SRI DHARMASTHALA MANJUNATHESHWARA COLLEGE, UJIRE-574240

(Autonomous)

(Re-Accredited by NAAC at 'A' Grade with CGPA 3.61 out of 4)

PG DEPARTMENT OF

CHEMISTRY

Syllabus of

M. Sc. Degree Programme in

Organic Chemistry

(CHOICE BASED CREDIT SYSTEM)

2020- 2021 onwards.

Approved by the BOS meeting held on 27th Aug. 2020

Approved by the Academic Council held on 10-11-2020

Preamble

Revision of Syllabus for the Two years Master Degree (Choice Based Credit System-Semester Scheme) Programme in Organic Chemistry.

The PG BOS in Organic Chemistry has prepared the revised Syllabus for M.Sc. Organic Chemistry (CBCS based) in its meeting held on 27 August 2020, as per the guidelines suggested by Mangalore University and University Grants Commission, New Delhi. It was resolved to implement this new syllabus from the academic year 2020-21.

In the present revised syllabus, the suggested course pattern includes Hard Core, Soft Core and Open Elective courses with 91 credits for the entire programme. The syllabus consists of 18 Hard Core courses including 12 theory (3 in each semester), 5 practicals (in III and IV semester) with 3 credits each and one Project work (in III Semester) with 4 credits, total of **55 credits**. It also consists of 3, 2, 2 and 3 (total 10 courses) Soft core theory courses respectively in I, II, III and IV semesters. Student shall opt any 2, 1, 1 and 2 (total 6 courses) courses respectively in I, II, III and IV Semesters. All the soft core theory papers are of 3 credits. Programme consists of 6 Soft Core practical courses (3 courses each in I and II semesters with 2 credits each) with a total of **30 credits** (6 theory x 3 credits + 6 practicals x 2 credits). BOS has also proposed 4 open electives (2 each in II & III Semesters) with 3 credits each (**6 credits)** to be offered to non-Chemistry students. Student shall opt any 1 course each in II and III Semesters respectively. All together **total credits** come to **91**.

The revised syllabus is designed to impart quality education by incorporating skill components with practical knowledge. The syllabus has been prepared in a participatory manner, after discussions with a panel of members consisting of subject experts, industrial experts and meritorious alumnus of the department by referring the existing syllabi, U.G.C. model curriculum and the syllabi of other Universities and National Institutes.

The syllabus is structured in a view to prepare the students for higher studies and employability. The curriculum imparts knowledge to the students on the skills required for contributing to the industry and academic Institutions. Organic Chemistry being an experimental science, sufficient emphasis is given in the syllabus for training in laboratory skills and instrumentation. The units of the syllabus are well defined. The number of

contact hours required for each unit is also given. A list of reference books is provided at the end of the each semester.

ELIGIBILITY FOR ADMISSION

B.Sc. Degree from recognized University, with Chemistry as one of the major/optional/special subjects, at UG level with 45% aggregate excluding languages (40% for SC/ST/Category–1 candidates). Mathematics in PUC is mandatory.

Faculty of PG Studies in Organic Chemistry: PGOCHE053

Programme Specific Outcomes:

PSO1: Show an ability to design, and carry out synthetic reactions, isolation and purification of products.

PSO2: Exhibit skills in problem solving, critical thinking and analytical reasoning.

PSO3: Effectively apply gained knowledge in smooth functioning of daily life.

PSO4: Show competency in teaching profession, industrial jobs..

PSO5: Show an ability to start small scale industries with the available resources.

PSO6: Accurately record and analyze the results of synthetic works.

PSO7: Behave ethically in issues that chemists face including an understanding of safe handling of chemicals, and issues like environmental, energy, health and medicine.

PSO8: Successfully clear exams like UPSC, UGC etc.

COURSE/CREDIT PATTERN

Semester	Credits (C)						Total
	Theory (T)			Practical (P)		Project (Pr)	
	Hard Core (H)	Soft Core (S)	Elective (E)	Hard Core (H)	Soft Core (S)	Hard Core (H)	
First	3T x 3C=9	2T x 3C=6	--	--	3P x 2C=6	--	21
Second	3T x 3C=9	1T x 3C=3	1T x 3C=3	--	3P x 2C=6	--	18+3*
Third	3T x 3C=9	1T x 3C=3	1T x 3C=3	2P x 3C=6	--	1Pr x 4C=4	22+3*
Fourth	3T x 3C=9	2T x 3C=6	--	3P x 3C=9	--	--	24
Total	36	18	6*	15	12	4	**85+6***

Total Credits from all the Four Semesters = 91

Total Hard Core credits = 36 (T) + 19 (P) = 55 = 60.4%

Total Soft Core credits = 18 (T) + 12(P) = 30 = 33.0%

*Open Elective Credits = 6 = 6.6% (Not to be considered for calculating the CGPA)

COURSE PATTERN AND SCHEME OF EXAMINATION

I Semester

Course Code	Course Title	No of Units	Evaluation IA + Exam	Teaching Hrs/ week	Exam Hrs	Credits
OC H 401	Inorganic Chemistry	3	30 + 70	3	3	3
OC H 402	Organic Chemistry	3	30 + 70	3	3	3
OC H 403	Physical Chemistry	3	30 + 70	3	3	3
OC S 404 OC S 405 OC S 406	Spectroscopy Methods of Analysis Environmental Chemistry (**Any two**)	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x2=6
OC P 407	Inorganic Chemistry Practicals-I	--	30 + 70	4	4	2
OC P 408	Organic Chemistry Practicals-I	--	30 + 70	4	4	2
OC P 409	Physical Chemistry Practicals-I	--	30 + 70	4	4	2

II Semester

Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
OC H 451	Advanced Inorganic Chemistry	3	30 + 70	3	3	3
OC H 452	Advanced Organic Chemistry	3	30 + 70	3	3	3
OC H 453	Advanced Physical Chemistry	3	30 + 70	3	3	3
OC S 454 **or** OC S 455	Spectroscopy and Analytical Techniques **or** Chemistry of Bio-molecules	3 3	30 + 70 30 + 70	3 3	3	3x1=3
CH E 456 **or** CH E 457 **or** CH E 458	Colour Chemistry: Applications in daily life **or** Environmental Chemistry for Sustainable future **or** Chemistry in the Community	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x1=3
OC P 459	Inorganic Chemistry Practicals-II	--	30 + 70	4	4	2
OC P 460	Organic Chemistry Practicals-II	--	30 + 70	4	4	2
OC P 461	Physical Chemistry Practicals-II	--	30 + 70	4	4	2

III Semester

Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
OC H 501	Organic Reaction Mechanisms	3	30 + 70	3	3	3
OC H 502	Organic Synthetic Methods and Reagents	3	30 + 70	3	3	3
OC H 503	Organometallic Chemistry	3	30 + 70	3	3	3
OC S 504 **or** OC S 505	Chemistry of Synthetic Drugs **or** Computational And Theoretical Chemistry	3 3	30 + 70 30 + 70	3 3	3	3x1=3
CH E 506 **or** CH E 507 or CH E 508	Biomolecules and Medicines **or** Chemistry of Materials or Food Chemistry	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x1=3
OC P 509	Organic Chemistry Practicals-III	--	30 + 70	6	6	3
OC P 510	Organic Chemistry Practicals-IV	--	30 + 70	6	6	3
OC P 511	Project Work & Dissertation	--	30 + 70	8	--	4

IV Semester

Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
OCH 551	Organic Synthetic Design and Green Techniques	3	30 + 70	3	3	3
OCH 552	Advanced Heterocyclic Chemistry	3	30 + 70	3	3	3
OCH 553	Photochemistry and Asymmetric Synthesis	3	30 + 70	3	3	3
OCS 554 OCS 555 OCS 556	Advanced Medicinal Chemistry Chemistry of Natural Products Industrial Organic Chemistry (**Any two**)	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x2=6
OCP 557	Organic Chemistry Practicals-V	--	30 + 70	6	6	3
OCP 558	Organic Chemistry Practicals–VI	--	30 + 70	6	6	3
OCP 559	Organic Chemistry Practicals–VII	--	30 + 70	6	6	3

BASIS FOR INTERNAL ASSESSMENT

Internal assessment marks in theory papers shall be based on two tests, seminar, assignment, class attendance and library usage. The tests may be conducted 8 and 14 weeks after the start of a semester. Average of two tests mark will be reduced to 20 marks and remaining 10 marks are allotted to seminar, assignment, class attendance and library usage. Practical internal assessment marks shall be based on test and records, 20 marks for experiment and 10 marks for record. The practical tests may be conducted 12 weeks after the start of a semester. Internal Assessment marks on Project work-Dissertation is based on presentation given on their project work.

THEORY QUESTION PAPERS PATTERN

Question Papers in all the four semesters shall consist of Two Parts, Part-A and Part-B. Part-A shall contain Twelve (12) short answer type questions drawn equally from all the 3 units (4 questions per unit). Nine out of Twelve questions are to be answered (marks: 9x2=18). Part B shall contain Six (06) brief and/or long answer questions carrying 13 marks each drawn equally from all the 3 units (2 questions per unit). There should be three sub-divisions per question (5+4+4). Four out of Six questions are to be answered selecting minimum of 1 question from each unit (marks: 13x4=52). Total marks of part A and B: 18+52=70.

M.Sc. Organic Chemistry

Time: 3 Hrs **Max. Marks: 70**

Answer any **nine** sub-divisions from **Question No.1** in **Part A** & any **four** questions from **Part B** selecting minimum of 1 question from each unit**.**

PART - A

Answer any Nine subdivisions

2x9= 18

1. a.
b. UNIT I
c.
d.

e.
f. UNIT II
g.
h.

i.
j.
k. UNIT III

l.

PART – B

Answer any **Four** questions selecting minimum of 1 question from each unit**.** 13x4 = 52

UNIT I

2. a.
b.
c. 5+4+4

3. a
b.
c. 5+4+4

UNIT II

4. a.
b.
c. 5+4+4

5. a.
b.
c. 5+4+4

UNIT III

6. a.
b.
c. 5+4+4

7. a.
b.
c. 5+4+4

M.Sc. Chemistry Open Elective Paper

Time: 3 Hrs **Max. Marks: 70**

Answer any **nine** sub-divisions from **Question No.1** in **Part A**& any **four** questions from **Part B**

PART - A

Answer any Nine subdivisions 2x9= 18

1. a.
b. UNIT I
c.
d.

e.
f. UNIT II
g.
h.

i.
j.
k. UNIT III
l.

PART – B

Answer any **Four** questions 13x4 = 52

UNIT I

2. a.
b.
c. 5+4+4

3. a
b.
c. 5+4+4

UNIT II

4. a.
b.
c. 5+4+4

5. a.
b.
c. 5+4+4

UNIT III

6. a.

b.

c. 5+4+4

7. a.

b.

c. 5+4+4

PRACTICAL EXAMINATION PATTERN

In the Practical Examination course, out of 70 marks, 10 marks shall be allotted for Viva voce and 60 marks for practical proper. In the III semester there shall be project work/dissertation of 70 marks. The Project work may be conducted either in the Department or in an Institution or Industry. Project report shall be valued for 70 marks.

I SEMESTER

OC H 401: INORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To understand the concept of ionic and covalent bond
2. To enable the students to grasp the chemistry of compounds of main group elements
3. To study the phenomenon of precipitation and complexometric titration

Course Outcomes:

CO1: Understanding the structure of ionic and covalent compounds and study of their properties

CO2: Knowledge on industrial and commercial applications of compounds of main group elements.

CO3: Use of organic precipitants and extraction techniques, masking and de-masking techniques, statistical treatment of errors

UNIT-I **15 Hrs**

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices - NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: Valence bond theory, resonance, hybridization, Bent's rules and energetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

UNIT-II **15 Hrs**

Compounds of Main Group elements

Higher Boranes - Classification, structures, types of bonding and M.O. description of bonding, framework electron counting, Wade's rules, carboranes and metallocarboranes, borazines and boron nitride

Graphite and intercalation compounds, carbides, silicates, zeolites.

Phosphazene polymers, P-O and P-S cage compounds, binary sulphur nitrides - S_4N_4, S_2N_2 and $(SN)_x$

Psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides.

UNIT-III **15 Hrs**

Precipitation phenomena: Precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Complexometric titrations: Titration curves with EDTA, feasibility of EDTA titrations, indicators for complexometric titrations, selective masking and de-masking techniques, industrial applications of masking.

Sampling techniques: Preparation of samples for analysis. Nature of errors, statistical treatment of errors, the student t-test and F-test, significant figures, rejection of data.

References:

1. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, 4th Edn., Pearson Education, 2013.
2. Inorganic Chemistry: Shriver, Atkins and Langford, 5th Edn., OUP, 2010.
3. Concise Inorganic Chemistry: J. D. Lee, 5th Edn., Blackwell Science, 2014.
4. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3rd Edn., Wiley, 2007.
5. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2nd Edn., Pearson Prentice Hall, 2005.
6. Inorganic Chemistry – A Unified Approach: W. W. Porterfield, Elsevier, 2nd Edn., 2005.
7. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th Edn., Wiley, 2014.
8. Quantitative Analysis: R. A. Day and A. L. Underwood, 6th Edn., Prentice Hall, 2012.
9. Analytical Chemistry: Dhruba Charan Dash, 1st Edn., PHI Learning Private Limited, 2011.
10. Basic Concepts of Analytical Chemistry: S. M. Khopkar, 3rd Edn., New Age International, 2008.

OC H 402: ORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To enable the students to understand concept of aromaticity and theory of bonding in organic molecules
2. To understand the methods of determining reaction mechanism and concept of reaction intermediates
3. To explicate the principles of stereochemistry of organic molecules

Course Outcomes:

CO1: Bonding in organic molecules, aromatic & non aromatic compounds, addition compounds, effect bonding on properties of acids and bases

CO2: Study of reaction mechanism and intermediates, carbocations, carbanions, free radicals and nitrenes

CO3: Stereochemistry of compounds and their properties – involving C-C, C-S, C-N and C-P bonds

UNIT–I **15 Hrs**

Bonding in organic systems: Theories of bonding-Molecular orbital theory. Electronic effects: Resonance, hyper-conjugation and tautomerism. Huckel molecular orbital theory. Frost circle and its application to simple π systems- ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, heptatrienyl systems.

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes & hetero-annulenes.

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules.

Weak chemical forces: Dipole-dipole, Induced dipole, vander Waals and hydrogen bonding. Solubility and solute-solvent interactions.

Structure and reactivity: Effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

UNIT-II **15 Hrs**

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods**,** Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects.

Reaction Intermediates: Detection, trapping, reactions and synthetic applications of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes .

A**liphatic Nucleophilic Substitution Reactions**: Mechanism and scope of aliphatic nucleophilic substitution reactions-SN1, SN2 and SNi. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions.

UNIT-III **15 Hrs**

Stereochemistry

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations. Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers.

References:

1. Organic Reactions and Their Mechanisms: P. S. Kalsi, New Age, New Delhi, 1996.
2. Advanced Organic Chemistry: J. March, 4th Ed., Wiley, NY, 2000.
3. Organic Reaction Mechanisms: R. K. Bansal, Tata McGraw Hill, New Delhi, 1978.
4. Organic Chemistry-Vol. I & II: Mukherji, Singh and Kapoor, Wiley Eastern, New Delhi, 1985.
5. Mechanism and Theory in Organic Chemistry: Lowry and Richardson Harper and Row, 1987.
6. Reaction Mechanisms in Organic Chemistry: Mukherji, Singh and Kapoor, McMillan, 1978.
7. Organic Chemistry: P. Y. Bruice, Pearson Education, New Delhi, 2002.
8. Organic Reaction Mechanism: R. K. Bansal, Wiley Eastern Limited, New Delhi, 1993.
9. A Guide Book to Mechanism in Organic Chemistry: Petersykes. Advanced Organic Chemistry: Carey and Sundberg, Part A & B, 3rd edition, Plenum Press, New York, 1990.
10. An Introduction to the Chemistry of Heterocyclic Compounds: Acheson, Wiley – Eastern, 1987.
11. Heterocyclic Chemistry: J. Joule & G. Smith, Van-Nostrand, ELBS, 1978.
12. Organic Chemistry: I. L. Finar, ELBS Longmann, Vol. I, 1984. Advanced General Organic Chemistry: S. K. Ghosh, Book and Alleied (P) Ltd., 1998.

OC H 403: PHYSICAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To explicate the principle and applications of chemical thermodynamics
2. To study the rate of composite reaction and to understand the factors affecting on reaction rate
3. To understand the theory and applications of quantum chemistry

Course Outcomes:

CO1: Concept of entropy, laws of Thermodynamics, Chemical potential and fugacity of molecules

CO2: Study of chain reactions, composite reactions, autocatalytic reactions and reactions in solutions including fast reactions

CO3: Role of quantum Chemistry in understanding properties of molecules

UNIT-I **15 Hrs**

Chemical Thermodynamics

Combined form of first and second law of thermodynamics, Maxwell's relations and significance. Thermodynamic equations of state. Gibbs – Helmholtz equation and its applications. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.

Nernst heat theorem: Its consequences and applications. Third law of thermodynamics – statements, applications.

Partial molar properties: Physical significance, determination of partial molar volume.

Chemical potential: Variation of chemical potential with temperature. Thermodynamic functions of mixing, Gibbs – Duhem equation, Gibbs – Duhem – Margules equation.

Thermodynamics of real gases

Concept of activity, choice of standard states, variation of activity and activity coefficient of a gas with pressure and temperature, activity of solids and liquids, concept of fugacity, variation of fugacity with pressure and temperature, fugacity of solids and liquids, fugacity of a gas in mixture of real gases, determination of fugacity of gas in a mixture

UNIT- II **15 Hrs**

Chemical Kinetics

Composite reactions: An overview of basic kinetic concepts and analysis of kinetic results - rates of simple and composite chemical reactions (reversible, parallel and consecutive first order reactions), Chain reactions (hydrogen-halogen reactions with comparison).

Theory of reaction rates- Collision theory of bimolecular reactions and limitations. Introduction to transition state theory.

Potential energy surfaces – Features & construction of them. Theoretical calculation of Ea.

Reactions in solution: Solvent effects on the reaction rates, Factors determining reaction rates in solution, reaction between ions (effect of dielectric constant and ionic strength), substitution and correlation effects- Hammet and Taft equations-linear free energy relations.

Fast reactions-Introduction, Study of fast reactions by-flow, relaxation and spectroscopic methods

UNIT-III **15 Hrs**

Quantum Chemistry

Introduction to Photoelectric and Compton effects, de-Broglie concept, uncertainty principle, operators, matrix representation and commutation relationships, Schroedinger equation, significance and characteristics of wave function, eigen functions and eigen values. Probabilities, normalisation and orthogonality. Postulates of quantum mechanics. Solution of Schroedinger wave equation for exactly solvable problems such as particle in a box (1D and 3D), particle in a ring, harmonic oscillator, rigid rotor and hydrogen atom (separation of r,θ,ϕ equations and their solutions), Angular momenta (commutations, relations, operators).

References:

1. Physical Chemistry: G. M. Barrow, 5th Edn., McGraw Hill, Int. St. 2008.
2. Atkin's Physical Chemistry: Peter Atkins, Julio De Paula, 9th Edn., OUP, 2011.
3. Thermodynamics for Chemists: S. Glasstone, 8th Edn., East-west, 2007.
4. Themodynamics: Rajaram, Kuriocose, 4th Edn., East-West, 2006.
5. Principles of Physical Chemistry: Puri, Sharma, Pathania, 46th Edn., Vishal Publishing, 2013.
6. Advanced Physical Chemistry: Gurudeep Raj, 35th Edn., Goel Publishing, 2009.
7. Chemical Kinetics: K. J. Laidler, 3rd Edn., Pearson Education, 2008.
8. Fundamentals of Chemical Kinetics: M. R. Wright, 1st Edn., Harwood Publishing, 1999.
9. Introductory Quantum Chemistry: A. K. Chandra, 4th Edn.,Tata McGraw Hill, 2009.
10. Quantum Chemistry: Ira N. Levine, 7th Edn., Prentice Hall, 2013.
11. Quantum Chemistry: R. K. Prasad, 4th Edn., New Age International Publications, 2012.
12. Quantum Chemistry: Donald Allan McQuarrie, 5th Edn., University Science Books, 2013.

OC S 404: SPECTROSCOPY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To acquaint the students with the basic concepts of Vibration-rotation & Raman spectroscopy.
2. To study the application of infrared and UV spectroscopy in the structural identification of organic molecules
3. To understand the theory and applications of ^{1}H and ^{13}C NMR spectroscopy

Course Outcomes:

CO1: Knowledge on Basics of Vibration-rotation & Raman spectroscopy

CO2: Knowledge on Electronic spectra of molecules

CO3: Nuclear magnetic applications and study of ^{1}H-NMR, ^{13}C-NMR spectra for identification of organic molecules

UNIT-I **12 Hrs**

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules). An introduction to Resonance Raman Spectroscopy.

UNIT–II **12 Hrs**

Application of infrared spectroscopy in the structural identification study- finger print region groups and functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, alcohols, ethers, phenols, amines and aromatic compounds). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, acids, esters, amides and anhydrides). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvents on vibrational frequencies, overtones, combination bands and Fermi resonance.

UV/Electronic Spectroscopy: Basic principle, Chromophores, auxochromes, Instrumentation and application. Factors affecting the positions of UV bands. Electronic

transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

UNIT-III **12 Hrs**

NMR Spectroscopy-^{1}H NMR: Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift, its measurements and factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nuclear Overhauser Effect. High resolution ^{1}H NMR spectroscopy. Applications of NMR spectroscopy in structure elucidation of organic molecules. Pulse techniques in NMR, two dimensional and solid state NMR. Use of NMR in Medical diagnostics.

^{13}C NMR: Chemical shift & factors affecting it, coupling constants, Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples.

References:

1. Fundamentals of Molecular Spectroscopy: Colin N .Banwell & Elaine M. McCash, 5th Edn., Tata McGraw Hill, 2014.
2. Organic Spectroscopy: W. Kemp, 3rd Edn., Pagrave Publishers, New York, 1991.
3. Introduction to Spectroscopy: Donald L. Pavia, Gary M. Lampman, G. Corge S. Kriz, 5th Edn., Cengage Learning, 2014.
4. Spectrometric Identification of Organic Compounds: Robert M. Silverstein, Francis X. Webster & David J. Kiemle, 8th Edn., Wiley, 2014.
5. Modern spectroscopy: J. Michael Hollas, 4th Edn., John Wiley and sons Ltd., 2004.
6. Spectroscopy of Organic Compounds: P. S. Kalsi, 3rd Edn., New Age, New Delhi, 2000.
7. Organic Structures from Spectra: L. D. Field & S. Sternhell & J. R. Kalman, 5th Edn., Wiley, 2013.

OC S 405: METHODS OF ANALYSIS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To study the principle and application of chromatographic techniques
2. To enable the students to have a sound knowledge on diffraction techniques
3. To explicate the theory and application of thermoanalytical and radiochemical methods of analysis

Course Objectives:

CO1: Chromatographic techniques for separation of components in a reaction mixture

CO2: Structural elucidation of crystals by XRD and Electron Diffraction techniques

CO3: Thermo- analytical methods for identification of samples and radiochemical analysis of samples

UNIT-I **12 Hrs**

Solvent Extraction: Distribution ratio & coefficient, efficiency of extraction, separation factor, methods of extraction – Batch, Continuous, Back, Synergistic methods.

Chromatography: General principle, efficiency of separation, retension time, capacity factor, column efficiency and column resolution, selectivity factor, Plate theory and Rate theory. Classification of Chromatographic techniques.

Thin layer chromatography: Theory and principle. Techniques; one, two- dimensional. Mechanism of separation. Methodology- Factors affecting RF values. Advantages and applications. Efficiency of TL plates, selection of stationary and mobile phases. Qualitative and quantitative analysis.

Gas Chromatography: Principles, columns, detectors - TCD, FID, ECD, GC-MS column efficiency, capacity factors, resolution. Practical aspects of GC.

HPLC: Principles, equipment, columns, detectors, choice of column, materials.

Ion exchange chromatography: Structures of resins, selectivity, capacity of resins, ion exchange equilibria, applications - removal of interfering ions, concentration and recovery of traces, anion and cation separations and application for the separation of lanthanides and actinides

UNIT-II **12 Hrs**

Diffraction Techniques

Introduction, production of X-ray, Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments – diffraction of X-rays by a crystalline powder (Debye-Scherrer and flat plate camera), powder diffractometer. Interpretation of powder patterns (analytical technique). Single crystal technique -: Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences. Crystalline X-ray diffractometer (4 angle), Intensities of diffracted X-rays and structural analysis, X-ray scattering atoms and molecules, Factors affecting X-ray intensities, introduction to Crystal structure analysis.

Electron Diffraction: Introduction, Theory of electron diffraction, Wierl equation and its significance(qualitatively), Elucidation of structure of simple gas molecules. Structure of surfaces - (Low and high Energy Electron Diffraction, Transmission electron microscopy (TEM), SEM.

UNIT-III **12 Hrs**

Thermoanalytical Techniques

Introduction, thermogravimetric analysis (TGA), types of thermogravimetric analysis, principle and method. Automatic thermogravimetric analysis, instrumentation, types of recording thermobalances, sample holders, factors affecting results and applications. Differential thermal analysis (DTA), principle of working, theory and instrumentation. Simultaneous DTA-TGA curves, factors affecting results and applications. Differential scanning calorimetry (DSC), principles, instrumentation and applications. Thermometric titration: introduction, apparatus and applications (Acid-base, precipitation, complexation, redox and non-aqueous titrations).

Radiochemical Methods of Analysis

Introduction, the nature of radioactivity, radiometric units, detection and measurements of radioactivity. Disintegration theory, rate of disintegration. Application in analytical chemistry, isotopic dilution analysis, activation analysis and prompt gamma neutron activation analysis (PGNAA). Radiometric analysis, radiometric titrations and applications

References:

1. Electroanalytical Chemistry: Vassos & Ewing, Wiley, N.Y., 1983
2. Principles of Electroanalytical Methods: Riley & Tomlinson, Wiley, N.Y.,1987.
3. Principles of Instrumental Analysis: Skoog, 7th Edn. Saunders College Pub., 2017
4. Instrumental Methods of Chemical Analysis: B.K. Sharma, 19th Edn., Goel, 2000.
5. Instrumental methods of chemical analysis: H. Kaur,9th Edn., Pragathi, 2013
6. Instrumental methods of chemical analysis: Gurudeep R. Chatwal and Sham K Anand, 5th Edn., Himalaya, 2013.
7. Instrumental Analysis by Skoog,Hollar and Crouch, Cengage Learning, 2012.
8. Instrumental Methods of Analysis: H. H. Williard, L. L. Merrit and J. J. Dean, 7th Edn., 2004.

OC S 406: ENVIRONMENTAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To give awareness on major air pollutants, their effects and methods of control
2. To render knowledge on waste water treatment, water analysis and desalination
3. To introduce toxicity of heavy metals, biochemical effects and major soil pollutants and their control

Course Outcomes:

CO1: Study of air pollution, pollutants and their control and safety measures

CO2: Identification of impurities in waste water and their removal

CO3: Identification of toxic and solid pollutants in environment and their treatment

UNIT-I **12 Hrs**

Environmental Chemistry: Introduction, environmental segments, classification of environmental pollution.

Air Pollution: Introduction, Air pollutants, Primary pollutants – Sources (CO, NOx, HC, SO_2, particulates). Particulates – Sources (Inorganic and organic particulate matters).Effects on: Humans, materials, vegetation and animals. Bhopal gas tragedy. Air quality standards, Sampling, monitoring and analysis: CO by gas chromatography, NOx by Spectrophotometric method using sulphanilamide and NEDA, SO_2 by pararosaniline (PRA), H_2S by colorimetric using ethylene blue, hydrocarbons by chemiluminescence, Control of air pollution: Control of particulate matter and gaseous pollutants.

Safety: Flammable material handling and firefighting equipment, control measures for toxic chemicals, industrial hygiene, safety in laboratories & plant, safety in the transportation & storage of chemicals.

UNIT-II **12 Hrs**

Water, Waste Water Treatment and Analysis: Hydrologic cycle, sources, chemistry of sea water, criteria & standards of water quality- safe drinking water, maximum contamination levels of inorganic & organic chemicals, radiological contaminants, turbidity, microbial contaminants.Water pollution control and management. Drinking water supplies, Trace elements in water. DO, COD, BOD, TOC. Monitoring techniques and methods: Determination of pH, conductance, fluoride, dissolved oxygen by Winkler's method, nitrate/nitrite by diazo coupling, chloride by Mohrs and Volhard's method, and

fluoride by Alizarin Visual method, Water contamination with cyanide, sulfide, sulphate, phosphate and total hardness. Analysis of Arsenic by Atomic absorption spectroscopy (AAS), cadmium and mercury by dithizone method, chromium by diphenyl carbazide method, lead by polarographic method. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis

UNIT-III **12 Hrs**

Soil pollution: Introduction, Origin and nature of soil, Sources of soil pollution Toxic chemicals in the environment: impact of toxic on enzymes, heavy metal pollution. Detergents- pollution aspects, eutrophication. Pesticides and insecticides- pollution of surface water, biochemical effects. Techniques for the analysis of soil - Lime Potentials: Moisture measurement by gravimetric method, pH using calomel glass electrode method, total nitrogen by kjeldhal method, determination of nitrate-nitrogen by Bratton and Marshal method, determination of potassium and sodium by Flame photometry, calcium by EDTA titration ,organic matter by combustion, total sulphur by oxidation as sulphate.

References:

1. Environmental Chemistry: Dr. H. Kaur, New edition, Pragathi prakshan, 2014.
2. Environmental Chemistry: A. K. De, 7th Edn., New Age, 2013
3. Environmental Pollution Monitoring and Control: Khopkar. S. M, New Age, 2013
4. Environmental Chemistry with Green Chemistry: Asim K. Das, 2010
5. A text book of Soil Chemical Analysis: P. R. Hesse, CBS Publishers, 2002
6. Physico chemical examination of water, sewage and industrial effluents: N. Manivasakam, Pragati Prakashan, 2008
7. Chemistry of Water Treatment, S. D. Faust and O.M. Aly, Butterworths, 1983.
8. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
9. Environmental Chemistry, I. Williams, John Wiley, 2001.

OC P 407: INORGANIC CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

1. Qualitative Analysis of mixtures of Inorganic Salts containing 4 metal ions and 2 anions (2 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).
2. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
3. Solvent extraction of Ni(II) and UO_2(II).
4. Preparation of Chrome alum/Chrome red/Lithopone/Mohr's salt
5. Paper chromatographic separation of mixtures of Ag(I), Hg2(II), Pb(II) / Hg(II), Cu(II), Pb(II), BI(II), Cd(II) / Fe(III), Al(III), Cr(III) / Ni(II), Co(II), Mn(II), Zn(II) / Li(I)
6. Spot test analysis

References

1. Vogel's Qualitative Inorganic Analysis: G.Svehla, 7th Edn., Longman, 2001.
2. Advanced Practical Inorganic Chemistry: Gurudeep Raj, 28th Edn., Goel Publishinh House, 2019.
3. Practical Inorganic Chemistry, Shika N Gulati, J L Sharma, Shagun Manocha, CBS Publishers & Distributors, 2017.

OC P 408: ORGANIC CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

Single stage organic preparations

1. Electrophilic substitution reactions–Preparations of p-nitroacetanilide, m-dinitrobenzene, p-nitroaniline, p-bromoaniline and picric acid.
2. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7–hydroxy-4-methyl-coumarin.
3. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
4. Oxidation reactions-Preparation of p-nitrobenzoic acid and adipic acid.
5. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
6. Alkylations–Preparations of nerolin and N-methyl anthranilic acid.
7. Acetylations–Preparations of β-D-glucose penta-acetate and 2-naphthyl acetate.
8. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
9. Condensation reactions–Condensations involving diethylmalonate and ethyl acetoacetate. Aldol condensation and Perkin reactions.
10. Halogenation reactions-Preparation of n-butylbromide & α,β-dibromocinnamic acid.

References

1. Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I & II Singh et al(TMH, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis et al Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss et al (Longman-ELBS, England), 1978.

OC P 409: PHYSICAL CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

(**Any 12 experiments are to be carried out)**

1. (a) Determination of transport number of Cd^{2+} and SO_4^{2-} ions by EMF method.
   (b) Determination of thermodynamic parameters of a cell reaction by EMF method.
2. Determination of pKa values weak acids by potentiometric/pH metric method
3. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate
4. Verification of Nernst equation for Ag^+, $Cu^{2+}$and Zn^{2+} species.
5. Determination of Solubility product and the Instability constant by potentiometric method.
6. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode.
7. Conductometric titrations of displacement and precipitation reactions.
8. Determination of equivalent conductance and dissociation constants of weak acid and base.
9. Determination of solubility of lead iodide at different T & hence molar heat of solution
11. Determination of hydrolysis constant of aniline hydrochloride.
11. Determination of degree of hydrolysis of CH3COONa and NH4Cl by conductivity method.
12. Determination of Critical Micelle concentration by conductometric method.
13. Determination of pH of buffer solutions with a pH meter & evaluation of pKa of acids
14. Verification of Walden`s rule (relation between viscosity of a solution and the electrical conductivity.
15. Study of variation of viscosity of a liquid with temperature
16. Determination of parachor value for CH_2 group and some elements by Surface Tension method,
17. Determination of the composition of a solution by S.T measurement.
18. Determination of the Critical Micelle Concentration by surface tension/spectrophotometric measurements.
19. Determination of the composition of Zinc Ferrocyanide complex by Potentiometric titrations. 20. Determination of Specific and molar refractivity of liquids and paracor value of a species by refractometric method.

References

1. Findlay's Practical Physical Chemistry: B. P. Levitt, 9th Edn., Longman, London, 2012.
2. Experimental Physical Chemistry: Das, Behera, 6th Edn., Tata McGraw Hill, New Delhi, 1983.
3. Advanced Practical Physical Chemistry: 33rd Edn., J. B. Yadav, Krishna Prakashan Media (P) Ltd, 2015.
4. Practical Physical Chemistry: 2nd Edn., B. Vishwanathan, P.S. Raghavan, Viva Books, 2012.
5. Experimental Physical Chemistry: 1st Edn., V.D Athawale, Parul Mathur, New age International, 2012.

II SEMESTER

OC H 451: ADVANCED INORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To enable the students to predict the spectral and structural properties of organic and inorganic molecules
2. To acquaint the students with reduction of oxide ores and reactions in non-aqueous solvents
3. To make the students to learn the advanced properties of 3d, 4d, 5d series elements, f-block elements and metal carbonyls.

Course Outcomes:

CO1: Predictions of spectral and structural properties of organic and inorganic molecules through symmetry elements and symmetry operation

CO2: Knowledge on metallurgical aspects of oxide ores and chemistry of reactions in non-aqueous media

CO3: Exposure to the Chemistry of d- & f- block elements and metal pi acceptor complexes

UNIT- I **15 Hrs**

Symmetry and Group Theory

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

UNIT-II **15 Hrs**

Metallurgy and redox potentials

Methods of reduction of oxide ores, chemical and electrolytic reductions, Ellingham diagram, Specialized techniques for the extraction of metals –Amalgamation,

Hydrometallurgy, Solvent Extraction, Ion exchange chromatography. Reduction potentials, Latimer and Frost diagrams – features and applications.

Reactions in non-aqueous media: Anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

Self Study: Liquid ammonia

UNIT-III **15 Hrs**

Chemistry of Ti subgroup and inner transition elements

Trends in oxidations states, stereochemistry and ionic sizes of metals; comparison of 3d, 4d and 5d series by taking Ti subgroup as an example. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

Metal Pi-acceptor complexes: Metal carbonyls – preparative methods, structure and bonding, reactions. Metal clusters- bi-, tri-, tetra-, penta- and hexanuclear metal clusters, bonding in metal clusters. Zintl ions and Chevrel phases.

References:

1. Symmetry and Spectroscopy of Molecules: K.Veera Reddy, 2nd Edn.,New Age Intl Publishers, 2009
2. Group Theory in Chemistry: M.S. Gopinathan, V. Ramakrishnan, 2nd Edn., Vishal Publishing, 2007
3. Symmetry and Group theory in Chemistry: R Ameta, 1st Edn., New Age, 2013.
4. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, 4th Edn., Pearson Education, 2013.
5. Inorganic Chemistry: Shriver, Atkins and Langford, 5th Edn., OUP, 2010.
6. Concise Inorganic Chemistry: J. D. Lee, 5th Edn., Blackwell Science, 2014.
7. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3rd Edn., Wiley, 2007.
8. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2nd Edn., Pearson Prentice Hall, 2005
9. Inorganic Chemistry – A Unified Approach: W. W. Porterfield, Elsevier, 2nd Edn., 2005.
10. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th Edn., Wiley, 2014.
11. Advanced Inorganic Chemistry: Satya Prakash, G. D. Tuli, S. K. Basu, R. D. Madan, Vol. II, 4th Edn., S. Chand, 2014.
12. Principles of Inorganic Chemistry: B. R. Puri, L. R. Sharma, K. C. Kalia, 31st Edn., Vishal Publishing, 2013.

OC H 452: ADVANCED ORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To enable students with important types substitution and addition reactions
2. To understand the mechanisms of free radical reactions and elimination reactions
3. To introduce students with heterocyclic compounds, their preparation and reactions

Course Outcomes:

CO1: Study of electrophilic and nucleophilic substitution reactions and addition to carbon-carbon, carbon- hetero multiple bonds

CO2: Exposure to free radical substitution reactions, autooxidations and coupling of alkynes, elimination reactions

CO3: Study of heterocyclic compounds with specific reference to the synthesis and reactions. Biologically important heterocycles

UNIT-I **15 Hrs**

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts.

Aromatic Electrophilic and Nucleophilic Substitution Reactions: General Mechanism of aromatic electrophilic substitution reactions, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Mannich reaction. Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- S_NAr, S_N1 & aryne mechanism.

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds.

Addition to Carbon-Hetero Multiple Bonds: Addition of Grignard reagents. Reformasky reaction, aldol condensation, Benzoin condensation, Knoevenagel condensation, Perkin reaction and Wittig reaction.

UNIT-II **15 Hrs**

Free Radical Reactions: Types, mechanisms of free radical substitution reactions & neighboring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead, reactivity of attacking radical and effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsdiecker reactions.

Elimination Reactions: Discussions of E1, E2 and E1cB mechanisms. Orientation during elimination reactions: Saytzeff and Hoffmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium.

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and Xanthate pyrolysis.

UNIT-III **15 Hrs**

Chemistry of Heterocyclic Compounds

Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Three membered heterocycles-structure, reactivity, synthesis and reactions of aziridines, epoxides, episulfides, diaziridines, oxaziranes and diazirines. Five membered simple and fused heterocycles- synthesis & reactions of derivatives of furan, pyrrole & thiophene. Six membered heterocycles- synthesis & reactions of derivatives of pyridine. Fused Heterocycles-Indole, Quinolines, Isoquinolines.

References:

1. Organic Reactions and Their Mechanisms: P. S. Kalsi, New Age, New Delhi, 1996.
2. Advanced Organic Chemistry: J. March, 4th Ed., Wiley, NY, 2000.
3. Organic Reaction Mechanisms: R. K. Bansal, Tata McGraw Hill, New Delhi, 1978.
4. Organic Chemistry-Vol. I & II: Mukherji, Singh and Kapoor, Wiley Eastern, New Delhi, 1985.
5. Mechanism and Theory in Organic Chemistry: Lowry and Richardson Harper and Row, 1987.
6. Reaction Mechanisms in Organic Chemistry: Mukherji, Singh and Kapoor, McMillan, 1978.
7. Organic Chemistry: P. Y. Bruice, Pearson Education, New Delhi, 2002.
8. Organic Reaction Mechanism: R. K. Bansal, Wiley Eastern Limited, New Delhi, 1993.
9. A Guide Book to Mechanism in Organic Chemistry: Petersykes. Advanced Organic Chemistry: Carey and Sundberg, Part A & B, 3rd edition, Plenum Press, New York, 1990.
10. Organic Chemistry: I. L. Finar, ELBS Longmann, Vol. I, 1984. Advanced General Organic Chemistry: S. K. Ghosh, Book and Alleied (P) Ltd., 1998.
11. An Introduction to the Chemistry of Heterocyclic Compounds: Acheson, Wiley – Eastern, 1987.
12. Heterocyclic Chemistry: J. Joule & G. Smith, Van-Nostrand, ELBS, 3rd Edn., 1995.

OC **H 453: ADVANCED PHYSICAL CHEMISTRY**

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To study the significance of partition function, thermodynamics properties in terms of partition function and the irreversible system
2. To understand ion-solvent interaction, different application of electrochemistry
3. To learn approximate methods in quantum chemistry, their application and application of HMO theory of linear conjugated systems and aromatic systems

Course Outcomes:

CO1: Applications of statistical and irreversible thermodynamics for various forces and phenomena

CO2: Knowledge on electrochemistry of solutions, ion-solvent interaction and applications of electrochemistry

CO3: Need for approximate methods for structure-property relationships

Unit -I **15 Hrs**

Statistical Thermodynamics: Micro and macrostates, phase space and ensembles. Concept of distribution - thermodynamic probability and most probable distribution - Maxwell-Boltzmann distribution law. Maxwell-Boltzmann statistics and applications, Bose-Einstein and Fermi-Dirac statistics. Partition functions - definitions and separations, evaluation of translational, rotational, vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Calculations of thermodynamic functions and equilibrium constant in terms of partition functions, entropy of monoatomic gas - Sackur-Tetrode equation.

Irreversible Thermodynamics- Entropy production in chemical reactions. Transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations. Electrokinetic phenomena and thermoelectricity. Irreversible thermodynamics for biological systems and non-linear regime.

UNIT-II **15 Hrs**

Electrochemistry of solutions: Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden`s rule. Debye-Huckel limiting law (DHL), its

modification and verification. Bjerrum theory of ion association, triple ion formation and its significance.

Ion-solvent Interaction: Ion-Solvation- Introduction, evidence for solvation, structural aspects of ion-solvent interaction -Born model and its limitations, structural treatment ion-dipole and ion-quadruple models. Spectroscopic and thermochemical approach to ion-solvent interaction. Solvation number – Introduction, methods of determination.

Ionic liquids-Introduction, models of simple ionic liquids, mixtures of simple ionic liquids. Electronic conductance of alkali metals dissolved in alkali halides.

Analytical Applications of Electrochemistry: Principles and Applications of Polarography, Cyclic voltammetry, Coulometry and Amperometry.

UNIT-III **15 Hrs**

Quantum Chemistry-II

Need of approximate methods in quantum chemistry. Approximate methods of solving Schroedinger equation for problems of chemical interest - variation and perturbation methods. Application of variation method to H & He atoms, the structure of many electron systems/atoms (secular equations & determinants), Spin-orbit interaction, antisymmetry and Pauli exclusion principle.

Conjugated and aromatic molecules: Huckel molecular orbital (HMO) theory of linear conjugated systems (ethene, allyl & butadiene systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, bond order & charge density. An introduction to Extended Huckel Theory and its simple applications (as a means to explain modern theoretical methods: Semi empirical and ab initio SCF methods).

References:

1. Physical Chemistry: G. M. Barrow, 5th Edn., McGraw Hill, Int. St. 2008.
2. Atkin's Physical Chemistry: Peter Atkins, Julio De Paula, 11th Edn., OUP, 2018.
3. Thermodynamics for Chemists: S. Glasstone, 8th Edn., East-west, 2007.
4. Thermodynamics for Chemists: Kuriocose and Rajaraman, 4th Edn., East-West, 2006.
5. Principles of Physical Chemistry: Puri, Sharma, Pathania, 46th Edn., Vishal Publishing, 2013.
6. Advanced Physical Chemistry: Gurudeep Raj, 35th Edn., Goel Publishing, 2009.
7. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.
8. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014
9. Modern Electrochemistry (Vol.1, 2A &2B): Bockris and Reddy, 2nd Edn., Plenum, New York, 1998.
10. Introductory Quantum Chemistry: A. K. Chandra, 4th Edn., Tata McGraw Hill, 2009.
11. Quantum Chemistry: Ira N. Levine, 7th Edn., Prentice Hall, 2013.
12. Quantum Chemistry: R. K. Prasad, 4th Edn., New Age International Publications, 2012.
13. Quantum Chemistry: Donald Allan McQuarrie, 5th Edn., University Science Books, 2013.

OC S 454: SPECTROSCOPY AND ANALYTICAL TECHNIQUES

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To interpret ESR spectrum of simple inorganic and organic free radicals and inorganic complexes and to apply NQR and Mössbauer Spectroscopy to study different compounds
2. To learn the principle, instrumentation and application of atomic absorption and emission spectrometer, molecular luminescence and nephelo & turbidometers
3. To know the basic principle of mass spectrometry and application of mass spectroscopic techniques in structural elucidation of organic molecules

Course Outcomes:

CO1: Structural elucidation of species containing unpaired electrons by ESR. Study of NQR, Mossbauer and photoelectron spectroscopic techniques and their applications

CO2: A to gain knowledge on Atomic Absorption Spectrometry, Emission Spectroscopy, Molecular Luminescence Spectroscopy and Light-Scattering methods for detection of metals, particles and particle size

CO3: Use of mass spectrometry in identification of organic compounds. Case studies of structural elucidations employing UV, IR, NMR and Mass spectral data of compounds

UNIT- I **12 Hrs**

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

Mössbauer Spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

Photoelectron spectroscopy: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications.

UNIT – II **12 Hrs**

Atomic Absorption Spectrometry: Principle, Theory, working of AAS instruments, analytical applications, interferences.

Emission Spectroscopy: Flame Emission Spectroscopy, plasma emission spectrometry, basic principles of flame photometry, evaluation methods in flame photometry, interferences.

Molecular Luminescence Spectroscopy: Theory of fluorescence and phosphorescence, instruments, flourescence and structure, fluorescence quenching, fluorimetry in quantitative analysis, phosphorescence method, applications in quantitative analysis.

Light-Scattering methods: Nephelometry and turbidimetry- theory, effects of concentration, particle size and wavelength on scattering, instrumentation and applications.

UNIT-III **12 Hrs**

Mass Spectrometry

Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy.

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules.

References:

1. H. Wlliard, L. L. Merrit and J. J. Dean, Instrumental methods of analysis,(7th Ed.) 1988.
2. B. K. Sharma, Instrumental Methods of Chemical Analysis (Goel publishing), 2000.
3. Skoog, Holler and Nieman: Principles of Instrumental Analysis, (Harcourt Afca), 2001.
4. Organic Spectroscopy-3rd Ed.-W.Kemp (Pagrave Publishers, New York), 1991.
5. Introduction to spectroscopy (3rd Ed)- Donald L. Pavia, Gary M. Lampman, G Corge S. Kriz, Thomson learning (Inc -2001, United states), Singapore.
6. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnil (Wiley) 1981.
7. Modern spectroscopy (4th Ed.) – J. Michael Hollas, John Wiley and sons Ltd. Chichester, West susex, England-2004.
8. Spectroscopy of Organic Compounds-3rd Ed.-P. S. Kalsi (New Age, New Delhi) 2000.
9. D. N. Satyanarayana: Electronic Absorption Spectroscopy and Related Techniques,
10. G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall, 2001

OC S 455: CHEMISTRY OF BIOMOLECULES

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn comparison of cell structures, structure and functions of lipids, and function and role of lipoproteins
2. To study properties of amino acids, their synthesis, structure and reaction of nucleic acids, use of enzymes in organic synthesis
3. To understand chemistry of important derivatives of monosaccharides and general methods of structural degradation of polysaccharides

Course Outcomes:

CO1: Knowledge on cell structures, structure and functions of lipids and function and role of lipoproteins

CO2: Studies on role of amino acids, proteins, nucleic acids and enzymes in biological processes

CO3: Study of monosaccharide's, di, tri and tetra saccharides, polysaccharide s and their functions and degradations

UNIT-I **12 Hrs**

Amino acids, Nucleic acids and Enzymes

Amino Acids: General structure, classification, specific rotation, distribution in proteins, location in proteins, physical properties, non-standard protein aminoacids and non protein aminoacids. General methods of synthesis of aminoacids with specific examples.

Nucleic acids: Introduction, RNA, DNA, Purines, pyrimidines: synthesis. Nucleosides and nucleotides, structure of nucleosides. Enzymatic hydrolysis of nucleic acids.

Enzymes: Enzymes in organic synthesis, α- Carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols-Transesterification. Enzymatic synthesis of α-amino acids and peptides.

UNIT- II **12 Hrs**

Carbohydrates

Configuration and conformation of monosaccharides, Chemistry of important derivatives of monosaccharides-ethers, esters, acetals, ketals, deoxysugars, aminosugars, Structure of disaccharides-maltose, cellobiose and sucrose. Structure of tri and tetrasaccharides.

General methods of structural degradation of polysaccharides-methylation, partial hydrolysis, periodate oxidation, Smith degradation and alkaline degradation techniques. Structures of cellulose, chitin, starch (amylose and amylopectin), glycogen, heparin and chondroitin. Hemicelluloses. Regenerated cellulose and cellulose derivatives.

UNIT-III **12 Hrs**

Biophysical Chemistry

Electrophoresis - Principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electro-osmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. "Salting In" and "Salting Out" of proteins. Effect of temperature and *p*H on the viscosity of bio-molecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension.

References:

1. Lehninger's Principles of Biochemistry, David L. Nelson, Michael Cox, W H Freemann · 2017
2. Harper, Harper's Illustrated Biochemistry, David Bender, Kathleen M. Botham, Peter J. Kennelly 29th Edition, 2012
3. Bioorganic Chemistry. H. Dugas, C. Penney., Springer New York, 2013
4. Fundamentals of Biochemistry, J. L. Jain, S. Chand & Company Ltd. 2004
5. Amino acids and Peptides- G. C. barret and D T Elmore (Cambridge university press),1998.
6. The Carbohydrates Vol. IA I B IIA and IIB – W. Pigman and D. Horton (Academic Press), 1970.
7. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York),1990.
8. Biophysical Chemistry- Principle and Technique – A. Upadhyay, K. Upadhyay and N.Nath, Himalaya Publishing House, Bombay, 2009.
9. Essentials of Physical Chemistry and Pharmacy – H. J. Arnikar, S. S. Kadam, K.N. Gujan, Orient Longman, Bombay, 1992.

Open Elective papers

CH E 456: COLOUR CHEMISTRY: APPLICATIONS IN DAILY LIFE

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To learn different dyeing techniques and dyes used in textile industry

LO2: To understand the role of pigments in surface coatings

LO3: To acquire the knowledge of colourants in cosmetics and other materials

Course Outcomes:

CO1: Will be able explain to the relation between colour and chemical constitution

CO2: Will realize the importance and technological application of pigments

CO3: Will be able to understand role of colourants in cosmetics and other materials

UNIT-I 12 Hrs

Synthetic Dyes

Introduction to Dyes: Definition of Dye or Dyestuff, Requisites of a True Dye, Historical development from natural to synthetic dyes, Important dyestuff intermediates.

Classification of Dyes based on application: Introduction, Direct dyes, Acid dyes, Basic dyes, Developed dyes, Mordant dyes, Vat dyes, Sulphur dyes, Disperse dyes, Reactive dyes Classification of Dyes based on Chemical Structure: Nitroso dyes, Nitro dyes, Azo dyes, Diphenylmethane dyes, Triphenylmethane dyes, Xanthene dyes, Heterocyclic Dyes.

Colour& its Chemical Constitution: Bathochromic &Hypsochromic Effect, Definition and concept of colour, Relationship between colour& chemical constitution, Witt's theory, Armstrong's theory, modern theories of colour& constitution. Introduction to Optical brighteners.

UNIT-II12 Hrs

Paints and Pigments

Definitions of pigment, extenders. Practical difference between dyes & pigments, Classification of pigments: White pigments (white lead, ZnO, lithopone, titanium dioxide), coloured pigments (Blue, red, yellow and green pigments), effect pigments, metal effect pigments, pearl luster pigments. General Chemical and Physical Properties & Applications. Paints and distempers: Requirements of a good paint, Emulsion, Latex,

Luminescent paints, Fire retardant paints, Varnishes, Enamels, Lacquers, Solvents and Thinners.

UNIT-III 12 Hrs

Colourants in Cosmetics and High Technology

Cosmetics: Introduction, Colourants for decorative cosmetics, Formulations and manufacturing of cream and lotions, lipstick and nail polish, shampoos, hair dyes and tooth pastes.

High technology colourants: Colour in Electronic Displays, Solar Energy Conversion and Optical Data Storage, Photographic Colour Chemicals, Digital Printing, Chromic Materials, colourants in plastics, ceramics and glass.

References:

1. Synthetic dyes: Gurdeep R. Chatwal, Himalaya Publishing House, 2009.
2. The chemistry of synthetic dyes: – Vol. V- Venkataraman, 1999
3. Colour chemistry, Robert M Christie, 2nd edition, 2015.
4. Chromic Phenomena: Technological Applications of Colour Chemistry, P. Bamfield and M. G. Hutchings, 2nd edition, RSC publishing, 2010.

CH E 457: ENVIRONMENTAL CHEMISTRY FOR SUSTAINABLE FUTURE

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: Detail studies on air, water and soil pollution.

LO2: Identification of toxic and solid pollutants in environment

LO3: Studies on impact of pesticides on human and ecosystem.

Course Outcomes:

CO1: Able to create an awareness on environmental pollutants.

CO2: Will be able to understand the importance of the environment.

CO3: Knowledge about Chemical toxicology.

UNIT-I **12 Hrs**

Air pollution

Composition of atmosphere, chemical and photochemical reactions in atmosphere, atmospheric stability, Qualitative study of environmental segments, Classifications of air pollutants, sources, sinks of atmospheric gases, control and effects of oxides of nitrogen, Oxides of sulphur, Carbon monoxide and Hydrocarbon pollutants. Greenhouse gases, acid rain, Ozone hole & CFC's, global warming, Photochemical smog & PAN. Bhopal gas tragedy, TCDD Accident at Italy.

UNIT-II **12 Hrs**

Water pollution

Water resources, Stages of hydrological cycle, Classifications of water pollutants and their effects- inorganic pollutants, toxic metals, organic pollutants, sewage and domestic waste its effects, sediments, synthetic detergents (Anionic surfactants, cationic surfactants, Non-ionic surfactants, builder, additive) and its effects, oxygen demanding wastes (DO, BOD, COD), Disease causing agents, Radioactive pollutants and its effects, plant nutrients-Eutrophication, types of Eutrophication, Thermal pollutants in water and its effects, Biological pollutants in water.

UNIT-III **12 Hrs**

Soil pollution and Chemical toxicology

Sources of soil pollution- By industrial waste, Urban waste, Radioactive pollutants, agriculture practices, metallic pollutants, biological agents, Mining activities, Municipal garbage, Soil sediments as pollutants and its effects. Pesticides pollutants- Classification, examples of pesticides. Effects on Man, animal, birds, aquatic biota, soil. Some pesticides accidents, Biochemical effects of Cadmium, Lead, Tetraethyl lead,Arsenic,mercury, Ozone and Pan, Cyanide and pesticides.

References:

1. Environmental Chemistry: A. K. De, 7th Edn., New Age, 2013
2. Environmental Chemsitry: H.Kaur, PragathiPrakashan 10thEdn 2016.
3. Environmental Chemistry with Green Chemsitry : Asim K Das,Books and Allied (P) Ltd.reprint 2015.
4. Environmental Chemistry, S. K. Banerji, Prentice Hall India, 1993.
5. Environmental Chemistry, I. Williams, John Wiley, 2001.
6. Environmental Chemistry (Green Chemistry and pollutants in eco system): Eric Lichtfouse, Jan Schwarzbauer, Didier Robert, Sprizer, 2005.

CH E 458: CHEMISTRY IN THE COMMUNITY

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To have a brief knowledge on water, food and conservation of chemical resources

LO2: To understand the concept of personal chemistry and atmospheric chemistry

LO3: To learn concepts of pesticide chemistry

Course Outcomes:

CO1: Awareness on quality of water, food and conservation of chemical resources

CO2: Knowledge on Human body's internal chemistry and atmospheric chemistry

CO3: Understanding role of fertilizer, insecticides and pesticides.

UNIT-I **12 Hrs**

Water: Quality of water, contaminants, purification and treatment; natural and municipal water purification.

Conserving Chemical resources: Use of resources, Conservation in nature and the community, metals; sources and replacement. Petroleum; separation, refining, as energy source, alternative energy sources

Understanding food: Food as energy and builder molecules. Vitamins and minerals in food, food additives, food preservatives, Artificial sweeteners, Artificial food colourants

UNIT-II **12 Hrs**

Personal Chemistry and choices

Human body's internal chemistry: Balance and Order, Elements in the Human Body, Cellular Chemistry, Enzymes. Acids, Bases and Body Chemistry, Chemistry at the Body's Surface: skin and hair, Drugs and Toxins in the Human Body

Chemistry and the atmosphere: Air, Atmosphere, Atmospheric Altitude, Air Pressure, Earth's Energy Balance, air pollution, smog, acid rain, pollution control and prevention

Personal choices and risk assessment:

UNIT-III **12 Hrs**

Pesticide Chemistry

Pesticides-General aspects and classification, Inorganic pesticides, Organic pesticides,

Insecticides- Arsenic compounds, chlorinated hydrocarbons, carbamates, organophosphorus compounds,

Fungicides-characteristics, classification, uses and impact on environment

Herbicides-Classification, mechanism of degradation and impact on environment

Alternative to chemical pesticides, biological control of pests, third and fourth generation of pest controller, integrated pest management, toxicology of pesticides.

References:

1. ChemCom- Chemistry in the community, Conrad L., Stanitski, 3rdEdn., Kendall/Hunt Publishing Company, 1998.
2. Environmental chemistry with Green chemistry, Asim K Das, Books and Allied (P) Ltd.
3. Environmental Chemistry: Dr. H. Kaur, New edition, Pragathiprakshan, 2014.
4. Environmental Chemistry: A. K. De, 7thEdn., New Age, 2013
5. The chemistry of food, Jan Velisek, Wiley Blackwell, 2013
6. Pesticide Chemistry- Crop Protection, Public health, Environmental safety, hideoOhkawa, Hisashi Miyagawa, Philip W Lee, Wiley-VCH Verlag GmgH& Co. KGaA, 2007
7. Pesticide Chemistry, GyMatolcsy, M Nadasy, V Andriska, Elsevier, 1988

OC P 459: INORGANIC CHEMISTRY PRACTICALS – II

Teaching Hours: 4 Hrs per week

1. Complexometric determination of Mn, Ca, Mg, Cu, Ni and Fe-Cr mixture
2. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using $Ce^{4+.}$
3. Analysis of Dolomite - insoluble residue by gravimetry and Ca, Mg by complexometry.
4. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
5. Analysis of solder - Pb and Sn by EDTA method.
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
10. Nephelometric determination of sulphate/phosphate.
11. Computer related practicals - Statistical analysis of data, determination of λ_{max}.

Reference:

1. Vogel's Text Book of Quantitative Chemical Analysis (5^{th} Ed), G. H. Jeffrey, J. Bassette, J.Mendham and R.C.Denny, Longman, 1999.
2. Advanced Practical Inorganic Chemistry: Gurudeep Raj, 28^{th} Edn., Goel Publishinh House, 2019.
3. Practical Inorganic Chemistry, Shika N Gulati, J L Sharma, Shagun Manocha, CBS Publishers & Distributors, 2017.

OC **P 460: ORGANIC CHEMISTRY PRACTICALS – II**

Teaching Hours: 4 Hrs per week

Separation and systematic qualitative analysis of binary mixtures of organic compounds.

References:

1. Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I & II Singh et al(TMH, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis et al Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss et al (Longman-ELBS, England), 1978.

OC P 461: PHYSICAL CHEMISTRY PRACTICALS – II

Teaching Hours: 4 Hrs per week

At least 12 experiments are to be carried out

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
2. Determination of degree of dissociation, Vant Hoff factor and molecular weight of an electrolyte by cryoscopy method using copper calorimeter/Dewar flask..
3. Heat of solution of a sparingly soluble compound in water by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Phase diagram of three component system (a) 3 liquids with single binodal curve, and b) two liquids and one solid
6. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of (a) order and rate constant and (b) Energy of activation.
7. Determination of a) Energy of activation & b) rate constant for the First and second order kinetics of reaction between potassium persulphate and potassium iodide.
8. Kinetics of sodium formate – iodine reaction.
9. Determination of the latent heat of evaporation of carbon tetrachloride.
10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
12. To study the adsorption of iodine on charcoal from alcoholic solution.
13. To study the effects of gelatin solution on the precipitation values.
14. Comparison of detergent action of detergents and determination of interfacial tension.
15. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene.
16. Study of association of benzoic acid in benzene/toluene.

Any other relevant experiments of interest.

Computer related Practicals

1. Use of Chem draw and Chem sketch for construction of molecules.
2. Use of Window excel for drawing graphs estimation of slope intercept.
3. Use of commercial software packages such as Mathcad, Matlab, Aspan Plus, Design II,

References:

1. Findlay's Practical Physical Chemistry: B. P. Levitt, 9th Edn., Longman, London, 2012.
2. Experimental Physical Chemistry: Das, Behera, 6th Edn., Tata McGraw Hill, New Delhi, 1983.
3. Advanced Practical Physical Chemistry: 33rd Edn., J. B. Yadav, Krishna Prakashan Media (P) Ltd, 2015.
4. Practical Physical Chemistry: 2nd Edn., B. Vishwanathan, P.S. Raghavan, Viva Books, 2012.
5. Experimental Physical Chemistry: 1st Edn., V.D Athawale, Parul Mathur, New age International, 2012.

III SEMESTER

OC H 501: ORGANIC REACTION MECHANISMS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn different name reactions in organic chemistry and synthetic applications of these name reactions in synthetic chemistry.
2. To learn the classification of molecular rearrangements and learnt different types of reaction mechanisms
3. To know advance name reactions and to have knowledge on the synthetic application of these name reactions

Course Outcomes:

CO1: Sound knowledge on mechanism and applications of name reactions which are being used continuously in synthetic chemistry.

CO2: Study of mechanistic treatment of nucleophilic, electrophilic, free radical rearrangements

CO3: Use of advanced name reactions in the synthesis of variety of chemical products

Unit-I **15 Hrs**

Organic Name Reactions-I: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction, Chichibabin reaction, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith Cyclopropronation reaction, Stork Enamine reactions, Bayil-Hillman reaction, Swern oxidation, Oppenauer oxidation, Yamada reaction, Suzuki coupling, Heck reaction, Bucherer reaction, Yamada reaction, and Mitsunobu reaction.

Unit-II **15 Hrs**

Molecular rearrangements and their synthetic applications:

Unifying principles and mechanisms of rearrangements taking place at an electron deficient and electron rich substrates. **Rearrangements taking place at carbon**: Wagner Meerwein, benzil-benzilic acid, Pinacol and semipinacol, Tiffeneau Demjanov, dienone phenol, Favorskii, Stevens, Wolff, Baker-Venkatraman, Payne rearrangement.

Rearrangements at nitrogen: Hofmann, Curtius, Lossen, Schmidt, Beckmann, Neber, rearrangement.

Rearrangements at oxygen: Baeyer-Villiger, Criegee, rearrangements. **Aromatic rearrangements:** Benzidine, Von Richter, Sommelet-Hauser, Smile's rearrangments

Unit-III **15 Hrs**

Named reaction for Organic Transformation: Alagar-Flynn-Oyamada reaction, Eschweiler-Clarke reaction, Barbier coupling reaction, Pschorr cyclization reaction, Blaise reaction, Dakin reaction, Barton-olefin synthesis, Corey-Kim reaction, Corey-Winter olefin synthesis, Fleming-Kumada oxidation, Houben-Hoesch reaction,, Nef reaction, Shapiro reaction, Staudinger reaction, Wacker-Tsuji oxidation, Leuckart-Wallach Reaction

References:

1. Advanced organic chemistry (structure and mechanism) by Ashitosh Kar , Medtect publications, 2017
2. Advanced Organic Chemistry-Part A & B: Francis A Carey and R. J. Sundberg, 5th Edn., Springer, 2007.
3. Organic Reactions Mechanisms: P. S. Kalsi and R. K. Parashar, Narosa Publishing House, 2011.
4. Synthetic Organic Chemistry: G. R. Chatwal, Himalaya Publishing House, Bombay, 2016.
5. Organic Chemistry, Vol. I-II: I. L. Finar, Longmann ELBS, London, 2000.
6. Advanced Organic Chemistry-Reaction Mechanisms: Reinhard Bruckner, Academic, 2005.
7. Organic Synthesis: Jagadamba Singh and L. D. S. Yadav, Pragathi Prakashan, 2014.
8. Reactions, Rearrangements and Reagents: S. N. Sanyal, 4th Edn., Bharati Bhawan (P&D), 2013.
9. Name Reactions for Functional Group Transformations: Jie Jack Li and E. J. Corey, Wiley-Interscience, 2007.
10. Organic synthesis Based on Name Reactions: A. Hassner and I. N. N. Namboothiri, 3rd Edn., Elsevier, 2012.
11. Name Reactions- A Collection of Detailed Reaction Mechanism: Jie Jack Li, 3rd Edn., Springer, 2006.
12. Name Reaction and Reagents in Organic Synthesis: Bradlfold P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Jr, John Wiley and sons, Inc., Hoboken, New Jersy, 2005.

OC H 502: ORGANIC SYNTHETIC METHODS AND REAGENTS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn concepts of oxidation reactions and reagent used for oxidation. To learn halogenation reactions
2. To understand catalytic hydrogenation, metal reductions and safety measures to be taken during the chemical reactions
3. To learn about activating groups, protecting groups and miscellaneous reagents and their usage in synthetic chemistry.

Course Outcomes:

CO1: Learning the concepts of oxidation reactions, reagent used for oxidation and halogenation reactions

CO2: Understanding catalytic hydrogenation, metal reductions and safety measures to be taken during the chemical reactions

CO3: Knowledge on activating groups, protecting groups and miscellaneous reagents and their usage in synthetic chemistry.

Unit-I **15 Hrs**

Oxidation Reactions: Introduction and different oxidative processes, Mechanism of oxidation reaction with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide, Dessmartin periodate and their synthetic importance in functional group transformation.

Halogenation: Halogenation of olefins, carbonyl compounds, Benzylic and Allylic halogenation, Dehalogenation reactions, dehydrogenation with S, Se, Pt, Pd, Ni.

Unit-II **15 Hrs**

Reduction Reactions and Safety measurements (MSDS)

Catalytic hydrogenation: Introduction, catalysts and solvents employed, reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis, and homogeneous catalytic hydrogenation. **Metal hydride reduction:** Reduction with $LiAlH_4$ & $NaBH_4$, Stereo chemistry of reduction & other functional groups, Functional group transformation during reduction, Reduction with diborane and related reactions.

Dissolving Metal Reductions: Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, Reduction with hydrazine, and its derivative, Wolf-Kishner reduction and related reactions, Reduction with arene sulphonyl derivative of hydrazine, Reaction with diimide and related compounds.

Unit-III : **15 Hrs**

Activating, Protecting and Miscellaneous Reagents

Carboxylic acid activating groups: DCC, EDC, HATU, HBTU, TBTU, CDI, BOP, T3P.

Protection of NH Groups: Acetic anhydride, Benzylchloride, Benzylchloroformate, Boc-anhydride and F-moc.

Protection of Carboxyl group: Alkyl esters, t-Butyl esters, Benzyl esters, Silyl esters, Oxazolines and Oerthoesters.

Protection of Hydroxyl (OH) and diols: as methylether, methoxymethyl ether, benzyloxymethyl ether, t-butylether. Protection using 3,4-Dihydro-2H-pyran, P-toluene sulphonyl chloride and Trialkyl chlorosilane. **Protection of 1,2 and 1,3-diols**: as acetals and ketals, as cyclic carbonates.

Protection of Aldehydes and Ketones: Using ethane and propane dithiols, Ethylene glycol. **Protection of double bonds and triple bonds.**

Miscellaneous Reagents: Lawesson reagent, DMF-DMA, Sodamide, NBS and Diazomethane.

References:

1. Reactions, Rearrangements and Reagents: S. N. Sanyal, 4th Edn., Bharati Bhawan (P&D), 2013.
2. Advanced Organic Chemistry-Part A & B: F. A. Carrey & R. J. Sundberg, 4th Edn., Springer, 2007
3. Modern Organic Reactions: H. O. House, W. A. Benjamin, 1972.
4. Organic Synthesis: R. E. Ireland, Prentice Hall India, 1969.
5. Art in Organic Synthesis: Anand, Bindra & Ranganathan, Wiley, 1970.
6. Modern Methods of Organic Synthesis: N. Carruthers and I. Coldham, Cambridge University, 2004.
7. Modern Reduction Methods: P. G. Anderson and I. J. Munslow, Wiley-VCH, 2008.
8. Protecting groups in Organic synthesis: T. W. Greene and P. G. M. Wuts, 3rd Edn., Willey, 1999..
9. Organic Synthesis: J. Singh and L. D. S. Yadav, 10th Edn., Pragathi Prakashan, 2014.
10. Modern organic Synthesis: An Introduction: G. S. Zweifel and M. H. Nantz, W. H. Freemen & Co. NY, 2006.
13. Advanced Organic Synthesis-Methods and Techniques: Richard S. Monson, Rhadon Academic Press, NY & London, 2012.

OC H 503: ORGANOMETALLIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To understand catalysis by organometallic compounds and application of reagents in various chemical reactions
2. To learn synthetic utility of various organometallic reagents like organolithium organosilicon, tin and boron compounds.
3. To study the mechanism of reaction in the presence of synthetic reagents and the synthetic utility of the reagents.

Course Outcomes:

CO1: Understand catalysis by organometallic compounds and application of reagents in various chemical reactions

CO2: Importance of synthetic utility of various organometallic reagents like organolithium, organosilicon, tin and boron compounds

CO3: Utilization of different types synthetic reagents in variety of chemical reactions.

Unit-I **15 Hrs**

Catalysis by Organometallic Compounds: Catalysis by Organometallic Compounds: 16 and 18-electron rules, oxidative addition,insertion, deinsertion and reductive elimination reactions. Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanationand isomerization of olefins.Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), carbonylation of alcohols- Monsanto acetic acid process.L-DOPA synthesis, alkene oligomerizations, The Reppe reaction.Polymerization of olefins andacetylenes: Ziegler-Natta catalyst systems. Fischer–Tropsch reaction, Water Gas Shift reactions.

Unit- II **15 Hrs**

Reagents in Organic Synthesis-I

Organometallic reagents: Preparation and properties of Organolithium and organo magnesium compounds. Their uses in organic synthesis and in the preparation of Organometallic compounds. Methods of preparation, reactivity and reactions. Properties,

preparations and reactions of Organozinc, Organocadmium and Organomercury compounds and organo indium reagents.

Silicon containing Reagents: Introduction, preparation reactions & stereochemistry, Peterson reaction.

Boron containing reagents: Introduction, preparations, Hydroborations, reactions of Organoboranes- Isomerization, oxidation, protonolysis, carbonylation, cyanidation. Synthesis of esters, E and Z alkenes, conjugated dienes and alkynes.

Organotin Compounds: Synthesis of Organostannanes and their utility in C-C bond forming reactions.

Unit-III **15 Hrs**

Reagents in Organic Synthesis-II

Use of the following reagents in Organic synthesis and functional group transformation- Gillman's reagent. Lithium dimethyl cuprate, Organopalladium reagents, Lithium diisopropyl amide (LDA), Dicyclohexyl carbodiimide (DCC), 1,3-dithiane (reactivity umpolong), Trimethyl silyl iodide, Tri-n-butyl tin hydride, Chloranil, DDQ, Selenium dioxide, Phase transfer catalyst, Baker's yeast, polyphosphoric acid.

References:

1. Organic Synthesis: Jagadamba Singh and L. D. S. Yadav, 10th Edn., Pragathi Prakashan, 2014.
2. Reactions, Rearrangements and Reagents: S. N. Sanyal, 4th Edn., Bharati Bhawan (P&D), 2013.
3. Principles and Applications of Organotransition Metal Chemistry: J. P. Collman, L. S. Hegedus, J. R. Norton and R. G. Finke, University Science Books, 1987.
4. Organometallic Chemistry: R. C. Mehrotra and A. Singh, New Age International, 1999.
5. Organometallic Chemistry of Transition Metals: R. H. Crabtree, Wiley , 1999.
6. Organic Name Reactions and Molecular Rearrangements: Gurudeep Raj, 3rd Edn., Krishna Prakashan Media (P) Ltd., 2011.
7. Advanced organic chemistry Part B : Reactions and synthesis, by Franc A Carey Richard J. Sundberg ,Fifth edition, Springer publications, 2007
8. Modern methods of organic synthesis by William Carruthers and Iain Coldham, Fouth Edition, Cambridge publications, 2017.

OC S 504: CHEMISTRY OF SYNTHETIC DRUGS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To enlighten knowledge on drug design, structure-activity relationship and pharmacokinetics.
2. To understand the classification and structure mode of action of anaesthetics, antibiotics, analgesics, anti-inflammatory and Cardiovascular agents
3. To gain knowledge on CNS depressants, Antihistaminic agents and antimalarials

Course Outcomes:

CO1: Imparting knowledge drug design, structure-activity relationship and pharmacokinetics.

CO2: Studying antibiotic, analgesics and anti-inflammatory agents in daily life

CO3: Absorbing the knowledge of CNS depressants, anticonvulsant, antimalarial drugs

UNIT I **12 Hrs**

Drugs : Introduction.. Drug design and relationship of functional groups to pharmacologic activity- introduction, relationship between molecular structure and biologic activity, selectivity of drug action and drug receptors, biologic targets for drug action, physicochemical properties of drugs, stereochemistry and drug action drug design-discovery and structural modification of lead compounds, physicochemical and biopharmaceutical properties of drug substances, pharmacokinetics- physicochemical factors affecting drug absorption, factors affecting the absorption of drugs from solid dosage forms and suspensions

General anaesthetics : Synthesis of Halothane, & Methohexital sodium. :

Local anaesthetics Synthesis and mode of action of Benzocaine & Procaine Hydrochloride,

UNIT-II **12 Hrs**

Antibiotics: Introduction, classification, mode of action of β-lactum antibiotics. Penicillin-Synthesis of Penicillin V, chemical degradation and bacterial resistance. Cephalosporians- Nomenclature, Classification, β-lactamase resistance. Structure and mode of action of Tetracyclins, Streptomycin and Chloramphenicol.

Analgesics and anti-inflammatory agents: Narcotic and Non-narcotic agents- Introduction and Mechanism of action, Synthesis of Ibuprofen, Acetaminophen, Phenyl butazone

Antihypertensive agents- Introduction, Mechanism of action, Synthesis of hydralazine derivatives.

Hypoglycemic agents- Introduction, Mechanism of action, Synthesis of Tolbutamide.

Anti-amoebic agents: Introduction, Classification and Mechanism of action. Synthesis of Metronidazole, Iodoquinol and Dimercaprol

UNIT-III **12 Hrs**

CNS depressants: Sedative and Hypnotic agents: Introduction, Classification. Synthesis of Barbitone, Methylphenobarbital, Butobarbitone, Pentobarbital, Phenobarbital. Benzodiazepine class: Triazolam, Flurazepam.

Anticonvulsant: Synthesis of Phenytoin sodium, Trimethadione and Carbamazepine

CNS stimulants: Introduction and classification. Synthesis and mechanism of action of Caffeine, Nikethamide, Phetermine, Methylphenidate.

Antihistaminic agents: Mechanism of action, Synthesis of Diphenhydramine HCI, Pyrilamine, Pheniramine

Anti-malarials: Etiology of malaria, Mechanism of action and SAR of Quinolines antimalarials. Synthesis of Chloroquin, Primaquin and Quinacrine

References:

1. Medicinal Chemistry: Ashutosh Kar, 4thEdn., Wiley-Eastern, New Delhi, 2006.
2. Foyes principles of medicinal chemistry 7thEdn: Thomas L Lemke, David A Williams Victorial F Rochem S. Willaim Zito, Lippincott Williams & Wilkins, 2013
3. Medicinal-Chemistry of Anticancer-Drugs: Carmen Avendano& J. C Menedez, Elsevier B.V, 2008.
4. The organic chemistry of drug synthesis Vol. I-VII: Daniel Lednicer, John Wiley & Sons Inc, 2007.
5. Medicinal Chemistry, a Molecular & Biochemical Approach: Thomas Nogrady& Donald F Weaver, 3rdEdn., Oxford University Press, 2005.
6. Advanced Practical Medicinal Chemistry: Ashutosh Kar, New Age International Pvt. Ltd., 2004.
7. Textbook of Organic Medicinal & Pharmaceutical Chemistry: Wilson, Giswold&Doerge 7th Edn., Lippincott Company, 1977.

8. Pharmacology & Pharmacotherapeutics-Part I and II: Satoskar and Bhandarkar 10th Edn., Bombay Popular Prakashan, 1986.
9. Principles of Medicinal Chemistry: Foye: 3rd Edn., Varghese Publishing House, 2008.
10. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi, 1996.
11. Burger's Medicinal Chemistry-Part–I-III: 4th Edn., Wolff, Wiley Eastern, NewYork, 1980.
12. Organic Chemistry-Vol. I and II: I. L. Finar, 6th Edn., Longman-ELBS, London, 2009.
13. Synthesis of Essential Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2006.
14. Synthesis of Best-Seller Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2016

OC S 505: COMPUTATIONAL AND THEORETICAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To enlighten the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction
2. To understand the theory of computational chemistry and computer aided drug design
3. To gain knowledge on learning the principles of computational chemistry and computer-based molecular design

Course Outcomes:

CO1: Conceptual knowledge on theories of quantum chemistry

CO2: Gain knowledge on use of SCF, Ab initio and DFT methods

CO3: Information on computer aided drug design

UNIT-I **12 Hrs**

Introduction: computational chemistry as a tool and its scope.

Potential energy surface: stationary point, transition state or saddle point, local and global minima.

Semiempirical Methods: Extended Huckel Method, Basic principle of SCF semi empirical methods, the Pariser-Parr-Pople Method, the CNDO, INDO and NDDO Method. Applications: Geometries, energies, frequencies and vibrational spectra, dipole moments, charges and bond orders, UV and NMR spectra, Ionization energies and electron affinities

UNIT-II **12 Hrs**

Ab initio theory: Basic principle: Hartree SCF method, Hartree-Fock equations; Basis sets; Post Hartree-Fock calculations: electron correlation, Moller Plesset approach, coupled cluster method

Density Functional Theory: Basic principle, Hohenberg-Kohn theorems, Kohn-Sham approach, exchange functionals, correlation functionals, hybrid functionals, use of Density Functional Theory in quantum chemistry.

UNIT-III **12 Hrs**

***In-silico* and Computer Aided Drug design**

Introduction to Computer aided drug design (CADD): History, Different techniques and applications, Introduction to Molecular Modelling, Lipinski's rule of five, Protein

preparation, Ligand preparation, Molecular Mechanics, force fields (Potential energy function), Energy Minimization Methods, and Conformational Analysis. Concepts of Virtual Screening, Drug likeliness, Screening-Counting Schemes, Functional Group Filters, Topological Drug Classification-Pharmacophore Point Filter-Focused Screening Libraries for Lead Identification, Pharmacophore Screening, Structure-Based Virtual Screening, Protein Structures, Computational Protein-Ligand Docking Techniques with the help of docking servers, Types-Rigid Docking, Flexible or induced fit Docking. Quantitative structure activity relationships: Basics, applications. ADMET properties prediction and analysis.

References:

1. Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Ed. Wiley & Sons, New York, 2004
2. F. Jensen, Introduction to Computational Chemistry, Wiley, New York, 1999
3. E.G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, 2nd Edn., Springer, 2011.
4. Elementary Quantum Chemistry by Frank L. Pilar, 2nd Edition, McGraw – Hill Publishing Company, 1990.
5. D.C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real- World Problems, John Wiley & Sons, 2001.
6. Gringauz, A. Introduction to Medicinal Chemistry: How Drugs Act and Why? John Wiley & Sons ,1997.

CH E 506: BIOMOLECULES AND MEDICINES

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To understand the chemistry and the uses behind the daily using drug molecules.
LO2: To study the importance of trace elements in the biological system and in medicines.
LO3: To understand the importance of amino acids, protein, nucleic acid, and vitamins and their uses in daily life.

Course Outcomes

CO1: Knowledge on drugs used in daily life and their proper usage.
CO2: Awareness on metals and their role in the body functions. Knowledge on metal based drugs.
CO3: Knowledge on biomolecules, their role and need in the functioning of the body.

UNIT-I 12 Hrs

Synthetic drugs

Introduction to drugs, chemotherapy, metabolites and antimetabolites, Prodrugs, analogs, agonists and antagonists. Introduction to medicines used in daily life-Antipyretics-Aspirin, analgesics-paracetamol and anti-inflammatory- Ibuprofen. Antibiotics -Amoxicillin, Cefexime and Streptomycin. Antidiabetics-Insulin and oral hypoglycemic agents. Antihistamines -Methapyrilene, Chlorpheniramine Antineoplastic agents – Mercaptopurine, Fluouracil, and Cis-platin. Anti-virals-Acyclovir, Amantadine. Local anti-infective drugs- Ciprofloxacin, Chloroquin.

UNIT-II 12 Hrs

Metals in Medicine

Inorganic compounds as therapeutic Agents: Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes).

Biological Trace elements: Introduction to trace elements in biological system, Biological classification of trace elements, essential trace elements. The trace elements in human

enzyme system-copper, iron zinc, cobalt, manganese. Clinical Significance of Essential Trace Elements, diseases due to metal deficiency.

UNIT-III 12 Hrs

Chemistry of Biomolecules

Amino Acids: General structure, classification, specific rotation, distribution in proteins, location in proteins, physical properties, non-standard protein amino acids and non protein amino acids.

Proteins: Classification, Structure of protein: primary, secondary, tertiary and quaternary structure and examples.

Nucleic acids: Introduction, RNA, DNA, Purines, Pyrimidines, Nucleosides and nucleotides, structure of nucleosides.

Vitamins: Introduction, Classification and Nomenclature-Source and Deficiency diseases-Biological, functions of Vitamins- Vitamin A1 & A2, VitaminB6 and B12, Vitamin C, Vitamin K1 and K2, Pantothenic acid, folic acid.

References:

1. Medicinal Chemistry: Ashutosh Kar, 4th Edn., Wiley-Eastern, New Delhi, 2006.
2. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby, Elsevier, 2006.
3. Essentials of Inorganic Chemistry For Students of Pharmacy, Pharmaceutical Sciences and Medicinal Chemistry by Katja A. Strohfeldt, John Wiley & Sons, Ltd, 2015.
4. Inorganic chemistry by Catherine E Housecraft and Alan G. Sharpe, Pearson-Prentice Hall, 2001.
5. Advanced Inorganic Chemistry (4th Edn) - Cotton and Wilkinson, 1999.
6. Natural Products Chemistry-Vol. I & II: G. R. Chatwal, Himalaya Bombay, 1990.
7. Fundamentals of Biochemistry by J L Jain, Nitin Jain &Sunjay Jain, S. Chand Publishing, 1979.

CH E 507: CHEMISTRY OF MATERIALS

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To gain knowledge on common materials used in day today life

LO2: To enable the students to grasp the chemistry of cements, ceramics and polymers

LO3: To study about bio-materials

Course Outcomes:

CO1: Knowledge on different types of cements, ceramics, polymers and superconductors

CO2: Ability to understand the industrial utility of materials

CO3: Knowledge on biological applications of materials

UNIT-I **12 Hrs**

Cementitious Materials

Raw materials, Portland cements; types, Non-Portland cements- high alumina cements, calcium sulfoaluminate cements, phosphate cements.

Chemicals in cement hydration; hydration process, set retarders and accelerators, plasticizers, slip-casting processing. Application of cementitious materials.

Ceramic Materials

Classification of ceramics, Examples and application of ceramics: oxides, carbides, borides, nitrides.

UNIT-II **12 Hrs**

Composite Materials

Definition, glass transition temperature, fiber for reinforced-plastic composite materials (i.e.glass fibers, carbon fibres, and aramid fibers); concretes and asphalt materials. Application of composite materials.

Bio-materials

Definition, Type of bio-materials; dense hydroxyapatite ceramics, bioactive glasses, bioactive glass ceramics and bioactive composites.

UNIT-III **12 Hrs**

Superconducting Materials

Definition of superconductivity, Critical temperature(Tc), Critical field, properties and classification of superconducting compounds, Examples of superconducting materials: Fullerenes, intermetallic superconductors. Application of superconducting materials.

Polymers– Classification, Polymer Processing and recycling, Conducting Polymers, Drug delivery polymers, Polymers for high temperature applications.

References:

1. Building Materials, S. K. Duggal, 3rd Ed., New Age International Publishers, 2008.
2. Cement Chemistry, HFW Taylor, 2nd Ed., Thomas Telford Publishing, 1997.
3. Essential of Materials Science and Engineering, Donald R. Askeland, Pradeep P. Fulay, 2nd Ed., Cengage learning, 2009.
4. Nature and Properties of Engineering Materials, Z. D. Jastrazebski, John Wiley Sons, 1989.
5. Polymer Science and Technology, Joel R. Fried, 3rd Ed., Prentice hall, 2014

CH E 508: FOOD CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To impart detailed knowledge on food, its nutritional aspects, food adulteration, artificial sweeteners, preservatives and colorants

LO2: To understand the science and few aspects of cooking

LO3: To know the science of metabolism, food factors and chemistry behind it

Course Outcomes:

CO1: Knowledge on food, nutrition and food additives

CO2: Understanding of science behind cooking

CO3: Information on food metabolism & impact of food factors on our body

UNIT-I **12Hrs**

Food, nutrition & food additives

Introduction, definition of food and nutrition, classification of foods- vitamins, proteins and carbohydrates. Knowledge on important nutrients in basic five food groups. Balanced diet, planning the menu, food pyramid. Food adulteration- common adulteration in food, food additives, food preservatives. Artificial sweeteners, artificial food colorants, artificial food flavors**.**

UNIT-II **12 Hrs**

The Science of cooking

Introduction to cooking, principles of cooking, sources of energy, heat transfer and materials for cooking, understanding the biology and chemistry behind cooking. The science behind measuring, time and temperature, taste and smell, heat & cold in cooking. Salt, fat, acid, heat: mastering the elements of good cooking, formation of toxins and role of antioxidants in our biological system.

UNIT-III **12 Hrs**

Eat right for good metabolism and health

Introduction to metabolism of food, the digestive process, improving the digestion, eating according to our metabolic types, how undigested food poisons the body, junk food & processed food chemistry, food factors causing anxiety the antianxiety food solution, food allergies. Foods to avoid: sugar, coffee, alcohol, nicotine. Antinutritional, toxic and other bioactive compounds in foods. Balancing the brain chemistry for a health life

References:

1. The chemistry of food, Jan Velisek, Wiley Blackwell, 2013.
2. The food lab-Better home cooking through Science, J Kenji Lopez-Alt, W.W. Noron& Company, 2015.
3. Foods: Facts and Principles – N Shakuntala Many & S. Swamy, 4thEdn. New AgeInternational, 1998.
4. Salt, Fat, Acid, Heat: Mastering the Elements of Good Cooking, by Nosrat&Samin, 2017.
5. The Science of Good Cooking , America's Test Kitchen Brookline, MA, 2012.

OC P 509: ORGANIC CHEMISTRY PRACTICALS- III

Teaching Hours: 6 Hrs per week

Quantitative determination of sugars, amino acids, phenols, carboxylic acids, amides, esters, aldehydes, ketones, urea by various methods. Determinations of acid and ester and acid and amide in mixtures of two.

Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide, unsaturation and nitro groups by various methods. Semi-micro analysis of Nitrogen, Halogen, Alkoxy, C-methyl and active hydrogens.

OC P 510: ORGANIC CHEMISTRY PRACTICALS- IV

Teaching Hours: 6 Hrs per week

Synthesis of one derivative each of Furan, Indole, Pyrazole, Quinoline, Thiazole, Acridine, Coumarin and Triazole containing heterocycles. Synthesis of Picric acid, Para red, Methyl red, Methyl orange, Flourescein, Eosin, Indigo.

Chromatographic techniques: TLC and column chromatography Elucidation of structure of organic compounds using UV, IR, NMR and Mass spectra.

References:

1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis: A. I. Vogel
2. Vogel's Text Book of Practical Organic Chemistry: Furniss et al., ELBS, London 1978.
3. Experimetal Organic Chemistry- Vol. I & II: P. R. Singh, Tata McGraw-Hill, 1981.
4. Practical Organic Chemistry: Dey & Sitaraman, IV Edn., Allied.
5. Laboratory Experiments in Organic Chemistry: Adam, Johnson & Wicon, McMillan, London, 1979.
6. Experimental Organic Chemistry: H. D. Durst & G. E. Goke, McGraw-Hill, 1980.
7. Practical Organic Chemistry- F. G. Mann and B. C. Saunders, M.A., 1936,
8. Advanced Practical Organic Chemistry (3rd ed.)-N.K. Vaishnoi, Vikas Publishing House Pvt. Ltd.

OC P 511: Project Work & Dissertation

8 Hrs per week

References:

1. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., 2002. An introduction to Research Methodology, RBSA Publishers.
2. Kothari, C.R., 1990. Research Methodology: Methods and Techniques. New Age International. 418p. 3.
3. Trochim, W.M.K., 2005. Research Methods: the concise knowledge base, Atomic Dog Publishing. 270p.

IV SEMESTER

OC H 551: ORGANIC SYNTHETIC DESIGN AND GREEN TECHNIQUES

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn about synthetic design, planning of organic synthesis and functionality of groups.
2. An introduction to disconnection approach to the synthesis, definition of terms, related to disconnection approach, principle, nature and use of protecting groups, introduction to combinatorial synthesis with example
3. To understand the principles of Green Chemistry, applications of microwave irradiation and of ultrasound in chemical processes, use of safer reagents, greener solvents and greener catalysts, greener synthesis of drugs

Course Outcomes:

CO1: Study of synthetic design, planning of organic synthesis and functionality of groups.

CO2: Illustration on basic principles and techniques used in disconnection approach

CO3: Knowledge on Principles of Green Chemistry and applications of different green techniques in chemical synthesis

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Unit-I **15 Hrs**

Synthetic Design: Carbon skeleton frame work, classification of carbon-carbon single &double bonds forming reactions and their use in carbon skeleton ring formation. Ring forming & ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, Friedel-Crafts reaction, 1,3-dipolar addition & Ene reaction in ring formation, Oxidative cleavage of rings & Retro Diel's-Alder reactions.

Planning of organic synthesis: Selection of starting materials and key intermediates during the synthesis. Synthesis of Cubane and Iswarane. Use of Robinson annulation, Dickmann cyclisation, Arndt-Eistert synthesis and Diel's- Alder reaction in organic synthesis. **Functionality**: Synthesis of 6- and 7- methoxy tetralones, biotin and penicillin-V with special reference to the introduction of functional groups. Stereo chemical consideration and stereo selectivity during organic synthesis.

Unit-II **15 Hrs**

General Introduction to Disconnection Approach. Basic principles and technologies used in disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C-X and two group. C-X disconnections.**Protecting groups**: Principle of protection of hydroxyl amino carboxylic and carbonyl groups.**C-C one group and C-C two group disconnections**: Use of C-C disconnections in the synthesis of 1,2-, 1,3-, 1,4-, 1,5- and 1,6- difunctionalised compounds.

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, retrosynthetic analysis of Benzocaine, 2,5-dimethylfuran, 2,4,6-trimethyl pyridine, Indole-2-carboxylate, 2-methyl-6-methoxy-indole-3-acetic acid, 6-methyl quinoline, Hydralazine, Benziodarone, Aphox, and Warfarin. **Illustrative Synthesis**: Juvabione, Longifolene, Prelog-Djerassi Lactone.

Unit-III: **15 Hrs**

Green Chemistry Techniques in Organic Synthesis

Green reagents: Dimethyl carbonate and Polymer supported reagents. . Green catalysts: Acid basic catalysts and Oxidation catalysts. .Aqueous phase reactions and photochemical reactions, application of phase transfer catalyst and crown ethers in green chemistry. Microwave assisted reactions in water and organic solvents. Solvent free (solid state) reactions. Synthetic applications of ultrasound. Reactions in neutral Ionic liquids : Hydrogenation, Diels – Alder, Heck reaction, O - and N - alkylation and methylene insertion reaction, , Supercritical Fluids (SCF) as media for chemical reactions.Greener synthesis of adipic acid, catechol, paracetamol, caprolactum, furfural. Common MCRs including Biginelli reaction, Hantzsch synthesis, etc. Click chemistry with examples.

References:

1. Modern Organic Reactions: H. O. House, W. A. Benjamin, 1972.
2. Organic Synthesis: R. E. Ireland, Prentice Hall India, 1969.
3. Art in Organic Synthesis: Anand, Bindra & Ranganath, Wiley, 1970.
4. Organic Synthesis a Disconnection Approach- Stuart
5. Advanced Organic Chemistry-Part A & B: Carrey & Sundberg, 4th Edn., Kluwer-Academic, 2001.
6. Modern Methods of Organic Synthesis: N. Carruthers, Cambridge University, 1996.

7. Environmental Chemistry with Green chemistry: Asim K. Das, Books and Allied (P) Ltd.
8. Green Chemistry: Environmentally Benign Reactions, V. K. Ahluwalia, Ane Books India, New Delhi, 2006.
9. New Trends in Green Chemistry, V. K. Ahluwalia and M. Kidwai, Anamaya Publishers, N. D
10. Microwaves in Organic Synthesis, Andre Loupy (Ed.), Wiley – VCH Verlag, Weinheim, 2002.
11. Green Chemistry, Samuel Delvin, IVY Publishing House, Delhi, 2006.
12. Introduction to Green Chemistry, Albert S. Matlack, Marcel Dekker, Inc., New York, 2001.
13. Green Chemistry: Frontiers in benign chemical synthesis and processes, Paul T. Anastas and Tracy C. Williamson (Eds.), Oxford University Press, Oxford, 1998

OC H 552: ADVANCED HETEROCYCLIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn nomenclature of heterocyles and have knowledge on four membered, five membered and six membered heterocyles
2. To learn mesoionic compounds, anthocyanins, flavones and heterocycles in functional group and ring transformation.
3. To know name reactions in heterocyclic chemistry and to have knowledge on the synthetic application of these name reactions

Course Outcomes:

CO1: Study of nomenclature of heterocyclic compounds and knowledge on four membered, five membered and six membered heterocycles

CO2: Learning on mesoionic compounds, anthocyanins, flavones and heterocycles in functional group and ring transformation.

CO3: Detailed information on name reactions in heterocyclic chemistry and their synthetic applications

Unit-I **15 Hrs**

Heterocyclic Chemistry-I

Structure, reactivity, synthesis and reaction of the following: Four membered heterocycles-Oxitanes, Azetidines and Thietanes; Five membered heterocycles- Thiazoles, Imidazoles, Pyrazolines, 1,2,4-Triazoles, 1,2,3-Triazoles, Oxadiazole, and Thiadiazols, Selenophenes, Tellurophenes. Six membered heterocycles-α and γ-Pyrones, 1,2,3- 1,2,4- and 1,2,5-Triazines, Pyrimidines and Pyrazines; Seven membered heterocycles-Azepines, Oxepines and Thiepines. Fused heterocycles: Benzofuran, Benzothiophene and Cumarines.

Unit-II **15 Hrs**

Heterocyclic Chemistry-II

Mesoionic compounds: Introduction, Synthesis and reactions of sydnones. **Anthocyanins and Anthocyanidins**: Introduction, structure and general methods of synthesis. **Flavones, Flavonols and Isoflavones**: Introduction, structure and synthesis of flavone, flavonal and

quercetin. Synthesis of Thymine, Cytosine, Adenine and Guanine. Structural elucidation and synthesis of Uric acid, Caffeine **Heterocycles in functional group and ring transformations:** Alkanes from thiophenes, dienes from pyrroles, alcohols from isooxazolines, conversion of coumarin to benzofuran, sydnone to pyrazole, chromones to pyrazoles, furans to pyridines, pyrrole to pyridines, pyrimidine to pyrazole, isatins to quinolines, indoles to quinoline. Dimroth and Cornforth rearrangements.

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Unit-III **15 Hrs**

Name Reactions in Heterocyclic Chemistry

Corey-Chaykovsky reaction, Hoch-Cambell aziridine synthesis, Blum aziridine synthesis, Bucherer carbazole synthesis, Hoffmann Loffler-Freytag reaction, Gewald aminothiophene synthesis, Gassman indole synthesis, Grabe-Ullmann carbazole synthesis, Fiesselmann thiophen, Fischer oxazole synthesis, Bockiheide reaction, Gabriel-Colman rearrangement, Gould-Jacobs reaction, Batcho–Leimgruber indole synthesis, and Meth–Cohn quinoline synthesis.

References:

1. An Introduction to the Chemistry of Heterocyclic Compounds: R. M. Acheson, Wiley Eastern, 2002.
2. Heterocyclic Chemistry: J. Joule & K. Mills, 5th Edn., Van Nostrand ELBS, 2010.
3. Name reactions in Heterocyclic Chemistry: Jie Jack Li, 3rd Edn., Springer.
4. Heterocyclic Chemistry: Raj K Bansal, 5th Edn., New Age International Publishers, 2014.
5. Comprehensive Heterocyclic Chemistry Vol. I-VI: Katritzky & Rees, Pergamon, 1984.
6. Principles of Modern Heterocyclic Chemistry: L. A. Paquette, Benjamin House, 1968.
7. Handbook of Heterocyclic Chemistry: A. R. Katrizky, C. A. Ramsden, J. A. Joule, V. V. Zhdankin, 3rd Edn., Elsevier, 2010.
8. Fundamentals of Heterocyclic Chemistry: L. D. Quin, J. A. Tyrell, Wiley, 2010.
9. Name Reactions- A Collection of Detailed Reaction Mechanism: Jie Jack Li, 3rd Edn., Springer, 2006.

OC H 553: PHOTOCHEMISTRY AND ASYMMETRIC SYNTHESIS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn about organic photochemistry, phtoreduction, photochemical isomerisation, photocylisation and photochemistry of alkenes benzenes and cycloalkanes.
2. To understand Pericyclic reactions, electocyclic reactions, cycloadditon reactions and sigmatropic reactions.
3. To learn about asymmetric synthesis, separation of enantiomers, chiral reagents and use of reagents in asymmetric synthesis.

Course Outcomes:

CO1: Learning photochemical reactions, their properties, kinetics and their rearrangement reactions.

CO2: Study of Pericyclic reactions, electocyclic reactions, cycloadditon reactions and sigmatropic reactions.

CO3: Learning about asymmetric synthesis, separation of enantiomers, chiral reagents and use of reagents in asymmetric synthesis

Unit I: **15 Hrs**

Organic Photochemistry: Bonding and antibonding orbital, σ and πorbitals, σ* and π* orbitals, singlet and triplet states, relative energies and excited states Light absorption and electronic transitions, Jablonski diagram,quantum yield, intersystem crossing, energy transfer, sensitizers.Photo oxidation,Photoreduction, Photochemical isomerisation. Norrish Type-I and Type-II reactions, Photoenols or Photoenolisation,Di-pi methane rearrangement, Lumiketone Rearrangement, Barton reaction, Hoffmann-Loeffler-Freytag Reactionand Photo Fries rearrangement, Paterno-Buchi reaction, Photochemistry of olefins, conjugated dienes, aromatic compounds.Applications of Photochemistry: Introductionto Photo imaging andphotochemical cells

Unit II **15 Hrs**

Pericyclic Reactions

Classifications of Pericyclic reactions, Theories of pericyclic reaction, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, 1,3,5,7-Octatetraene, allyl systems and 2,4-

pentadienyl system. Molecular orbital symmetry. Woodward-Hoffmann correlation diagram and FMO approach.

Electrocyclic Reactions: Introduction, Con- rotatory and dis-rotatory Process, 4n and 4n+2 systems. Reactions of cations and anions, formation and cyclisation of Dipolar molecules. Selection rules for electrocyclic reaction.

Cycloaddition reaction: Suprafacial and Antrafacial addition, 4n and 4n+2 systems, 1,3-dipolar cyclo additions. Diels-Alder reaction. Selection rules for cycloaddition reaction

Sigmatropic reactions: Classification, FMO analysis of [1,3] and [1,5] H shift. Sigmatropic shift of alkyl group. Selection rules for sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

UNIT III: 15 Hrs

Asymmetric Synthesis: Introduction, Seperation of enantiomers by resolution, The chiral pool. Asymmetric synthesis: Chiral auxillaries, alkylation of chiral enolates, enantimeric excess. Chiral reagents and chiral catalysts, CBS reagent and reaction. Asymmetric diels alder reaction, Proline as asymmetric catalyst. Asymmetric hydrogenation, resolution of BINAP, Improving enantiomeric excess by recrystallization, Asymmetric Epoxidation, Asymmetric Dihydroxylation and Asymmetric Heck reaction.

References:

1. Organic Reaction Mechanism: V. K. Ahluwalia and R. K. Parashar, 4th Edn., Narosa Publishing House, 2011.
2. Photochemistry and Pericyclic Reactions: Jagadamba Singh and Jaya Singh, New Age International Publishers, 3rd Edn., 2012.
3. Pericyclic Reactions: S. M Mukherji, The McMillan, 1979.
4. Frontier Orbital and Symmetry Controlled Pericyclic Reactions: Ratan Kumar Kar, Booka and Allied Pvt. Ltd. 2010.
5. Modern Methods of Organic synthesis: W. Carruthers and I. Coldham, 4th Edn., Cambridge University Press, 2004.
6. Advanced Organic chemistry: J. March, 5th Edn., John Wiley and sons, 2007.
7. Mechanisms in Advanced Organic Chemistry: R. P. Narain, New age International (P) Ltd., 2008.
8. Organic Chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers, 2nd Edn., Oxford University Press, 2012.

OC S 554: ADVANCED MEDICINAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To learn about antineoplastic agents antimetabolites, cardiovascular agents and antiarrythmic agents and their mode of action.
2. To study antiviral drugs anti-inflammatory drugs, antihypertensive agents and their mode of action.
3. To have knowledge on industrial pharmacy, different methods of extraction, separation, purification and different processes involved in drug delivery system.

Course Outcomes:

CO1: Basic knowledge on antineoplastic agents, antimetabolites, cardiovascular agents and antiarrhythmic agents and their mode of action

CO2: Study of antiviral drugs, anti-inflammatory drugs, antihypertensive agents and their mode of action

CO3: Knowledge on industrial pharmacy, different methods of extraction, separation, purification and processes involved in drug delivery system

Unit I: **12 Hrs**

Anti-neoplastic agents: Introduction and Classification. Methotrexate, Mercaptopurine, 6-thioguanine (6TG), Fluorouracil, Cytarabine. Alkylating agents-classification-Mechlorethamine, Chlorambucil, Cyclophosphamide. Alkyl sulfonates: Busulfan. Nitrosoureas: Lomustine. Cisplatin and Carboplatin.

Cardiotonic drugs: Introduction and classification. Digoxin, Amrinone, Milrinone.

Antiarrhythmic Drugs: Introduction and classification: Quinidine, Procainamide, Propranolol.

Antianginal Drugs: Introduction and classification: Nitroglycerine, Pentaerythritol tetranitrate, Propranolol, Diltiazem, Verapamil.

Unit II **12 Hrs**

Antiviral Drugs: Introduction & classification. Synthesis of Etraverine (NNRTI), Darunavir (antiviral Protease Inhibitor) and Raltegravir (HIV Integrase inhibitor). Mode of action of Raltegravir. **Antiinflammatory:** Types: COX-I and COX-II. Examples: Synthesis of Celecoxib, Indomethacin and Dichlofenac sodium. Mode of action of

Celecoxib. **Cholinesterase Inhibitors for Alzheimer Disease:** Synthesis Donepezil, Rivastigmine and Galantamine. Mode of action of Donepezil. **Antihypertensive agents-** Introduction, synthesis and mechanism of action of Hydralazine derivatives. Synthesis of Olmesartan, Candesartan and Aliskiren. **Proton pump inhibitors:** Synthesis of Rabeprazole, Pantaprazole, and Ranitidine. Mode of action of Rabeprazole. **Quinolone Antibacterials**: Synthesis of Nalidixic acids and Ciprofloxacin. Mode of action of Ciprofloxacin.

Unit III **12 Hrs**

Industrial processing and techniques

Industrial Processing: Introduction to industrial processing-patents, R&D, quality control and quality assurance. Process development in synthetic chemistry(milligrams to tons): Literature survey, selection of reagents, solvents and catalyst. Reaction optimization in multistep synthesis, scale up studies and documentation.

Industrial Techniques: extraction-methods of extraction, continuous extraction, soxhlet extraction. Distillation- methods of distillation, azeotropic, steam, extractive distillation and factional distillation. Techniques of Crystallization-cooling crystallization, seeding crystallization and anti-solvent crystallization. Drying techniques-- -tray drying, fluidized drying, spray drying

References:

1. Medicinal Chemistry: Ashutosh Kar, 4th Edn., Wiley-Eastern, New Delhi, 2006.
2. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi, 1996.
3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby, Elsevier, 2006.
4. The Organic Chemistry of Drug Synthesis Vol. VII: Daniel Lednicer, John Wiley & Sons Inc., 2007.
5. Modern Drug Synthesis: Jie Jack Li and D. S. Johnson, Wiley, 2010.
6. Medicinal and Pharmaceutical Chemistry: H. Singh and V. K. Kapoor, Vallabh Prakashan New Delhi, 996.
7. Solvents and Solvent Effects in organic Chemistry: Christian Reichardt, 3rd Edn., Wiley-VCH, 2004.
8. The chemistry of process development in Fine chemical & Pharmaceutical Industry by C. Somerswara Rao, Asian Books Private Limited, 2006
9. Pharmaceutical process Chemistry, Kunisuke Izawa and Toshiro Konoike, Wiley-VCH publication, 2010.
10. Synthesis of Best-Seller Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2016

OC S 555: CHEMISTRY OF NATURAL PRODUCTS

Teaching Hours: 3 hrs per week

Learning Objectives:

1. To learn about introduction to alkaloids, structure elucidation, stereochemistry of alkaloids, and synthesis of few alkaloids.
2. To study terpenoids, isoprene rules, methods of structure determination synthesis of terpenoids, diterpenoids and prostaglandins.
3. To learn about steroids, Blanc's rule, chemistry of different steroids and steroidal hormones.

Course Outcomes:

CO1: Learning on structural features of structure, synthesis and stereochemistry of alkaloids

CO2: Detailed knowledge on natural product terpenoids, diterpenoids and prostaglandins

CO3: Study of chemistry of different steroids and steroidal hormones.

Unit-I **12 Hrs**

Alkaloids: Definition, Classification and isolation of alkaloids, general methods of structural determination of alkaloids, detailed study of structure elucidation, stereochemistry, rearrangement, Synthesis and biogenesis of the following alkaloids- Papaverine, Cinchonine, Quinine, Morphine and Reserpine.

Terpenoids: Introduction, classification, isoprene rules, methods of structure determination. Structural elucidation & synthesis of geraniol, menthol, α-pinene, camphor and farnesol. **Diterpenoids**: Abietic acid. Triterpenoids: Squalene.

Unit-II **12 Hrs**

Amino Acids: General structure, classification, specific rotation, distribution in proteins, location in proteins, physical properties, non-standard protein aminoacids and non protein aminoacids. General methods of synthesis of aminoacids with specific examples.

Peptides & Proteins: Peptide bond formation and synthesis of polypeptides, Amino and carboxy protecting groups in peptide synthesis, Solid phase peptide synthesis-Merrifield method, Peptide structure determination-Sequence and End group anaysis (N-Terminus and C-Terminus), Secondary, Tertiary and Quaternary structure of proteins.

Unit-III **12 Hrs**

Steroids: Introduction and Nomenclature of steroids, Blanc's rule, Barbier-Wieland degradation, Oppenauer oxidation, Diel's hydrocarbon, Chemistry of Cholestrol, Ergosterol, Vitamin-D &bile acids. Steroidal hormones: Chemistry of Oestrone, esterdiol, estriol and their chemical relationship. Progesterone, androsterone and testosterone-Structure and Synthesis of Cortisone, Cortisol and Aldosterone.

References:

1. Natural Products Chemistry-Vol. I & II: G. R. Chatwal, Himalaya Bombay, 1990.
2. Chemistry of Natural Products-Vol. I & II: O. P. Agarwal, Goel Gorakhpur, 1985.
3. Organic Chemistry-Vol. I-II: I. L. Finar, Longmann ELBS London, 2000.
4. Chemistry of Natural Products: Sujatha V. Bhat, B. A. Nagasampige and M. Sivakumar, 2nd reprint, Springer, 2006.

OC S 556: INDUSTRIAL ORGANIC CHEMISTRY

Teaching Hours: 3 hrs per week

Learning Objectives:

1. To learn about classification and nomenclature of synthetic polymers, different types of polymerization and techniques used in polymerization.
2. To understand the concept of color, and constitution of dyes, synthesis of dyes, pesticides and insecticides.
3. To learn about different heterocyclic compounds as agrochemicals, plant growth regulators and veterinary products.

Course Outcomes:

CO1: Understanding different types of polymerization techniques and kinetics of polymerization.

CO2: Conceptual knowledge on color and constitution of dyes, synthesis of dyes, pesticides and insecticides.

CO3: Usage of different heterocyclic compounds as agrochemicals, plant growth regulators and veterinary products.

Unit-I **12 Hrs**

Synthetic polymers: Classification and Nomenclature, Properties of polymers (molecular weight, Glass transition temperature, Solubility and Viscosity). Methods of polymerization, Mechanism and Stereochemistry, Addition polymerization (Anionic, Cationic and Free radical process), Condensation and Stepwise polymerization, Coordination polymerization, Study of polyesters, polyamides, Phenol-Formaldehyde resins, Urea-Formaldehyde resins, Epoxy resins, Polyurethanes, Polycarbonates, Synthetic rubber. Structural features and manufacture of natural rubber and Regenerated cellulose. Ziegler-Natta catalyst. Ring opening polymerization. Mechanism of co polymerization.

Polymerization process & some individual polymers:Polymerization in homogeneous &heterogeneous systems - Gas phase polymerization- Bulk polymerization and Polymer precipitation, suspension and emulsion polymerization- Solid phase polymerization. Properties, Structure and applications of Polythene, Polypropylene, PVC, Polystyrene & Acrylic polymers, Teflon, Nylon(polyamides), polyesters(terylines),caprolactum based polymers.

Unit-II **12 Hrs**

Dyes: Color and constitution (electronic concept). Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes, Orange –II, Mordant brown, Congo red and methyl orange; Triphenylmethane dyes- Malachite green, Rosaniline, Crystal violet and Phenolphthalein; Cyanin dyes- Ethyl Red, Cyanin blue and Quinaldine; Reactive dyes and Optical brighteners-Tinapal and Blankophor. Pigments: Fast violet, Lake red and Orange R.

Pesticides and Insecticides: Introduction and classification. Natural insecticides-Nicotine, Pyrethrins, Rotenone and Allethrin; Organic insecticides-DDT, Methoxychlor, BHC, Aldrin, Malathion and Parathion. Fumigants and repellants-general studies.

Unit III: 12 Hrs

Heterocyclices in Agrochemicals

Introduction to heterocycles in agrochemicals.

Herbicides: Triazine herbicides, Pyrimidynyl and Triazinylsulfourea, triazolopyrimidine, imidazoline, pyridazinones, thiadiazoles, and pyridine class of herbicides.

Plant growth regulators: Indole and pyrimidine.

Fungicides: Triazoles, benzimidazoles, pyrimidines, pyrazole carboxamide, Sulfenyl derivatives. Dicarboximides. Heterocyclic organophosporous reagents.

Insecticides: Pyridine and thiazole, pyrazole and pyrimidine, Organo phosphorus compounds.

Veterinary Products: Antimicrobials, Antiprotozoals, Ectoparasiticides.

References:

1. Text Book of Polymer Science: F. W. Billmeyer, 3rd Edn., Wiley, 2012.
2. Polymerscience: V. R. Gowariker, N. V. Vishwanathan & T. Shridhar, 1st Edn., New Age International (P) Ltd. Publishers, Reprint 2012.
3. Text Book of Polymer Science Vol. I-III: M. S. Bhatnagar, 1st Edn., S. Chand Publication, Reprint 2010.
4. Synthetic Dyes – Vol. I- Venkataraman, 1999.
5. Oragnic Chemistry Vol. I: I. L. Finar, 4th Edn., Longmann ELBS London, 2000.
6. Comprehensive Heterocyclic Chemistry-Vol. I: A. R. Katritzky, C. W. Rees, Elsevier, 1997.
7. Bioactive Heterocyclic compound classes:Agrochemicals- by Clemens Lamberth and Jurgen Dingers, WILEY-VCH, 2012.

OC P 557: ORGANIC CHEMISTRY PRACTICALS- VI

Teaching Hours: 6 Hrs per week

Multi-step synthesis of Pharmaceutical compounds and Analytical Techniques: Synthesis of heterocyclic compounds such as Thiophene, Indole, Imidazole, Pyrazole, Pyrazoline, Thiazole, Oxazole, 1,2,4-oxadizole, 1,3,4-oxadiazole, Pyrimidine, Pyridine, Quinoline, Quinazoline and fused heterocyclic systems such as Imidazothiazole, Imidazopyridine, Thiazolopyridine derivatives of pharmaceutical interest by 4 to 5 step synthesis. Characterization and interpretation of these derivatives by spectroscopic techniques such as IR, UV, ^{1}H NMR, ^{13}C NMR and mass spectral data.

Combined spectral solving problems: Elucidation of structure of organic compounds using UV, IR, NMR and Mass spectra.

References:

1. Elementary Practical Organic Chemistry-Vol. III quantitative Organic Analysis: A. I. Vogel
2. Vogel's Text Book of Practical Organic Chemistry: Furniss et al., ELBS, London 1978.
3. Experimetal Organic Chemistry- Vol. I & II: P. R. Singh, Tata McGraw-Hill, 1981.
4. Practical Organic Chemistry: Dey & Sitaraman, IV Edn., Allied.
5. Laboratory Experiments in Organic Chemistry: Adam, Johnson & Wicon, McMillan, London, 1979.
6. Experimental Organic Chemistry: H. D. Durst & G. E. Goke, McGraw-Hill, 1980.
7. Practical Organic Chemistry- F. G. Mann and B. C. Saunders, M.A. 1936
8. Advanced Practical Organic Chemistry (3rd ed.)-N.K. Vaishnoi, Vikas Publishing House Pvt. Ltd.

OC P 558: ORGANIC CHEMISTRY PRACTICALS –VI

Teaching Hours: 6 Hrs per week

Separation, purification, analysis and derivatization of ternary mixture of organic compounds, Identification, separation and qualitative analysis of the individual compounds and preparation of suitable derivative for each component, identification of derivative by m.p., TLC and spectral techniques.

References:

1. Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.
2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.
3. Experimental Organic Chemistry–Vol.I & II Singh et al(TMH, New Delhi)1981.
4. Semimicro Qualitative Organic Analysis–Cheronis et al Wiley-Eastern, New Delhi) 1964.
5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss et al (Longman-ELBS, England), 1978.

OC P 559: ORGANIC CHEMISTRY PRACTICALS- VII

Teaching Hours: 6 Hrs per week

Isolation and Characterization of natural products like Caffeine, Recinoleic acid, Azelic acid, Piperine, Hespiridine, Cysteine, Casein, Lycopene and enzymes like Lipase and Sucrase. Extraction of Groundnut oil and Coconut oil. Determination of Saponification and Iodine values of oils and fats. Isolation of Carotines. Purification by paper, Column and TLC. Characterization of natural products by oxidation studies & derivatization of natural products.

References:

1. Elementary Practical Organic Chemistry-Vol. III Quantitative Organic Analysis: A.I Vogel
2. Vogel's Text Book of Practical Organic Chemistry- Furniss et al.; ELBS, London, 1978.
3. Experimental Organic Chemistry- Vol. I &II- P. R. Singh, Tata McGraw-Hill , 1981.
4. Practical Organic Chemistry- IV Ed- Dey & Sitaraman; Allied.
5. Laboratory Experiments in Organic Chemistry-Adam, Johnson & Wicon; McMillan, London, 1979.
6. Experimental Organic Chemistry- H. D. Durst & G. E. Goke; McGraw-Hill, 1980

VALUE ADDED COURSES

CERTIFICATE COURSE ON APPLICATIONS OF CHEMISTRY SOFTWARE AND RESEARCH METHODOLOGY

Total Teaching hours: 40 Hrs

Unit I: 20 Hrs

Computer applications for chemists

Chemsketch 6 Hrs

Writing the structures of simple and complex organic and inorganic molecules, prediction of molecular weight, elemental values, IUPAC names. Use of different arrows, symbols, glassware cliparts. Writing reactions of simple organic conversions. Writing reaction mechanisms of few organic reactions-Nitration, sulphonation, halogenations, Vilsmeir Hack formylation, preparation glucosozone. Drawing 3D structure of the molecules.

Origin Graphing and Analysis for Chemistry: 4 Hrs

Plot of Mathematical functions and equations- trigonometric functions, logarithmic functions, exponential functions. Drawing of the geometries of atomic and molecular orbitals using mathematical operations using origin. Plot of radial and angular part of wave function as a function of r for s, p and d orbitals.

Microsoft Excel® 6 Hrs

Basics of excel®: Basics, Excel® in important analytical and general data analysis: Least-squares fitting to a general straight line, smoothing, Non-linear data fitting, pH calculations, Titrations of monoprotic acids and bases, Precipitation titrations, Redox titrations, Spectrometric p*Ka* determination.

Mercury program for visualizing crystal structures 4 Hrs

Introduction, Loading structures, Editing a structure, Creation and display of centroids, least-squares mean planes and Miller planes, crystal packing. Measurement of distances, angles and torsion angles involving atoms, centroids and planes, Displaying and saving powder diffraction patterns, Finding hydrogen bonds and other nonbonded contacts.

Unit II 20 Hrs

Research, Industrial pharmacy and Safety

Fundamentals of research 6 Hrs

Introduction to research, Hypothesis setting, Literature review, Web Search tools: Spectral analysis tools (Spectral Database for Organic Compounds - SDBS), Writing a Research Paper, Journals search and publishing article, Citation Software for detection of Plagiarism, Report writing and scientific editing tools.

Industrial pharmacy: 10 Hrs

Introduction to industrial processing and documentation. Monitoring of reactions by different methods, product isolation and purification techniques. Scale up studies in industrial process development.

Chemical and hazardous materials safety 4 Hrs

Chemical safety guidelines, material safety data sheets, types of chemical hazards, acid handling safety, flammable liquid safety, liquid solvents toxins and irritants, reactives and explosives.Chemical laboratory safety guidelines.

References

1. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., 2002. An introduction to Research Methodology, RBSA Publishers.
2. Kothari, C.R., 1990. Research Methodology: Methods and Techniques. New Age International. 418p. 3.
3. Trochim, W.M.K., 2005. Research Methods: the concise knowledge base, Atomic Dog Publishing. 270p.
4. Wadehra, B.L. 2000. Law relating to patents, trademarks, copyright designs and geographical indications. Universal Law Publishing.
5. http://sdbs.db.aist.go.jp/sdbs/cgi-bin/cre_index.cgi
6. Robert de Levie, 2001, How to use excel® in analytical chemistry and in general scientific data analysis, Cambridge University Press, UK, ISBN 0-511-04037-7 (ebook)
7. https://www.ccdc.cam.ac.uk/Community/csd-community/freemercury/
8. P. K. Ghosh and P.K. Shukla, Atomic Electronic structure, PHI Learning, Delhi.
9. Chemical Safety Manual for Small Businesses, A Publication of the American Chemical Society Committee on Chemical Safety and Division of Small Chemical Businesses, ISBN 0-8412-6984-X