SOLAPUR UNIVERSITY, SOLAPUR

SCHOOL OF CHEMICAL SCIENCES

M. Sc. II, Sem.-III & IV ORGANIC CHEMISTRY SYLLABUS (Choice Based Credit System-CBCS)

(w.e.f. June, 2016)

SOLAPUR UNIVERSITY, SOLAPUR M. Sc. II, ORGANIC CHEMISTRY COURSE SYLLABUS CHOICE BASED CREDIT SYSTEM (CBCS) (w.e.f. June 2016)

A two-year duration **M. Sc. Organic Chemistry** course syllabus has been prepared as per the CBCS semester system. M. Sc. II, SEM-III & SEM-IV Organic Chemistry syllabus will be implemented from June 2016. The syllabus has been prepared taking into consideration the syllabi of other Universities, SET, NET, UGC guidelines, and the specific inputs of the Expert Committee Members from Pune University, Pune, Shivaji University Kolhapur and Dr. BAMU, Aurangabad.

General Structure of the Course:

The course will be of four semesters spread over two academic years. Each semester will have four theory papers of 70 marks for university external examination and 30 marks for internal examination of each semester and two practical's of 70 marks, 30 marks for internal practical of each semester. The distribution of marks is mentioned below

Theory Paper (Semester exam), 16 X 70+30 marks
Practicals (semester end exam.), 8 X 70+30 marks
Tutorials for each semester, 4 X 25

Total: 2500 marks

Ratio of marks (Theory: Practical): (73:27)

Semester	Paper Code	Title of the Paper	Semester exam		L	Т	P	Credit s	
I		Hard core	Theory	IA	Total				
	HCT-101	Inorganic Chemistry -I	70	30	100	4		-	4
	HCT-102	Organic Chemistry -I	70	30	100	4		-	4
	HCT-103	Physical Chemistry -I	70	30	100	4		-	4
		Soft Core (Any one)							
	SCT-104A	Analytical Chemistry -I	70	30	100	4		0	4
	SCT-104B	Chemistry in Life Sciences	70	30	100	4		0	4
		Practicals							
	HCP-I	Inorganic Chemistry	35	15	50	-	-	2	
	HCP-I	Organic Chemistry	35	15	50	-	-	2	6
	HCP-II	Physical Chemistry	35	15	50	-	-	2	
		Soft core (Any one)							
	SCP-IIA	Analytical Chemistry	35	15	50	-	-	2	2
	SCP-IIB	Analytical Chemistry	35	15	50	-	-	2	2
	T-1	Tutorial					25		1
		Total for 1st semester	420	180	600		25		25

II		Hard core							
	HCT-201	Inorganic Chemistry -II	70	30	100	4		-	4
	HCT-202	Organic Chemistry -II	70	30	100	4		-	4
		Soft core (Any one)							
	SCT-203A	Physical Chemistry -II	70	30	100	4		-	4
	SCT-203B	Green Chemistry	70	30	100	4		-	
		Open elective (Any one)							
	OET-204A	Instrumental Methods of	70	30	100	4		-	4
		Analysis							
	OET-204B	Medicinal Chemistry -I	70	30	100	4		-	
		Practicals							
	HCP III	Inorganic Chemistry	35	15	50	-	-	2	4
	HCP III	Organic Chemistry	35	15	50	-	-	2	4
		Soft core (Any one)							
	SCP IVA	Physical Chemistry	35	15	50	-	-	2	
	SCP IVB	Physical Chemistry	35	15	50	-	-	2	2
		Open elective (Any one)							
	OEP IVC	Analytical Chemistry	35	15	50	-	-	2	2
	OEP IVD	Medicinal Chemistry	35	15	50	-	-	2	2
	T-2	Tutorial					25		1
_		Total for 2 nd semester	420	180	600		25		25

III		Hard core							
	HCT-301	Advanced Organic Chemistry-I	70	30	100	4		_	4
	HCT-302	Advanced Spectroscopic Methods	70	30	100	4		-	4
		Soft core (Any one)							
	SCT-303A	Photochemistry and Pericyclic Reactions	70	30	100	4		-	4
	SCT- 303B	Medicinal Chemistry-II	70	30	100	4		-	
		Open elective (Any one)							
	OET- 304A	Drugs and Heterocycles	70	30	100	4		-	
	OET- 304B	Unit operations of chemical Engineering	70	30	100	4		-	4
		Practicals							
	HCP -V	Organic Mixture (Ternary)	70	30	100	-	-	4	4
	SCP -VIA	Preparation (2 Stages)	35	15	50	-	-	2	2
		Open elective (Any one)							
	SCP -VIB	Spectral Problems	35	15	50	-	-	2	2
	OEP- VIC	Colum chromatography	35	15	50	_	_	2	
	T-3	Tutorial					25		1
		Total for 3 rd semester	420	180	600		25		25

IV		Hard core							
	HCT-401	Advanced Organic Chemistry-II	70	30	100	4		-	4
	HCT-402	Stereo Chemistry	70	30	100	4		-	4
	HCT-403	Chemistry of Natural Products	70	30	100	4		-	4
		Soft Core (Any one)						-	4
	SCT-404A	Applied Organic Chemistry	70	30	100	4		-	
	SCT-404B	Chemical Industries	70	30	100	4		-	
		Practicals							
	HCP -VII	Preparations (3 Stages)	70	30	100	-	-	4	4
	HCMP-VIII	Major Project/In plant training & Spectral Problems	70	30	100	-	-	4	4
	T-4	Tutorial					25		1
		Total for 4 th semester	420	180	600		25		25
		Total			2500				100

L = Lecture **T** = Tutorials **P** = Practical

4 Credits of Theory = 4 Hours of teaching per week

2 Credit of Practical = 4 hours per week

HCT = **Hard** core theory,

SCT = **Soft** core theory,

HCP = **Hard** core practical

SCP = **Soft** core practical,

OET = **Open** elective theory,

OEP = Open elective practical,

HCMP = **Hard** core main project

Nature of Examination:

Each semester will have theory external examination of four papers of 70 marks each (2.5 hrs. duration). The practical examination of Semesters I to IV will be conducted at the end of the each Semester. Duly certified copy of laboratory record must be produced at the time of examination.

Practical Examination of M. Sc. II

The practical examination will be of 3 days for each semester.

Practical experiments: 60
Oral 05
Journal: 05

Project work / In-plant training Report:

60**+10 marks for presentation

** The valuation of project/ In plant training report to be done by both external and internal examiners at the time of examination. Valuation of Tutorials is to be done in each semester by the teaching faculty involved in organic chemistry course.

Nature of question paper (M. Sc. II):

Time: 2.5 hours Maxi Marks 70

Instructions

- 1. Attempt 05 questions.
- 2. Section I (question 1) is compulsory
- 3. Attempt any two questions from section II and any two questions from section III.
- 4. Answers to all 05 questions (from section I, II, III) should be written in the one and the same answer book.
- 5. All questions carry equal marks.
- 6. Figures to the right indicate full marks.
- 7. Use of log tables and calculators is allowed.

Question Paper Section I

Q 1. Answer the following (14 sub-questions)

Marks 14 (1 x 14)

Multiple choice / fill in the blanks / define the term / True-False, predict the product, provide the reagent and conditions etc.

Sub-questions (i) to (xiv)

S	Sub-questions (i) to (xiv)	
	Section II	
Q 2.	a)	Marks 07
	b)	Marks 07
Q 3.	a)	Marks 07
	b)	Marks 07
Q 4.	a)	Marks 07
	b)	Marks 07
	Section III	
Q 5.	a)	Marks 05
	b)	Marks 05
	c)	Marks 04
Q 6.	a)	Marks 05
	b)	Marks 05
	c)	Marks 04
Q 7. V	Write short notes on (any three)	Marks 14
	a)	
	b)	
	c)	
	d)	

N.B. In sections II and III, the sub-questions (a, b, and c) in a given question should be from different topics of the syllabus.

At least 25 % questions should be problem oriented, where-ever possible, in view to train students for the SET/NET/GATE and other competitive examinations. These questions should test the understanding of candidate rather than the memory. The question paper should cover all the Units included in the syllabus of the respective paper and the weightage of the questions should correspond to the number of lectures allotted to the respective Units / Topics.

M. Sc. II SEMESTER-III (Organic Chemistry) PAPER NO. HCT-301 ADVANCED ORGANIC CHEMISTRY-I

Credit: 04 Hours: 60

UNIT-I (a) Methods of determining reaction mechanism:

(15)

Kinetic & non-kinetic methods: Hammett equation, & its modification. Taft equation.

(b) Free radical reactions:

Types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at aromatic substrates, neighboring group assistance. Reactivity for aliphatic and aromatic substitution at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic hydrogenation (NBS), Oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction. Free radical rearrangement, Hunsdiecker reaction.

UNIT-II Rearrangements

(15)

Pummerer, Payne, Eschenmoser fragmentation, Brook, Wagner-Meerwein, Wolf, Semipinacol, Epoxide rearrangement with lewis acid, Tiffeneau-Demjanov, von Richter, Wittig, Neber, Smiles, Fries, Curtius, Lossen, Schmidt, Steven, Hofmann, Iodolactonisation.

UNIT-III Name Reactions

15hrs

Darzen, Prins, Henry, Strecker amino acid synthesis. Bamford-Steven, Baylis-Hillmann, Corey-Fuchs Reaction, Julia Olefination, Mukaiyama aldol, Mitsunobu, Corey-Winter olefination, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubb's metathesis), Aldol-Tishchenko reaction (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli.

UNIT-IV Application of following reagents & reaction in synthesis. 15hrs Complex metal hydrides, lithium dialkyl cuprate, Trimethyl silyl iodide, tributyl tin hydride, peracids, lead tetraacetate, PPA, Diazomethane, ozone, Hoffmann-Loffler-Fretag reactions, Selenium dioxide, periodic acid, Iodoisobenzyl diacetate.

References

- 1. A guide book to Mechanism in Organic Chemistry (Orient- Longmens)- Peter Sykes
- 2. Organic Reaction Mechanism (Benjamin)-R. Bresslow
- 3. Mechanism and Structure in Organic Chemistry(Holt Reinhartwinston)- B. S. Gould

- 4. Organic Chemistry (McGraw Hill)-Hendrikson, Cram and Hammond
- 5. Basic principles of Organic Chemistry (Benjamin) J. D. Roberts and M. C. Caserio.
- 6. Reactive intermediates in Organic Chemistry 9 Jojn Wiley) N. S. Issacs.
- 7. Organic reaction mechanism (Mc Graw Hill) R. K. Bansal
- 8. Advanced organic chemistry, part B:Reaction and synthesis by Francis A. Carey, Richard Y. Sandburg.
- 9. Organic Chemistry by Clayden, Greeves, Warren and Wothers.

PAPER NO. HCT -302 ADVANCED SPECTROSCOPIC METHODS

Credit: 04 Hours: 60 UNIT-I IR Spectroscopy 15 hrs

Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols, ethers, phenols, amines, ketones, aldehydes, esters, amides, acids, anhydrides, conjugated carbonyl compounds etc. Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; combination and Fermi resonance bands. FTIR, of gases; solids and polymeric materials.

UNIT-II ¹H NMR 15 hrs

Recapitulation of basic principle, Fourier Transform technique, Use of Integration in the quantative determination of isomers, Chemical Shift Factors affecting on chemical shifts (inductive, resonance and anisotropic effect and solvent effect with examples), chemical shift of different types of protons (alkane, alkene, alkyne and allene, aromatic protons)

Spin-Spin coupling: Coupling constant and its mechanism, factors affecting coupling constants (dihedral angle, Karplus equation-graph, electronegativity, bond order, hybridization, bond angle with examples), Chemical equivalence and non equivalence, rate processes. Ramsay mechanism of spin coupling, roofing effect with example, different spin systems with examples (AB, AM, AX, ABX/AMX etc.), calculations of line intensities and chemical shifts in AB spin system, Effect of high field NMR for simplification of spectra, , Shift reagents. Spin decoupling and Nuclear Overhauser effect (NOE) with examples. Resonance of other nuclei- ¹⁹F & ³⁴P.

UNIT-III (a) ¹³C NMR 15 hrs

Elementary ideas, instrumental difficulties, FT technique advantages and disadvantages. Proton Noise Decoupling technique advantages and disadvantages, off-resonance technique, factors affecting chemical shifts, analogy with ¹H NMR, calculations of chemical shift of hydrocarbons, different types of carbons (alkene, alkyne, allene, carbonyl, nitrile, oxime and aromatic carbons and effect of substituent on chemical shifts of carbons. Chemical shifts of solvents

b) Two dimensional (2D)

NMR techniques, principle and pulse technique, DEPT, H- H COSY, H- C COSY (HETCOR, HMQC, HMBC, HSQC), interpretation of 2D spectra and examples.

UNIT-IV Mass spectrometry

15 hrs

Theory, instrumentation various methods of ionization (field ionization, FAB, MALDI, californium plasma), different detectors [magnetic analyzer, ion cyclotron analyzer, quadruple mass filter, time of flight (TOF)]. Importance of HRMS, Rules of fragmentation of different functional groups, factors controlling fragmentation. Fragmentation of alkanes alkenes, nitriles ,aromatic and carbonyl compounds etc.

Problems: Based on joint application of UV, IR, ¹H and ¹³C NMR, 2D and Mass (including reaction sequence).

References:

- 1. Introduction to Spectroscopy D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
- Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6 Ed. John Wiley and Sons.
- 3. Absorption spectroscopy of organic molecules V. M. Parikh
 - 4. Spectroscopic methods in organic chemistry D. H. Williams and I. Flemming Mc Graw Hill.
- 5. Nuclear Magnetic Resonance Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
- 6. One and Two dimensional NMR Spectroscopy -- Atta-Ur-Rehman, Elsevier (1989).
- 7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
- 8. Organic structural spectroscopy- Joseph B. Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
- 9. Organic structures from spectra- Field L. D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.
- 10. NMR spectroscopy of Organic compounds. Jackmann and Sternhell S.
- 11. Spectroscopy: Donald L. Pavia, Gary M. Lampman.

PAPER NO. SCT - 303A

PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Credits: 04 60 Hrs.

UNIT-I Molecular Orbital Theory:

(15)

Aromaticity in benzenoids, alternant and non-alternant hydrocarbons, **Huckel,s** rule, energy level of pi molecular orbitals and concept of Aromaticity, Calculation of energies of orbitals in cyclic and acyclic systems. Determination energies and stabilities of different systems. Calculation of charge densities. PMO theory and reactivity index.

UNIT-II Pericyclic Reactions-I

(15)

Features and classification of pericyclic reactions, Phases, nodes and symmetry properties of molecular orbital in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical reactions.

Electrocyclic reactions: Con-rotation and dis-rotation, electrocyclic closure and opening in 4n and 4n+2 systems, Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by: (i) Symmetry properties of HOMO of open chain partner; (ii) Conservation of orbital symmetry and orbital symmetry correlation diagram and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

UNIT-III Pericyclic Reactions-II

(15)

(a) Cycloaddition reactions: Suprafacial and antarafacial interactions. (π 2-cycloadditions. Cycloreversions. Stereochemical aspects in supra–supra, antara-supra and antara-antara (π 2 and π 4 cycloadditions. Diels-Alder reaction. Woodward-Hoffmann selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by 1) Conservation of orbital symmetry and orbital symmetry correlation diagrams 2) Fukui Frontier Molecular Orbital (FMO) theory and (3) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and it's explanation by FMO theory. Examples of cycloaddition reactions. (b) Sigmatropic reactions: [1,j] and [i,j] shifts. Suprafacial and antarafacial shifts. Selection rules for [i,j] shifts. Cope, degenerate Cope and Claisen rearrangements. Explanation for the mechanism of sigmatropic reactions by 1) symmetry properties of HOMO 2) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

UNIT- IV Photochemistry: Photochemistry of (π, π^*) transitions: Excited state of alkenes, cis-trans isomerisation, photochemistry state, electrocyclisation and Sigmatropic rearrangements, di π -methane rearrangement.

Intermolecular reactions: photocycloadditions, photodimerasation of sample and conjugated olefins, addition of olefins to α , β unsaturated carbonyl compounds, excimers and exiplexes. Photoaddition reactions. Excited states of aromatic compounds, photodimerisation of benzene, photosubstitution reactions of aromatic compounds and Photo-Fries rearrangement.

Photochemistry of (n, \pi^*) transitions: Excited state of carbonyl compounds, hemolytic cleavage of α -bond-Norrish type I reaction in acyclic, cyclic ketones and strained cycloalkanediones.

Intermolecular abstraction of hydrogen: Photo reduction and photo oxidation-influence of temperature, solvent, nature of hydrogen donors and structure of the substrate.

Intramolecular abstraction of hydrogen: Norrish type II reaction in ketones, esters and 1, 2-diketones.

Addition to C-C multiple bonds: Paterno-Buchi reaction, photodecarboxylation, photochemistry of alkyl peroxides, hypohalites and nitriles. Barton reaction. Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides. Chemiluminescent reactions. Oxidative coupling.(15)

Recommended Books:

- 1. Lehar and Merchand: Orbital Symmetry
- 2. R. B. Woodward and Hoffman: Conservation of Orbital symmetry.
- 3. Photochemistry and pericyclic reactions by Jagdamba Shingh
- 4. Cixon and Halton: Organic photochemistry
- 5. Arnold: Photochemistry
- 6. N. Turro: Modern Molecular Photochemistry
- 7. Rohatgi- mukherji: Fundamentals of photochemistry.
- 8. Ginsburg: Nionbenzoid aromatic compound
- 9. A. Streitfwieser: Molecular orbital theory for organic chemistry.
- 10. E. Cler: The aromatic sextet.
- 11. Lloyd: Carbocyclic non- benzoid aromatic compounds.
- 12. G. M. Bandger; The structure and reactions of aromatics compounds
- 13. W. B. Smith; Molecular orbital methods in Organic Chemist

PAPER NO. OET - 303B MEDICINAL CHEMISTRY-II

Credits: 04 60 Hrs

UNIT-I Basic consideration of drug activity

Definition and Introduction of following terms-Drug, Prodrug, Hard and Soft drugs, agonists, antagonists, affinity, efficacy, potency, isosterism, bioisosterism, pharmacophores, lead molecule, lethal dose (LD50) and effective dose (ED50) (i) Factors affecting bioactivity, (ii) Theories of drug activity, (iii) Structure activity relationship (SAR), QSAR (2D and 3D method) and Hantzsch equation (iv) Drug receptor mechanism.

UNIT-II (a)Pharmacokinetics

- (i) Drug absorption, Distribution and deposition of drugs.
- (ii) Excretion and elimination of drugs, Bioavailability.

(b) Pharmacodynamics

(i) Mechanism of drug action: Enzyme stimulation and enzyme inhibition, antimetabolites, membrane active drugs, chelation; (ii) Drug metabolism and inactivation: Factors affecting drug metabolism, pathways of drug metabolism [Metabolicreaction (Phase I) and conjugation reaction (Phase II)].

UNIT-IV Synthesis and Utilities of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

- **A. Anti inflammatory Drugs:** (a) Naproxen (b) Ibuprofen (c) Oxaprozin (d) Diclofenac Sodium (e) Rofecoxib (f) Celecoxib.
- **B.** Anti-hypertensive Drugs: (a) Verapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadil fumarate.
- C. Drugs acting on CNS: (a) CNS Stimulant : Dextro-amphetamine
- (b) Respiratory Stimulant: Doxapram
- (c) CNS anti-depressant : (i) Chlorpromazine (Antipsychotic) (ii) Diazepam (Anxiolytic)
- (iii) Phenobarbitol (Antiepileptic)

D Anesthetic Drugs:

- (a) General: Ketamine (b) Local: (i) Lidocaine (ii) Procaine
- **E. Antibiotics:** (a) Chloramphenicol (b) Ampicillin (c) Amoxycillin (d) Cefepime (e) Cefpirome (f) Antimycobactrial: Ethambutol (g) Antiviral: Acyclovir (h) Antimicrobial: Sulfamethoxazole
- **F. Antidiabetics :** (a) Troglitazone (b) Chlorpropamide (c) Tolbutamide
- **G.** Antineopastic Drugs: (a) Antagonist: Fluorouracil (b) Alkylating agents: i) Chlorambucil (ii) Cis-Platin

- FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A.
 Williams, Victoria F. Roche and S. William Zito.
- 2. Introduction of Medicinal Chemistry: A. Gringuage, Wiley-VCH.
- 3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby.
- 4. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
- 5. Medicinal Chemistry: David J. Triggle.
- 6. Essentials of Medicinal Chemistry IInd: Andrejus Korolkovas, WileyVCH

(OPEN ELECTIVE) PAPER NO. OET-304A DRUGS AND HETEROCYCLES

Credits: 04 60 Hrs.

UNIT-I Drug Design

(10)

Development of new drugs, procedures followed in drug design, concepts of prodrugs and soft drugs, factors affecting bioactivity, resonance, inductive effect, isosterism, bioisosterism, spatial considerations. History and development of QSAR, Concepts of drug receptors, applications of computers in drug design, Molecular modeling, Applications of combinatorial Chemistry in drug design.

UNIT- II Study of the following type of drugs: (20)

- a. **Antibiotics:** Preparation of semi synthetic penicillin, conversion of penicillin into cephalosporin, general account of tetracycline and macaracyclic antibiotics. (no synthesis)
- b. **Antimalarials**: Trimethopim, role of folic acid and its inhibition, mechanism of cell wall synthesis and inhibition.
- c. Analgesic and antipyretics; Paracetamol, Meperidine, Methadone, Aminopyrine
- d. **Anti-inflammatory**; Ibuprofen, Oxyphenbutazone, Dichlorophenac, Indomethacin, Arachidonic acid.
- e. **Antitubercular and anti leprotic**; Ethanbutol, Isoniazide, Dasone, mechanism, Pathways, inhibition of cyclooxygen.
- f. Anaesthetics; Lidocaine, Thiopental, mechanism of action.
- g. **Antihistamines**; Phenobarbiton, Fenediazole, Diphenylhydramine, mechanism of action.
- h. **Tranqulisers**: Diazepam, Trimeprazin, mechanism of action.
- i. Anti AIDS drugs: Cause, antimetabodies and anti-AIDS drugs.
- j. Cardiovascular Drugs: Synthesis of dilliazem, quindine, methyldopa, atenolol, Oxyprenol
- k. **Anti-neoplastic drugs:** Cancer chemotherapy, alkylating agents, mitolic inhibition, carcinolytic antibiotics and antimetabiotics, mode of action and synthesis of some important drugs.

Heterocycles

UNIT-III (15)

a) Small Ring Heterocycles

Three-membered and four-membered heterocycles-synthesis and chemical reactions of aziridines, oxiranes, thiranes, azetidines, oxitanes and thietanes.

(b) Five Membered HeterocyclesSynthesis and reactions including medicinal applications of furan, pyrrole, thiophene and benzopyrroles, benzofurans and benzothiophenes, imidazole, oxazole, thiazole, pyrazoles.

UNIT- IV (15)

(a)Six- Membered Heterocycles with one hetero atom:

Synthesis and reactions of pyridine, quinolines, isoquinoline, purines, , coumarins and chromones.

(b)Six member heterocycles with two hetero atoms:Pyridazines, pyrimidines, quinazolines, quinoxalines, diazines.

Books Suggested

- 1. Burger: Medicinal Chemistry
- 2. A . Kar: Medicinal chemistry (Wiley East)
- 3. W. O. Foye: Principals of medicinal chemistry
- 4. Wilson, Gisvold and Dirque: Text book of Organic medical and pharmaceutical Chemistry
- 5. Pharmaceutical manufacturing encyclopedia
- 6. R. M. Acheson: An introduction to chemistry of heterocyclic compounds (Interscience)
- 7. Joule and Smith: Heterocyclic chemistry (Van Nossstrand)
- 8. R.K. BANSAL: Heterocyclic chemistry (Wiley E)
- 9. L.A. Paquitte: Principals of modern heterocyclic chemistry
- 10. M.H. Palamer: The structure and reactions of heterocyclic compounds.
- 11. A.R. Katrtzhy and A.V. Bootton: Advances in Heterocyclic chemistry (A.P.)
- 12. Finar: Organic chemistry (Vol. 1 and 2)
- 13. Conn and Stumf: Outline of Biochemistry
- 14. Williams, Introduction to the chemistry of enzyme action.
- 15. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman Academic

Press.

- 16. Stralegies for Organic Drug Synthesis and Design. D. Lednicer, John Wiley.
- 17. Heterocyclic Chemistry Vol. 1-3, R. R. Gupta, M. Kumar, and V. Gupta, Springer Verlag.
- 18. The Chemistry of Heterocycles, T Eicher and S. Hauptmann, Thieme.
- 19. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, Chapman ans Hall.
- 20. Heterocyclic Chemistry, T. L. Gilchrist, Longman Scietific Techinal
- 21. Contemporary Heterocyclic Chemistry, G. R. Newkome and W. W. Poudler, Wiley.
- 22. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.
- 23. Comprehensive Heterocyclic Chemistry, A. R. Katrizky and C. W. Rees, eds, Pergamon Press.
- 24. Introduction to Medicinal Chemistry, Alex Gringuaz

(OPEN ELECTIVE) PAPER NO. OET- 304B UNIT OPERATIONS OF CHEMICAL ENGINEERING

Credits: 04 60 Hrs.

Unit I:

A) Heat Exchangers

Introduction; Shell and Tube Heat Exchanger, Shell side and tube side passes ;Classification of Shell and Tube Heat Exchangers-Fixed tube sheet heat exchanger, Fixed tube sheet 1-2 heat exchanger, Internal floating head heat exchanger, U-tube heat Exchanger, Kettle Reboiler.

B) Evaporation

Introduction; Types of evaporators-Jacketed, Horizontal and Vertical tube evaporators, forced Circulation evaporation; Entrainment separators; Effect of various parameters on Evaporation; Multiple effect evaporators and its Economy.

Unit II:

A) Distillation

Introduction; Boiling and Distillation; Vapor liquid equilibria; Azeotropic mixture; Flash/Equilibrium distillation; Steam distillation; Vacuum distillation; Extractive distillation; Batch and Continuous distillation; Equipment and working of Rectifier/Fractionating column-Bubble cap plate, Sieve-plate, Valve plate, Downcomers.

B) Extraction

Introduction; Selection of solvent for Extraction; Extraction with agitation and its Equipments-Mixer Settler, Spray column, packed column, Sieve column, Rotating disc Contactor, pulse column; Extraction with reflux.

C) Leaching

Introduction; solid liquid leaching- Batch plant for extraction of oil from seed, Bollman extractor, Rotocel extractor; continuous leaching Equipments-Dorr Agitator, Dorr thickener, Continuous counter- current extraction.

Unit III:

A) Filtration

Introduction; Principles of cake filtration; Types of filtration-Constant rate, Constant pressure filtration; Filter aids; washing filter cake; Filtration Equipment – centrifugal filtration, Rotary drum filter.

B) Crystallization

Introduction; Supersaturation, Methods of supersaturation, The Miers supersaturation theory and its limitation; Nucleation, Homogeneous Nucleation; crystal growth; Caking of crystal; Crystal hydrates and Solvates; Deliquescence and Hygroscopicity; Efflorescence; crystallization equipment-Agitated tank crystallizer, Swenson -walker crystallizer, vacuum crystallizer, Oslo cooling crystallizer.

Unit IV:

A) Crushing, Grinding, Drying and Mixing

Equipment for crushing-Blake Jaw crusher, Gyratory crusher; Equipment for grinding – Hammer mill, Revolving mill, Ball mill; Equipment for drying processes-Tray, Tunnels, Drum, Rotary, and Spray driers, Equipment for mixing processes-propeller, turbines.

B) Mechanical Separation and Beneficiation

Introduction; Screening sieves- equipment and use, Removal of solid from gases-Cyclone, Hydrocyclone, Dust filters- electrostatic dust precipitators, colloidal particles and their removal- scrubbers.

- 1. F.A. Henglein: Chemical Technology (Pergamon)
- 2. J.M. Coulson, J.F. Richardson,: Chemical Engineering Vol I, II,III (Pergamon)
- 3. R.N. Shreve: The Chemical Process industry (MGH)
- 4. W.L. Badger and J.T. Bandchero: Introduction to Chemical Engineering (MGH).
- 5. O.A. Hougen, K.M. Watson and R.A. Ragetz: Chemical Process Principle Vol I II (JW).
- 6. Prakash G. More, Comprehensive Industrial Chemistry, Pragati prakashan, Meerut (Uttar Pradesh)

SEMESTER-IV (Organic Chemistry) PAPER NO. HCT- 401 ADVANCED ORGANIC CHEMISTRY-II

Credits: 04 60 Hrs.

UNIT-I Protecting Groups

Protection and deprotection of hydroxyl, carbonyls in aldehydes and ketones, amines, carboxylic acids, alkenes and alkynes.

UNIT-II Disconnection Approach

Introduction to:

Grounding of organic chemistry for understanding retrosynthesis;

Retrosynthetic analysis and designing of the synthesis;

Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enentioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

C-C Disconnections

i) One group C-C Disconnections:

Alcohols (including stereoslectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

ii) Two group C-C Disconnections:

Diels-Alder reactions, 1,3 difunctionalized compounds and α , β -unsaturated compounds, control in carbonyl condensations, 1,5 difunctionalized compounds, Michael addition and Robbinson annealation.

UNIT-III Transitional metals complexes in organic synthesis

(A.) Palladium Heck arylation, allylic activation, carbonylation, wacker oxidation, isomarization formation N-aryl and N-alkyl bond transmetalation, allyl deprotection in peptides, coupling reactions: Stille coupling, Sonogashira and Suzuki coupling reactions and their importance

Iron:- Reactions of Iron carbonyls, ferrocenes, Fe-cyclopentadiene complex, protection of dienes, isomerization

Mn & Co:- Manganese and Co-carbonyls in hydroformylation, carboxylations, synthesis of silane complexes and their applications Pausal-khand reactions and its applications protection of alkynes by Co_2CO_8 .

UNIT-IV Organoboranes:- preparation and properties of organoborane reagents e.g. RBH, R₂B,9-BBN,catechol borane. Thexyl borane, cyclohexyl borane, ICPBH₂,

IPC₂BH, Hydrboration-mechanism, stereo and regeoselectivity, uses in synthesis of primary, secondary tertiary alcohols, aldehydes, ketones, alkenes. Synthesis of EE, EZ, ZZ dienes and alkyenes. Mechanism of addition of IPC₂BH. Allyl boranes- synthesis, mechanism and uses

- 1. Organic Synthesis: The Disconnection Approach: Stuart Warren
- 2. Designing Organic Synthesis: Stuart Warren
- 3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
- 4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
- 5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others
- 6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
- 7. Some Modern Methods of Organic Synthesis: W. Carruthers
- 8. Organic Synthesis: M. B. Smith
- 9. Principles of Organic Synthesis: R. Norman and J. M. Coxan.
- 10. Advanced Organic Chemistry: Jerry March
- 11. Organic Chemistry: Clayden, Greeves, Warren and Wother

PAPER NO. HCT - 402 STEREOCHEMISTRY

Credits: 04 60 Hrs.

UNIT-I

Conformation and reactivity in acyclic compounds and of cyclohexanes.

Stability and reactivity of diastereoisomers. Curtin- Hammett principle.

The shapes of the rings including six membered: Shapes of five, and seven eight membered rings, Reactivity of six member ring system, Conformational effects in medium sized rings, Concept of I strain.

UNIT-II

Fused and Bridged rings: Fused bicyclic ring systems:

Cis- and trans- decalins and nine methyl decalines and perhydraphenanthrene, perhydroanthracene. Bridged rings, Nomenclature stereo chemical restrictions. The Bredts rule, Reactivities.

Stereochemistry of Allenes, spiranes and biphenyls

UNIT-III Newer methods of Stereo selective synthesis

Introduction and Stereoselective and stereospecific reactions. Enantioselective synthesis (Chiral approach) reactions with hydride donors, catalytic hydrogenation via chiral hydrazones and oxazolines, enatiotopic and diastereotopic atoms, groups and faces. Use of calculations of optical purity and enantiomeric excess.

UNIT-IV Asymmetric Synthesis

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP, Hydroboration- Ipc₂BH, IpcBH₂, Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation- (DHQD)₂PHAL & (DHQ)₂PHAL, Felkin-Anh model, Zimmermann-Traxler transition state model, Proline catalyzed asymmetric reactions.

- 1. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
- 2. Stereochemistry: Conformation and Mechanism: P. S. Kalsi
- 3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
- 4. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
- 5. Organic Chemistry: Clayden, Greeves, Warren and Wothers
- 6. Organic Synthesis: M. B. Smith

PAPER NO. HCT- 403 CHEMISTRY OF NATURAL PRODUCTS

Credits: 04 60 Hrs.

UNIT-I Steroids

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progestrone.

- **UNIT-II** (a) Structure, stereochemistry, synthesis and biogenesis of Hardwickiic acid, Camptothecin and Podophyllotoxin. (Ref. 1 to 4 and 11)
- **(b) Structure determination and Synthesis** of i) Reserpine (Woodward synthesis) Ref. 5, 6 ii) Taxol Ref. 6 iii) Estrone and Mifepristone Ref. 6, 7 iv) Strychnine (Overman's synthesis) Ref. 6 v) Fredericamycin A Ref. 5. **(15)**

UNIT-III Biogenesis – The building blocks and construction mechanism of

- (i). Terpenoids Mono, Sesqui, Di and Triterpenoids and cholesterol
- (ii) Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and trytophan.
- (iii) The Shikimate pathway cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbers, isoflavanoids and terpenoid quinones. Ref. 8, 9, 10.
- (iv) Arachidonic acid Prostagladins & thromboxanes. (15)

UNIT-IV Synthesis and Biological Functions – involving vit. B1, B2, B6, Biotin, Folic acid, Riboflavin, Prostaglandins. (15)

- 1. J. Am Chem. Soc. 88, 3888 (1966).
- 2. M. C. Wani and M.E. Wall J. Org. Chem. 34, 1364 (1969)
- 3. (i) Tetrahedron Letters, 3751 (1964)
 - (ii) Tetrahedron Letters, 2861 and 2865 (1968)
- 4. Chemistry of Natural products-Kalsi
- 5. Principles of organic synthesis by R.O.C. Norman and J. M. Coxon; Chapman and Hall
- 6. Classics in organic synthesis K.C. Nicolaou and E.J. Sorensen
- 7. J. Indian Inst. Sci. 81, 287 (2001).
- 8. Medial Natural Products A Biosynthetic approach by Paul M. Dewick 2nd edition (Wiley)

- 9. Secondary metabolism J. Mann, 2nd edition.
- 10. Chemical aspects of Biosynthesis J. Mann (1994)
- 11. i) J.C.S. Perkin Transactions II, 288-292, (1973)
 - ii) J. Am. Chem. Soc. Vol. 77, 432-437, (1955).
- 12. Apsimon: The Total synthesis of natural products.
- 13. Manskey and Holmes: Alkaloids
- 14. A.A. Newmen: Chemistry of Terpenes.
- 15. P. D B.Mayo: The Chemistry of natural products.
- 16. Simonson: Terpenes.
- 17. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry
- 18. Woguer: Vitamins and Co- enzymes.
- 19. Bently: Chemistry of natural products,
- 20. Fieser and Fieser: Steroids
- 21. Finar: Organic chemistry Vol. II and I
- 22. J.B. Hendrickson: The molecules of nature.
- 23. Peter Bernfield: The biogenesis of natural products,
- 24. R.T. Slickenstaff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.
- 25. The Chemistry of natural products: by Nakanishi

(SOFT CORE) PAPER NO. SCT- 404A APPLIED ORGANIC CHEMISTRY

Credits: 04 60 Hrs.

UNIT-I

(a) Application of the following in synthesis

Merrifield resin Solid phase synthesis of polypeptide & oligonucleotides, enzyme catalyzed reaction in synthesis., Cyclodextrins, Calixerins.

(b)Synthesis and applications of perfumery: 2-Phenylehanol, vanillin and other food flavours and synthetic musk. **(15)**

UNIT-II Green Chemistry:- (i) Introduction and basic principles (ii) multicomponent reactions. (iii) Applications of Microwave and Ultrasonication in Organic Synthesis (iv) Reactions in aqueous media (v) Use of ionic liquids. (15)

UNIT-III Non benzenoid aromatic Compounds:

Aromaticity in Non- benzenoids compounds, **Annulenes** and hetroannulenes, fullerene C60, Tropone, tropolone azulene, fulvene, tropylium salts, ferrocene, three and five membered systems, bonding in fullerenes. (15)

UNIT-IV Advanced Carbohydrate Chemistry

Introduction of sugars, structures of triose, tetrose, pentose, hexose. Fisher projection, D-and L-configuration, Conversion of Fisher projection to furanose and pyranose form, Haworth Structure, 4C_1 and 1C_4 Conformations, anomeric effect, Reactions of five and six carbon sugars, glycoside formation, acetonide formation, reduction, synthesis of D-glyceraldehyde, Killani-Fischer Synthesis, glucal formation and reactions, Ferrier and Hanesian Reaction, Ferrier rearrangement. (15)

- 1. Organic Chemistry R. P. Morrison and R. N. Boyd
- 2. Organic Chemistry I. L. Finar, Volume –II
- 3. New Trends in Green Chemistry V. K. Ahluwalia and M. Kidwai Anamaya Publishers (2004).
- 4. Supramolecular Chemistry vol. 17 (1-2), pp. 47-55, January-March 2005.
- 5. Modern synthetic reactions H. O. House (Benjamin)
- 6. Organic chemistry J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press)
- 7. Designing of organic synthesis S. Warren (Wiley)
- 8. Some modern methods of organic synthesis W. Carruthers (Cambridge)
- 9. Organic synthesis M. B. Smith
- 10. Advanced organic chemistry, Part B F. A Carey and R. J. Sundberg 5th edition

PAPER NO. SCT- 404B

CHEMICAL INDUSTRIES

Credits-04 60 hr

Unit I:

A) Metallurgy Industry

15hr

Extraction and applications of metal alloys

- a) Iron and steel: Iron, steel alloy, tool steel, stainless steel.
- b) Aluminum

B) Cement Industry

Introduction; Classification and Manufacturing processes of Cement and Lime; Setting and Hardening process.

C) Glass Industry

Introduction; Physical and Chemical properties; Characteristics of glass; Raw material Manufacturing process of glass; Ceramic-Raw material, Manufacturing process of White ware, Glazing.

Unit II:

A) Paints and Pigments Industries

15hr

Paints- Introduction; Classification of paints; Constituents of paints; Formulation of paints; Mixing of paints; Manufacturing processes of paints; Failure of paints; Varnishes, Enamals, Emulsion paints- Constituents.

Pigment- Manufacturing processes of zinc oxide and titanium dioxide, properties and application

Special paints- Luminescents paints, Heat resistant paints, cellulose paints.

B) Dyes

Classification of dyes according to the mode of applications and according to the chemical constitution; Methods of preparation of commercial dyes of different classes with suitable examples; Typical manufacturing processes of dyes; Fluorescent brightening agents

Unit III:

Agrochemicals:

15hr

- a) Organo chlorine pesticides: BHC, Aldrin, Dialdrin, Endosulphan,
- b) Organo phosphorus pesticides: Malathion, monocrotophos, Dimethoate, chloropyriphos.
- c) Carbamates: Carbaryl, Bygon, Ziram, Zineb, Maneb.
- d) Insect pheromones and Repellants: Pheromone, general introduction and application in integrated pest management (no synthesis), Repellant: Survey and synthesis of following repellants: N,N Diethyl-3-methyl benzamide, N,N, Diethylenebenzamide, 2-ethyl-1,3, hexanediol, Butopytranexyl, Dimethylcarbamate, Dimethylpthalate

Unit IV:

Petrochemicals 15hr

Crude oil, Natural gas, Petroleum hydrocarbons- Types and source of crude oil; Refining various petroleum fractions- Thermal cracking, Recycle cracking, Thermal cracking of fuel; outline of chemicals derived from natural gases/ paraffin hydrocarbon-Ethylene, Propylene Butylenes, Benzene, Toluene.

- 1. F.A. Henglein: Chemical Technology (Pergamon)
- 2. R.W. Thomas & P.Farago: Industrial Chemistry (HEB)
- 3. R.N. Shreve: Chemicals Process Industrial (MGH)
- 4. Riegel's: Industrial Chemistry (Reinhold)
- 5. D.S.T: Perspectives in science and technology Vol I & II (Vilas)
- 6. W.H. Dennis: Foundation of iron and steel metallurgy (Elsevier)
- 7. Prakash G. More, Comprehensive Industrial Chemistry, Pragati Prakashan, Meerut (Uttar Pradesh)
- 8. Kirk R Smith: Biofuels: Air pollution and Health: A Global Review (Kluwer Academic/Plenum publisher
- 9. Plant oil as fuels- Present state of science and future developments Edited by N. Martini and J.S. Sebeli Springer Verlag 1998.

M. Sc. II Organic Chemistry Practicals: Practicals V –VIII

V) Qualitative Analysis

Separation, purification and identification of compounds of THREE components mixtures, chemical tests. derivatives etc.by microscale technique.

IR spectra to be used for functional group identification. TLC and Column Chromatography.

VI & VII) Two stage and Three stage Organic preparations starting with 5g or less. (TLC Analysis is recommended)

- 1. Preparation of Benzanilide by Beckmann rearrangement.
- 2. Preparation of Antharanilic acid.
- 3. Preparation of Phthalimide.
- 4. Preparation of N- Bromosuccinamide.
- 5. Preparatin of p- Aminobenzoic acid.
- 6. Preparation of p- chloronitrobenzene by Sandmeyer reaction.
- 7. Preparation of p- Iodonitrobenzene by Sandmeyer reaction.
- 8. Pinacol- Pinacolone rearrangement.
- 9. Preparation of Acetophenones by Fries rearrangement
- 10. Preparation of aromatic aldehydes by Vilsmer Hack reaction or R. T.
- 11. Wittig reaction.
- 12.Preparation of Benzopyrazole (Other suitable experiments may be added)

HCMP VIII Major Project/In Plant training: Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, new methods etc. and Spectral Analysis.

Reference books.

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- 4. Organic Synthesis Collective Volumes by Blat.
- 5. Reagents in Organic Synthesis by Fieser and Fieser.
- 6. Organic Practicals by Ahluwalia.
- 7. Systematic Lab Experiments in Organic Chemistry by Arun Sethi. (New Age).