information from infrared and mass spectrum to determine the structures of organic compounds.
5. Ethers, Epoxides and Sulphides	<ul style="list-style-type: none"> • Physical properties, nomenclature and synthesis of ethers • Cleavage of ethers by HBr and HI • Reactions of ethers • Sulphides • Synthesis of epoxides acid- and base- catalyzed ring opening of epoxides reactions of epoxides with Grignard and organolithium reagents 	2.5	<ul style="list-style-type: none"> • Draw and name ethers and heterocyclic ethers, including epoxides. • Predict relative boiling points and solubilities of ethers. • Explain how ether solvents stabilize electrophilic reagents and why they are compatible with organometallic reagents. • Determine the structures of ethers from their spectra and explain their characteristic absorptions and fragmentations. • Devise efficient laboratory syntheses of ethers and epoxides, including <ul style="list-style-type: none"> ○ the Williamson ether synthesis ○ alkoxymercuration-demercuration ○ peroxyacid epoxidation ○ base-promoted cyclization of halohydrins ○ predict the products of reactions of ethers and epoxides, including cleavage and autoxidation of ethers ○ acid- and base-promoted opening of epoxides ○ reactions of epoxides with organometallic reagents • Use the knowledge of the mechanisms of ether and epoxide reaction to propose mechanisms and products for similar reactions the student has never learnt before.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
6. Conjugated Systems, Orbital Symmetry and Ultraviolet Spectroscopy	<ul style="list-style-type: none"> • Stability of dienes. • Molecular orbital picture of a conjugated system and an allylic system • Allylic cations and radicals • 1,2- and 1,4- addition to conjugated dienes • Kinetic versus thermodynamic control in HBr addition to 1,3-butadiene • SN₂ reactions of allylic halides and tosylates • The Diels-Alder reaction 	2.5	<ul style="list-style-type: none"> • Show how to construct the molecular orbitals of ethylene, butadiene, and the allylic system. Show the electronic configurations of ethylene, butadiene, and the allyl cation, radical and anion. • Recognize reactions that are enhanced by resonance stabilization of the intermediates, such as free-radical reactions and cationic reactions. Develop mechanisms to explain the enhanced rates and observed products and draw resonance forms of the stabilized intermediates. • Predict the products of Diels-Alder reactions, including the orientation of cycloaddition with unsymmetrical reagents and the stereochemistry of the products. • Predict which cycloadditions will be thermally allowed and which will be photochemically allowed by comparing the molecular orbitals of the reactants. • Use values of λ_{max} from UV-visible spectra to estimate the length of conjugated system and compare compounds with similar structure.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
7. Aromatic Compounds	<ul style="list-style-type: none"> • Structure, properties and molecular orbitals of benzene • Aromatic, antiaromatic and nonaromatic compounds • Huckel's rule. Aromatic heterocyclic and polyaromatic compounds 	2	<ul style="list-style-type: none"> • Construct the molecular orbitals of a cyclic system of p orbitals similar to benzene and cyclobutadiene. • Use the polygon rule to draw the energy diagram for a cyclic system of p orbitals and fill in the electrons to show whether a given compound or ion is aromatic or antiaromatic. • Use Hückel's rule to predict whether a given annulene, heterocycle or ion will be aromatic, antiaromatic or nonaromatic. • Determine whether the lone pairs are used in the aromatic system and predict whether the nitrogen atom is strongly or weakly basic for heterocycles containing nitrogen atoms • Recognize fused aromatic systems such as polynuclear aromatic hydrocarbons and fused heterocyclic compounds and use the theory of aromatic compounds to explain their properties. • Name aromatic compounds and draw their structures from the names. • Use IR, NMR, UV and mass spectra to determine the structures of aromatic compounds. Predict the important features of the spectra of an aromatic compound.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
8. Reactions of Aromatic Compounds	<ul style="list-style-type: none"> • Electrophilic aromatic substitution • Halogenation, nitration and sulphonation of benzene • Activating and deactivating groups and their effects on the orientation of electrophilic aromatic substitution • Effect of multiple substitution • Friedel-Crafts alkylation and acylation • Nucleophilic aromatic substitution • Side-chain reactions of benzene derivatives 	5	<ul style="list-style-type: none"> • Predict products and propose mechanisms for the common electrophilic aromatic substitutions: halogenation, nitration, sulfonation and Friedel-Crafts alkylation and acylation. • Draw resonance structures for the sigma complexes resulting from electrophilic attack on substituted aromatic rings. Explain which substituents are activating and which are deactivating and show why they are ortho, para-directing, or meta-allowing. • Predict the position(s) of electrophilic aromatic substitution on molecules containing substituents on one or more aromatic rings. • Design syntheses that use the influence of substituents to generate the correct isomers of multisubstituted aromatic compounds. • Determine which nucleophilic aromatic substitutions are likely and propose mechanisms for both the addition-elimination type and the benzyne type. • Predict the products of Birch reduction, hydrogenation and chlorination of aromatic compounds and use these reactions in syntheses. • Explain how the reactions of side chains are affected by the presence of the aromatic ring, predict the products of side-chain reactions, and use these reactions in syntheses. • Predict the products of oxidation and substitution of phenols and use these reactions in syntheses.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
9. Ketones and Aldehydes	<ul style="list-style-type: none"> • Nomenclature and physical properties of ketones and aldehydes • Their synthesis including using 1,3-dithianes, from carboxylic acids, nitriles and acid chlorides • Nucleophilic addition reactions: the Wittig reaction, hydration, formation of cyanohydrins and imines • Condensation with hydroxylamines and hydrazines • Formation of acetals. Use of acetals as protecting groups. Oxidation of aldehydes. Reduction of aldehydes and ketones 	5	<ul style="list-style-type: none"> • Name ketones and aldehydes and draw the structures from their names. • Interpret the IR, NMR, UV and mass spectra of ketones and aldehydes and use spectral information to determine the structures. • Write equations for syntheses of ketones and aldehydes from alcohols, alkenes, alkynes, carboxylic acids, nitriles, acid chlorides, dithianes and aromatic compounds. • Propose effective single-step and multistep syntheses of ketones and aldehydes. • Predict the products of reactions of ketones and aldehydes with the following types of compounds (give mechanisms where appropriate): <ul style="list-style-type: none"> ○ hydride reducing agents; Clemmensen and Wolff-Kishner reagents ○ Grignard and organolithium reagents ○ phosphorus ylides ○ water ○ hydrogen cyanide ○ ammonia and primary amines ○ hydroxylamine and hydrazine derivatives ○ alcohols ○ oxidizing agents • Use the knowledge of the mechanisms of ketone and aldehyde reactions to propose mechanisms and products of similar reactions the student has never seen before. • Show how to convert ketones and aldehydes to other functional groups. • Use retrosynthetic analysis to propose effective multistep syntheses using ketones and aldehydes as intermediates and protecting the carbonyl group if necessary.

Topic	Content	Number of lecture hours	Expected outcome – upon completion of this course, the student should be able to:
10. Amines	<ul style="list-style-type: none"> • Nomenclature, structure, physical properties and basicity of amines. Amine salts as phase-transfer catalysts. Reactions of amines with ketones and aldehydes. Aromatic substitution of arylamines and pyridine. Alkylation and acylation of amines. Hofmann and Cope eliminations. Reactions of arenediazonium salts. Syntheses of amines. 	4	<ul style="list-style-type: none"> • Name amines and draw the structures from their names. • Interpret the IR, NMR and mass spectra of amines and use the spectral information to determine the structures. • Explain how the basicity of amines varies with hybridization and aromaticity. • Show the contrast of physical properties between amines and their salts. • Predict the products of reactions of amines with the following types of compounds (propose the mechanisms where appropriate) : <ul style="list-style-type: none"> ○ ketones and aldehydes ○ alkyl halides and tosylates ○ acid chlorides ○ sulfonyl chlorides ○ nitrous acid ○ oxidizing agents ○ arylamines with electrophiles • Give examples of the use of arenediazonium salts in diazo coupling reactions and in the synthesis of aryl chlorides, bromides, iodides, fluorides and nitriles. • Illustrate the uses and mechanisms of the Hofmann and Cope eliminations, and predict the major products. • Use your knowledge of the mechanisms of amine reactions to propose mechanisms and products of similar reactions the student has never seen before. • Show how to synthesize amines from other amines, ketones and aldehydes, acid chlorides, nitro compounds, alkyl halides, nitriles and amides. • Use retrosynthetic analysis to propose effective single-step and multistep syntheses of compounds with amines as intermediates or products, protecting the amine as an amide, if necessary.
TOTAL		36	