SOLAPUR UNIVERSITY,

SOLAPUR

SCHOOL OF CHEMICAL

SCIENCES

M.Sc.II- ORGANIC CHEMISTRY SYLLABUS

(Choice Based Credit System – CBCS)

(w.e.f. June, 2016)

M. Sc.-I (Chemistry) (Semester–I and Semester–II) As per CBCS Pattern w.e.f. Academic year-2015-2016

Semester-I

Paper	Type of Course	Name of the Paper	Total	Total	Total	Hours/
Number			Marks	Hours	Credits	Week
Paper-I	Core	Inorganic Chemistry-I	100	60	4	4
Paper-II	Core	Organic Chemistry-I	100	60	4	4
Paper-II	Core	Physical Chemistry-I	100	60	4	4
Paper-IV	Core	Analytical Chemistry-I	100	60	4	4
Practical Co	ourse-I	Inorganic Chemistry	50	60	2	4
		Organic Chemistry	50	60	2	4
Practical Co	ourse-II	Physical Chemistry	50	60	2	4
		Analytical Chemistry	50	60	2	4
	Seminar –I		25		1	4
			625		25	36

Semester-II

Paper	Type of Course	Name of the Paper	Total	Total	Total	Hours/
Number			Marks	Hours	Credits	Week
Paper-V	Core	Inorganic Chemistry-II	100	60	4	4
Paper-VI	Core	Organic Chemistry-II	100	60	4	4
Paper-VII	Core	Physical Chemistry-II	100	60	4	4
Paper-VIII	Core	Analytical Chemistry-II	100	60	4	4
Practical Co	urse-III	Inorganic Chemistry	50	60	2	4
		Organic Chemistry	50	60	2	4
Practical Co	urse-IV	Physical Chemistry	50	60	2	4
		Analytical Chemistry	50	60	2	4
	Seminar –II		25		1	4
			625		25	36

M. Sc.-II (Organic Chemistry) Syllabus (Semester-III and Semester-IV) Semester System CBCS pattern (w.e.f. June 2016)

Semester-III

Paper Number	Type of Course	Name of the Paper	Total Marks	Total Hours	Total Credits	Hours/ Week
Paper-IX	Core	Advanced Organic Chemistry-I	100	60	4	4
Paper-X	Core	Advanced Spectroscopic Methods	100	60	4	4
Paper-XI	Core	Photochemistry and Pericyclic Reactions	100	60	4	4
	Elective –I	Drugs and Heterocycles	100	60	4	4
Paper-XII	Elective –II	Medicinal Chemistry	100	60	4	4
Practical Cou	rse-V	Qualitative Analysis of Ternary Mixture	100	120	4	8
Practical Cou	rse-VI	i) Organic Preparation ii) Spectral Problems	100	120	4	8
	Seminar –III		25		1	4
	Total		625		25	36

Semester –IV

Paper Number	Type of Course	Name of the Paper	Total Marks	Total Hours	Total Credits	Hours/ Week
Paper-XIII	Core	Advanced Organic Chemistry-II	100	60	4	4
Paper-XIV	Core	Stereo Chemistry	100	60	4	4
Paper-XV	Core	Chemistry of Natural Products	100	60	4	4
	Elective -I	Applied Organic Chemistry	100	60	4	4
Paper-XVI	Elective -II	Chemical Industries	100	60	4	4
Practical Co		Organic Preparations	100	120	4	12
Practical Co	urse-VIII	i) Project work ii) Spectral Problem	100	120	4	12
	Seminar-IV		25		25	4
	Total		625		32	36

Summary:

Course	No. of Papers	Total	Examination Pattern		Total Credits
		marks	UA	IA	
Core	14	1400	980	420	56
Elective	04 (any two)	200	140	60	08
Practical	08	800	560	240	32
course					
Seminars	04	100	-	100	04
TOTAL		2500	1680	820	100

SOLAPUR UNIVERSITY, SOLAPUR M. Sc. ORGANIC CHEMISTRY COURSE SYLLABUS SEMESTER 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 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	1600 marks
Practicals (semester end exam.), 8 X 70+30 marks	800 marks
Seminars for each semester, 4 X 25	100 marks
	Total: 2500 marks

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

M. Sc. Part I* Chemistry

(* This course is common for Polymer, Organic and Physical Chemistry courses).

Semester I

Theory Courses:

Paper No	0.	Title of Papers	
CH 101	(I)	Inorganic Chemistry-I	70+30 = (100 marks)
CH 102	(II)	Organic Chemistry-I	70+30 = (100 marks)
CH 103	(III)	Physical Chemistry-I	70+30 = (100 marks)
CH 104	(IV)	Analytical Chemistry-I	70+30 = (100 marks)

Semester II

Paper No.	Title of Papers	
CH 201 (V)	Inorganic Chemistry-II	70+30 = (100 marks)
CH 202 (VI)	Organic Chemistry-II	70+30 = (100 marks)
CH 203 (VII)	Physical Chemistry-II	70+30 = (100 marks)
CH 204 (VIII)	Analytical Chemistry-II	70+30 = (100 marks)

Practical Course: (Semester end examination) Practicals I & II for semester I Practical Examination will be of 4 days for each semester

Inorganic Chemistry Practicals:	(35 + 15) = 50 marks
Organic Chemistry Practicals:	(35 + 15) = 50 marks
Physical Chemistry Practicals:	(35 + 15) = 50 marks
Analytical Chemistry Practicals:	(35 + 15) = 50 marks

Practicals III & IV for semester II

Inorganic Chemistry Practicals:	(35 + 15) = 50 marks
Organic Chemistry Practicals:	(35 + 15) = 50 marks
Physical Chemistry Practicals:	(35 + 15) = 50 marks
Analytical Chemistry Practicals:	(35 + 15) = 50 marks

M. Sc. Part II Organic Chemistry: Semester III

Theory Courses:

Paper No.	Title of Papers	
ORG CH 301 (IX)	Advanced Organic Chemistry-I	(70 + 30) = 100 marks
ORG CH 302 (X)	Advanced Spectroscopic Methods	(70 + 30) = 100 marks
ORG CH 303 (XI)	Photochemistry and Pericyclic	
	Reactions	(70 + 30) = 100 marks
ORG CH 304 (XII) E	EleI: Drugs and Heterocycles	(70 + 30) = 100 marks
E	le .:- II Medicinal Chemistry	(70 + 30) = 100 marks

Semester IV

Paper No.	Title of Papers	
ORG CH 401 (XIII)	Advanced Organic Chemistry-II	(70 + 30) = 100 marks
ORG CH 402 (XIV)	Stereochemistry	(70 + 30) = 100 marks
ORG CH 403 (XV)	Chemistry of Natural Products	(70 + 30) = 100 marks
ORG CH 404 (XVI) EleI:	Applied Organic Chemistry	(70 + 30) = 100 marks
EleII:	- Chemical Industries	(70 + 30) = 100 marks

Practical Course: (Semester end examination) Practicals V to VIII

Semester III

ΡV	Organic Mixture	(70 + 30) = 100 marks
P VI	i) Organic Preparation	
	ii) Spectral Problems (50)	(70 + 30) = 100 marks

Semester IV

P VII	Organic Preparations	60 + Oral 05 marks + Journal 05 marks +
		Internal $30 = 100$ marks
P VIII	Project work/In-plant	60 marks + presentation 10 +
		Internal (spectral problem) $30 = 100$ marks

Nature of Examination:

Each semester will have theory external examination of four papers of 70 marks each (3 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. I Semester I and II

The practical examination will be of 4 days (one day for each specialization). The distribution of marks for an each specialization (50 marks) will be as under,

Practical experiments:	30
Oral	03
Journal:	02
Internal Practical	15
Total	50 (for each specialization practical)

Practical Examination of M. Sc. II

The practical examination will be of 3 days for each semester. The distribution of marks for each P V, VI, and VII is (70 marks) as under,

Practical experiments:60Oral05Journal:05;whereas distribution of marks for P VIII will be;Project work / In-plant training Report:60**+10 marks for presentation

** The valuation to be done by both external and internal examiners at the time of P VIII examination. Valuation of Seminars is to be done in each Semester by the Teaching Faculty involved in teaching Organic Chemistry course.

Nature of question paper (for M. Sc. I and II):

Time: 03 hours

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.

Maxi Marks 70

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)

	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. 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. ORG CH-301 (IX) Advanced Organic Chemistry-I

Credit: 04

Hours: 60

(15)

15hrs

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

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

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.15hrsComplex metal hydrides, lithium dialkyl cuprate, Trimethyl silyl iodide, tributyl tinhydride, 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. ORG CH 302 (X) Advanced Spectroscopic methods

Credit: 04

UNIT-I IR Spectroscopy

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-II¹H NMR

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.

15 hrs

15 hrs

Hours: 60

UNIT-III (a) ¹³C NMR

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-¹H-¹³C COSY (HETCOR, HMQC, HMBC, HSQC), interpretation of 2D spectra and examples.

UNIT-IV Mass spectrometry

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).

Books:

- Introduction to Spectroscopy D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
- 2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster,
 - 6th 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.
- Nuclear Magnetic Resonance Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
- 6. One and Two dimensional NMR Spectroscopy- Atta-Ur-Rehman, Elsevier (1989).
- Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998).
- 8. Organic structural spectroscopy- Joseph B. Lambert, Shurvell, Lightner, Cooks,

15 hrs

15 hrs

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-ORG CH-303 (XI) Photochemisty and Pericyclic Reactions

Credits: 04

60 Hrs.

(15)

(15)

(15)

UNIT-I Molecular Orbital Theory:

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

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

(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, π^*) **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 oxidationinfluence 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. ORG CH 304 (XII)(A) **Drugs and Heterocycles**

Credits: 04

UNIT-I Drug Design

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. Trangulisers: Diazepam, Trimeprazin, mechanism of action.
- i. Anti AIDS drugs: Cause, antimetabodies and anti-AIDS drugs.
- j. Cardiovascular Drugs: Synthesis of dilliazem, quindine, methyldopa, atenolol, Oxvprenol
- k. Anti-neoplastic drugs: Cancer chemotherapy, alkylating agents, mitolic inhibition,

60 Hrs.

(10)

carcinolytic antibiotics and antimetabiotics, mode of action and synthesis of some important drugs.

Heterocycles

UNIT- III

a) Small Ring Heterocycles

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

(15)

(b) Five Membered Heterocycles Synthesis 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, pyrazines, 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.
- 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

Paper No. ORG CH 304 (XI)(B) MEDICINAL CHEMISTRY

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

Reference Books:

1. 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

SEMESTER-IV (Organic Chemistry) Paper No-ORG CH-401 (XIII) 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. $RBH_2, R_2BH, R_3B, 9$ -BBN, catechol borane. Thexyl borane, cyclohexyl borane , ICPBH₂, IPC_BH, 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 IPC_BH. Allyl boranes- synthesis, mechanism and uses

Reference Books:

- 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. ORG CH- 402 (XIV) 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.

Reference Books:

- 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. ORG CH-403 (XV) 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)

Books:

- 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).
- 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

Paper No. ORG CH- 404(A) (XVI) Applied Organic Chemistry

Credits: 04

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)**

60 Hrs.

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, Dand L-configuration, Conversion of Fisher projection to furanose and pyranose form, Haworth Structure, ${}^{4}C_{1}$ and ${}^{1}C_{4}$ Conformations, anomeric effect, Reactions of five and six carbon sugars, glycoside formation, acetonide formation, reduction, synthesis of Dglyceraldehyde, Killani-Fischer Synthesis, glucal formation and reactions, Ferrier and Hanesian Reaction, Ferrier rearrangement. (15)

Referance Books:

- 1. Organic Chemistry R. P. Morrison and R. N. Boyd
- 2. Organic Chemistry I. L. Finar, Volume -II
- 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)
- 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
- Advanced organic chemistry, Part B F. A Carey and R. J. Sundberg 5th edition (2007)

ORG CH – 404 (XVI) (B) Chemical Industries

Credits-04

Unit I:

A) Metallurgy Industry

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

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:

- 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

60 hr

15hr

15hr

15hr

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.

Reference Books

- 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

A) Qualitative Analysis

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

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

C) 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.
- (Other suitable experiments may be added)

D) Project: Literature survey. Studies of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, new methods etc..

E). Spectral Analysis

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).