GUJARAT TECHNOLOGICAL UNIVERSITY

Pharm.D.

1st year

Subject Name: Pharmaceutical Organic Chemistry
Subject Code: 818804

Scope: This subject deals with general methods of preparation and reaction of organic compounds. Reactivity of organic compounds is also included here. The course emphasizes on mechanism and orientation of reactions.

Objectives:

This course is designed to impart a very good knowledge about

a. IUPAC/Common system of nomenclature of simple organic compounds belonging to different classes of organic compounds;

b. Some important physical properties of organic compounds;

c. Free radical/ nucleophyllic [alkyl/ acyl/ aryl] /electrophyllic substitution, free radical/ nucleophyllic / electrophyllic addition, elimination, oxidation and reduction reactions with mechanism, orientation of the reaction, order of reactivity, stability of compounds;

d. Some named organic reactions with mechanisms; and e. Methods of preparation, test for purity, principle involved in the assay, important medicinal uses of some important organic compounds.

TeachingScheme (Hours)				**EvaluationScheme(Marks)**				**Totalmarks**
Theory	**Tutorial**	**Practical**	**Total**	**Theory**		**Practical**		
				External	**Internal**	**External**	**Internal**	
3	1	3	7	70	30	70	30	200

Sr. No.	**CourseContents**	**Hours**	**Module Weightage**
1	Structures and Physical properties: a. Polarity of bonds, polarity of molecules, M.P, Inter molecular forces, B.P, Solubility, non ionic solutes and ionic solutes, protic and aprotic Solvents, ion pairs, b. Acids and bases, Lowry bronsted and Lewis theories c. Isomerism	**9**	**10%**
2	Nomenclature of organic compound belonging to the following classes Alkanes, Alkenes, Dienes, Alkynes, Alcohols, Aldehydes, Ketones, Amides, Amines, Phenols, Alkyl Halides, Carboxylic Acid, Esters, Acid Chlorides And Cycloalkanes.	**8**	**9%**
3	Free radicals chain reactions of alkane : Mechanism, relative reactivity and stability	**6**	**6.5%**
4	Alicyclic compounds : Preparations of cyclo alkanes, Bayer strain theory and orbital picture of angle strain.	**3**	**3.5%**

5	Nuclophilic aliphatic substitution mechanism: Nucleophiles and leaving groups, kinetics of second and first order reaction, mechanism and kinetics of SN2 reactions. Stereochemistry and steric hindrance, role of solvents, phase transfer catalysis, mechanism and kinetics of SN1 reactions, stereochemistry, carbocation and their stability, rearrangement of carbocation, role of solvents in SN1 reaction, Ion dipole bonds, SN2 versus SN1 solvolyses, nucleophilic assistance by the solvents.	**7**	**8%**
6	Dehydro halogenation of alkyl halides: 1,2 elimination, kinetics, E2 and E1 mechanism, elimination via carbocation, evidence for E2 mechanism, absence of rearrangement isotope effect, absence hydrogen exchange, the element effect, orientation and reactivity, E2 versus E1, elimination versus substitution, dehydration of alcohol, ease of dehydration, acid catalysis, reversibility, orientation.	**5**	**5.5%**
7	Electrophillic and free radicals addition: Reactions at carbon-carbon, double bond, electrophile, hydrogenation, heat of hydrogenation and stability of alkenes, markownikoff rule, addition of hydrogen halides, addition of hydrogen bromides, peroxide effect, electrophillic addition, mechanism, rearrangement, absence of hydrogen exchange, orientation and reactivity, addition of halogen, mechanism, halohydin formation, mechanism of free radicals additon, mechanism of peroxide initiated addition of hydrogen bromide, orientation of free addition, additions of carbene to alkene, cyclo addition reactions.	**6**	**6.5%**
8	Carbon-carbon double bond as substituents: Free radical halogenations of alkenes, comparision of free radical substitution with free radical addition, free radical substitution in alkenes, orientation and reactivity, allylic rearrangements.	**4**	**4.5%**
9	Theory of resonance: Allyl radical as a resonance hybrid, stability, orbital picture, resonance stabilisation of allyl radicals, hyper conjugation, allyl cation as a resonance hybrid, nucleophyllic substitution in allylic substrate, SN1 reactivity, allylic rearrangement, resonance stabilisation of allyl cation, hyper conjugation, nucleophilic substitution in allylic substrate, SN2 nucleophilic substituion in vinylic substrate, vinylic cation, stability of conjugated dienes, resonance in alkenes, hyper conjugation, ease of formation of conjugated dienes, orientation of elimination, electrophilic addition to conjugated dienes, 1,4- addition, 1,2-versus 1,4-addition, rate versus equilibrium, orientation and reactivity of free radical addition to conjugated dienes.	**6**	**6.5%**
10	Elecrophilic aromatic substitution: Effect of substituent groups, determination of orientation, determination of relative reactivity, classification of substituent group, mechanism of nitration, sulphonation, halogenation, friedel craft alkylation, friedel craft acylation, reactivity and orientation, activating and deactivating O,P,M directing groups, electron release via resonance, effect of halogen on electrophilic aromatic substitution in alkyl benzene, side chain halogination of alkyl benzene, resonance stabilization of benzyl radical.	**6**	**6.5%**

11	Nucleophilic addition reaction: Mechanism, ionisation of carboxylic acids, acidity constants, acidity of acids, structure of carboxylate ions, effect of substituent on acidity, nucleophilic acyl substitution reaction, conversion of acid to acid chloride, esters, amide and anhydride. Role of caboxyl group, comparison of alkyl nucleophilic substitution with acyl nucleophilic substitution.	**5**	**5.5%**
12	Mechanism of aldol condensation, claisen condensation, cannizzaro reaction, crossed aldol condensation, crossed cannizzaro reaction, benzoin condensation, perkin condensation. Knoevenagel, Reformatsky reaction, Wittig reaction, Michael addition.	**5**	**5.5%**
13	Hoffman rearrangement: Migration to electron deficient nitrogen, Sandmeyer's reaction, basicity of amines, diazotisation and coupling, acidity of phenols, Williamson synthesis, Fries rearrangement, Kolbe reaction, Reimer tieman's reactions.	**5**	**5.5%**
14	Nucleophilic aromatic substitution: Bimolecular displacement mechanisms, orientation, comparison of aliphatic nucleophilic substitution with that of aromatic.	**4**	**4.5%**
15	Oxidation reduction reaction.	**5**	**5.5%**
16	Study of the following official compounds- preparation, test for purity, assay and medicinal uses of Chlorbutol, Dimercaprol, Glyceryl trinitrate, Urea, Ethylene diamine dihyrate, Vanillin, Paraldehyde, Ethylene chloride, Lactic acid, Tartaric acid, citric acid, salicylic acid, aspirin, methyl salicylate, ethyl benzoate, benzyl benzoate, dimethyl pthalate, sodium lauryl sulphate, saccharin sodium, mephensin.	**6**	**6.5%**

CourseMaterials: (Latest edition)

Text books

a. T.R.Morrison and R. Boyd-Organicchemistry,

b. BentleyandDriver-Text book of Pharmaceutical chemistry

c. I.L.Finer- Organicchemistry, the fundamentalsof chemistry

Referencebooks

a. Organicchemistry– J.M.Cram and D.J.Cram

b. Organicchemistry-Brown

c. Advancedorganicchemistry- JerryMarch, Wiley

d. Organicchemistry-Cram and Hammered, PineHendrickson

Pharm.D.1st yearPHARMACEUTICALORGANICCHEMISTRY

Practical (3 Hours / Week; 6 Credits, 90 Hours)

Sr. No.	Experiments
1	**Introduction to the various laboratory techniques through demonstration involving synthesis of the following compounds (at least 8 compounds to be synthesised):** 1. Acetanilde / aspirin (Acetylation) 2. Benzanilide / Phenyl benzoate (Benzoylation) 3. P-bromo acetanilide / 2,4,6 – tribromo aniline (Bromination) 4. Dibenzylidene acetone (Condensation) 5. 1-Phenylazo-2-napthol (Diazotisation and coupling) 6. Benzoic acid / salicylic acid (Hydrolysis of ester) 7. M-dinitro benzene (Nitration) 8. 9, 10 – Antharaquinone (Oxidation of anthracene) / preparation of benzoic acid from toluene or benzaldehyde 9. M-phenylene diamine (Reduction of M-dinitrobenzene) / Aniline from nitrobenzene 10. Benzophenone oxime 11. Nitration of salicylic acid 12. Preparation of picric acid 13. Preparation of O-chlorobenzoic acid from O-chlorotolune 14. Preparation of cyclohexanone from cyclohexanol
2	**Identification of organic compounds belonging to the following classes by :** Systematic qualitative organic analysis including preparation of derivatives Phenols, amides, carbohydrates, amines, carboxylic acids, aldehyde and ketones, Alcohols, esters, hydrocarbons, anilides, nitrocompounds.
3	**Introduction to the use of stereo models:** Methane, Ethane, Ethylene, Acetylene, Cis alkene, Trans alkene, inversion of configuration.

Course material:

Text book and Reference book: (Latest edition)

1. Practical Organic Chemistry by Mann and Saunders.
2. Vogel's text book of Practical organic Chemistry
3. Advanced Practical Organic Chemistry by N. K. Vishnoi
4. Introduction to Organic Laboratory techniques by Pavia, Lampman and Kriz

Scheme of PracticalExamination

	Internal/Sessional	External
Synopsis	05	15
MajorExperiment	10	25
MinorExperiment	03	15
Viva	02	15
Max.marks	**20**	**70**
Duration	**3 hours**	**4 hours**

Note: Total sessional marksis30(20forpracticalsessionalplus10marksforregularity,promptness,viva-voce and record maintenance)