M.Sc. Organic Chemistry



SRI DHARMASTHALA MANJUNATHESHWARA COLLEGE (AUTONOMOUS), UJIRE – 574 240

M. Sc. DEGREE PROGRAMME

in

ORGANIC CHEMISTRY

CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME

(EFFECTIVE FROM ACADEMIC YEAR 2016-17)



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 (CREDIT BASED SEMESTER SCHEME)

Approved by the BOS meeting held on 31 August 2019



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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 revised Syllabus for M.Sc. Organic Chemistry (CBCS based) in its meeting held on 15 September 2017. It was resolved to implement this syllabus from the academic year 2018-19.

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**.



COURSE OBJECTIVES

The revised syllabus provides a skeleton of Organic Chemistry within which students can choose the topics relevant to industry and research/analytical skills. The syllabus takes into account to enhance the knowledge and skills which help students build their career in research and industrial field across the world. The syllabus is designed in such a way that the students can excel in the present changing, evolving, challenging and competing scientific environment.

The syllabus aims to enable students to:

- Prepare the students to gain sound knowledge on principles and methodologies of Organic Chemistry.
- Understand and analyze the problems using the acquired scientific knowledge.
- Develop the capacity to adopt effectively and implement the information available with them.
- Acquire good laboratory skills and practice safety measures when using equipment and chemicals as well as the safe disposal of chemical waste.
- Apply the basic knowledge in everyday life to solve the problems and for the betterment of society.
- Use the knowledge for a safe and sustainable future and to develop the entrepreneurial skills.

OUTCOMES

M.Sc. Organic Chemistry course involves chemical and scientific theories such as Inorganic, Organic, Physical, Analytical Chemistry and focusing more on Organic Chemistry aspects.

The students undertaking this course;

- Will be able to plan, design and carry out synthetic reactions, isolation and purification of products, as well as accurately record and analyze the results of synthetic works.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Will utilize the knowledge gained effectively for the smooth functioning of daily life and use this as a basis for ethical behavior in issues facing chemists including



an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.

- Will be competent to take up teaching profession, industrial jobs and beside these one can easily clear the UGC/NET/KSET and Civil service examinations.
- Will be able to start small scale industries with the available resources



COURSE/CREDIT PATTERN

	Credits (C)						
	Theory (T)		Practical (P)		Project	Tatal	
Semester						(Pr)	10101
	Hard Core	Soft Core	Elective (E)	Hard Core	Soft Core	Hard Core	
	(H)	(S)		(H)	(S)	(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

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	Spectroscopy	3	30 + 70	3		
OC S 405	Methods of Analysis	3	30 + 70	3	3	3x2=6
OC S 406	Environmental Chemistry	3	30 + 70	3		
	(Any two)					
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

I Semester

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	Chemistry of Life or Environmental Chemistry	3 3	30 + 70 30 + 70	3 3	3 3	3x1=3
OC P 458	Inorganic Chemistry Practicals-II		30 + 70	4	4	2
OC P 459	Organic Chemistry Practicals-II		30 + 70	4	4	2
OC P 460	Physical Chemistry Practicals-II		30 + 70	4	4	2



Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
OC H 501	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	Advanced Heterocyclic Chemistry	3	30 + 70	3	3	3
OC S 504 or	Chemistry of Synthetic Drugs or	3	30 + 70	3	3	3x1=3
OC S 505	Bioorganic Chemistry	3	30 + 70	3		
CH E 506 or	Medicines in Daily Life or	3	30 + 70	3	3	3x1=3
CH E 507	Chemistry of Materials	3	30 + 70	3		
OC P 508	Organic Chemistry Practicals-III		30 + 70	6	6	3
OC P 509	Organic Chemistry Practicals-IV		30 + 70	6	6	3
OC P 510	Project Work & Dissertation		30 + 70	8		4

III Semester

IV Semester

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

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Time: 3 Hrs

Answer any Nine subdivisions

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

2x9=18 $\begin{array}{c}
1. a. \\
b. \\
c. \\
d.
\end{array} \quad UNIT I$ $\begin{array}{c}
e. \\
f. \\
g. \\
h.
\end{array} \quad UNIT II$ $\begin{array}{c}
i. \\
j. \\
k. \\
l.
\end{array} \quad UNIT III$



10

<u> PART – B</u>

Answer any Four o	uestions selecting	minimum of 1	auestion from	each unit.	13x4 = 52
i mo woi ung i oui g	acoulous selecting	minimum of 1	question nom	cucii unit.	$13 \times 1 = 32$

<u>UNIT I</u>

2 . a.		
b.		
с.	5+4+	-4
3. a		
b.		
с.	5+4+	-4
4	<u>UNIT II</u>	
4. a.		
D.	5 . 4 .	1
с.	3+4+	•4
5 a		
b		
с.	5+4+	-4
	<u>UNIT III</u>	
6 . a.		
b.		
с.	5+4+	-4
7 . a.		
b.		
с.	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

Rationale /Learning Objectives:

- To understand the concept of ionic and covalent bond
- To enable the students to grasp the chemistry of halogens and noble gases
- To study the phenomenon of precipitation and complexometric titration

UNIT-I

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

Halogens and Noble gas chemistry: Interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides.

Oxy and peroxy acids of N, P and S. Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

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

UNIT-III

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



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15 Hrs

15 Hrs

15 Hrs

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.

Quantitative Analysis: R. A. Day and A. L. Underwood, 6th Edn., Prentice Hall, 2012.
 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

Rationale /Learning Objectives:

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

UNIT-I

Bonding in organic systems: Theories of bonding-Valence and molecular orbital approaches. Resonance, hyper-conjugation and tautomerism, Huckel molecular orbital theory and its application to simple π systems- ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, heptatrienyl systems. Calculation of the total $\pi \Box$ energy and M.O. coefficients of the systems.

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

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

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

UNIT-II

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

Reaction Intermediates: Generation, structure, stability, reactivity, detection, trapping and reactions of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes.

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions- $S_N 1$, $S_N 2$ and $S_N i$. 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: 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



15 Hrs

15 Hrs

15 Hrs

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 Chemistry: P.Y.Bruice, Pearson Education Pvt. Ltd., New Delhi, 2002.

2. Stereochemistry, Conformation and Mechanism: P.S.Kalsi, Wiley Eastern, New Delhi, 1993.

3. Stereochemistry of Carbon Compounds: E.L.Eliel, Tata McGraw Hill, New. Delhi, 1994.

4. Advanced Organic Chemistry-Reactions, mechanisms & structure: J.March, Wiley, NY, 2000.

- 5. Organic Chemistry Vol. -1, 2 &3: Mukherji, Singh and Kapoor, Wiley Eastern, 1994.
- 6. A guide book of mechanisms in Organic Chemistry: P.Sykes, Orient- Longman, 1985.

7. Organic Chemistry: R.T. Morrison and R.N. Boyd, Prentice Hall, New Delhi, 1994.

8. Organic Chemistry.: S.H. Pine et al., 4th Edn, McGraw-Hill, London, 1987.

9. Advanced Organic Chemistry: R.A. Carey and R.J. Sundberg, Plenum, New York, 1990.

10. Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.

11. A Text book of Organic Chemistry: Tewari, Vishnoi and Mehrotra, Vikas, New Delhi, 1998.

12. A Text book of Organic Chemistry: R.K. Bansal, 3rd Edn., New Age, New Delhi, 1997.

13. Organic Chemistry: F.A. Carey, 3rd Edn, Tata McGraw Hill, New Delhi, 1996.

- 14. Organic Chemistry: H. Pine Hendrickson, Cram and Hammond, Mc Graw Hill, 1987.
- 15. Organic Chemistry: I.L. Finar, ELBS Longmann, Vol. I, 1984.

16. Advanced Organic Chemistry: Dr. Jagdamba Singh, Pragati Prakashan, 2014.



OC H 403: PHYSICAL CHEMISTRY

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To explicate the principle and applications of chemical thermodynamics
- To study the rate of composite reaction and to understand the factors affect on reaction rate
- To understand the theory and applications of quantum chemistry

UNIT-I: Chemical Thermodynamics

Concept of Entropy, Physical significance, entropy change in an ideal gas. Variation of entropy with Temperature, Pressure and Volume. Entropy change in reversible and irreversible processes. Free energy, Helmholtz's and Gibbs free energies, Gibbs – Helmholtz equation and its applications. Maxwell's relations and significance. Thermodynamic equations of state. 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.

Fugacity: Relationship between fugacity and pressure. Determination of fugacitygraphical method. Activity and activity coefficient: Variation of activity and fugacity with temperature and pressure.

UNIT- II: 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). Transition state theory and its applications. Auto catalytic reactions (Hydrogen-Oxygen reaction). Reactivity - selectivity principles (Hammond's postulate & Curtin-Hammet principle).

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, molecular beam, and spectroscopic and analytical methods

UNIT-III: 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



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15 Hrs

15 Hrs

15 Hrs

(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.
- Quantum Chemistry: Donald Allan McQuarrie, 5th Edn., University Science Books, 2013.



OC S 404: SPECTROSCOPY

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To acquaint the students with the basic concepts of microwave and vibration spectroscopy
- To study the application of infrared and UV spectroscopy in the structural identification of organic molecules
- To understand the theory and applications of ¹H and ¹³C NMR spectroscopy

UNIT-I

12 Hrs

Microwave Spectroscopy- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond length, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibration Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO₂& H₂O). Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches.

UNIT-II

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 λ_{max} . Application of UV spectroscopy in the structural study of organic molecules.

UNIT-III: NMR Spectroscopy

¹H 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, A₂B₂), 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 ¹H NMR spectroscopy. Applications of NMR



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12 Hrs

12 Hrs

spectroscopy in structure elucidation of organic molecules. Pulse techniques in NMR, two dimensional and solid state NMR. Use of NMR in Medical diagnostics.

¹³C 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.



OC S 405: METHODS OF ANALYSIS

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

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: 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: 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



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12 Hrs

12 Hrs

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, 3rd Edn. Saunders College Pub., 1985;
- 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.
- Instrumental Methods of Analysis: H. H. Williard, L. L. Merrit and J. J. Dean, 7th Edn., 1988.



OC S 406: ENVIRONMENTAL CHEMISTRY Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

UNIT-I

Air Pollution, Analysis & Control Methods: Qualitative study of environmental segments, air pollutants, sources, prevention & control, Green house gases & acid rain. Carbon monoxide, industrial sources & tranportation sources. Ozone hole & CFC's, global warming. Photochemical smog & PAN. Catalytic converters for mobile sources, Air quality analysis, Bhopal gas tragedy. Analysis of air pollutants, Dispersion of air pollutants-weather, wind speed and acidity.

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

UNIT-II

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. Public health significance & measurement of colour, turbidity, total solids, acidity, fluoride, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate & different forms of nitrogen in natural & polluted water. Significance of DO, BOD, COD & TOC. Water purification for drinking & industrial purposes, disinfection techniques, demineralization, sewage analysis, desalination processes & reverse osmosis.

UNIT-III

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.

Solid pollutants: Treatment and disposal. Treatment of industrial liquid wastes. Sewage and industrial effluent treatment. Radioactive wastes and its control. Composition of soil-inorganic and organic components.

Soil pollution: Classification of pollutants and their characteristics, sources, prevention and control, sampling and monitoring techniques.

References:

- 1. Environmental Chemistry: A. K. De, 7th Edn., New Age, 2013
- 2. Environmental Chemistry, S. K. Banerji, Prentice Hall India, 1993.



12 Hrs

12 Hrs

12 Hrs

- 3. Chemistry of Water Treatment, S. D. Faust and O.M. Aly, Butterworths, 1983.
- 4. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
- 5. Environmental Chemistry, I. Williams, John Wiley, 2001.
- 6. Environmental Pollution Analysis S.M. Khopkar, (Wiley Eastern), 2010.



OC P 407: INORGANIC CHEMISTRY PRACTICALS – I Teaching Hours: 4 hrs per week

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).

References

1. Vogel's Qualitative Inorganic Analysis : G.Svehla, 7th Edn., Longman, 2001

OC P 408: ORGANIC CHEMISTRY PRACTICALS – I Teaching Hours: 4 hrs per week

Single and two stage organic preparations

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, and picric acid

2. Alkylations-Preparations of nerolin and N-methyl anthranilic acid.

3. Acetylations–Preparations of β -D-glucose penta-acetate and 2-naphthyl acetate.

4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole and 7–hydroxy-4-methyl-coumarin.

5. Diazotisation reactions-Preparations of iodo, chloro and azo compounds.

- 6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
- 7. Condensation reactions–Condensations involving diethylmalonate and ethyl

acetoacetate. Aldol condensation and Perkin reactions.

8. Oxidation reactions-Preparation of p-nitrobenzoic acid and adeipic acid.

9. Halogenation reactions-Preparation of n-butylbromide & α , β -dibromocinnamic acid.

10.Oxidation reactions-Preparation of adipic & p-nitrobenzoic acids and p-benzoquinone.

11.Reduction reactions–Reductions of nitro compounds and carbonyl compounds.

References

- 1. Laboratory Manual in Organic Chemistry: R. K. Bansal (New Age, New Delhi)1990.
- 2. Experimental Organic Chemistry-Vol. I & II-P. R. Singh et al (TMH New Delhi)1981
- 3. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic Analysis- B. S. Furniss et al., (Longman-ELBS, London), 1989.
- 4. Systematic Lab Experiments in Organic Chemistry- Arun Sethi (New Age International Publishers-2010)

OC P 409: PHYSICAL CHEMISTRY PRACTICALS - I

Teaching Hours:4 hrs per week

Any 12 experiments are to be carried out

- 1. Potentiometric titration of halides in mixtures (Cl⁻, Br⁻ and I⁻) with silver nitrate
- 2. Potentiometric determination of redox potentials.
- 3. Potentiometric determination of dissociation constants of weak acids
- 4. Potentiometric and conductometric acid –base titrations in partial & non-aqueous media.
- 5. Conductometric titrations of displacement and precipitation reactions



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- 6. Determination of equivalent conductances and dissociation constants of weak acids.
- 7. Determination of solubility of lead iodide at different T & hence molar heat of solution
- 8. Determination of pH of buffer solutions with a pH meter & evaluation of pK_a of acids
- 9. Analysis of a binary mixture and determination of molar refraction of a solid and the composition of chloroform and acetone in its azeotropic mixture by refractometry
- 10. Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity
- 11. Study of variation of viscosity of a liquid with temperature
- 12. Determination of parachor value for CH₂ group by S.T method, the composition of a solution by S.T measurement and the CMC of a soap solution by S.T measurement.
- 13. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
- 14. Determination of degree of hydrolysis of CH₃COONa and NH₄Cl.
- 15. Determination of hydrolysis constant of aniline hydrochloride.
- 16. Verification of Nernst equation for Ag^+ , Cu^{2+} and Zn^{2+} species.
- 17. Determination of transport number of ions by emf method (Ag ⁺,Cd ²⁺,NO₃ ²⁻,SO₄ ²⁻ etc.)

References

- 1. Findlay's Practical Physical Chemistry: B. P. Levitt, 9th Edn., Longman, London, 1973.
- 2. Experimental Physical Chemistry: Das, Behera, 6th Edn., Tata McGraw Hill, New Delhi, 1983.
- Advanced Practical Physical Chemistry: 33rd Edn., J. B. Yadav, Krishna Prakashan Media (P) Ltd, 2015.
- 4. Experiments in Physical Chemistry: 1st Edn., J.C.Ghosh, Bharathi Bhavan, 1974.
- 5. Practical Physical Chemistry: 2nd Edn., B. Vishwanathan, P.S. Raghavan, Viva Books, 2012.
- 6. 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

Rationale /Learning Objectives:

- To enable the students to predict the spectral and structural properties of organic and inorganic molecules
- To acquaint the students with structure, types of bonds and preparatory methods in boranes, inorganic polymers, cage compounds and metal carbonyls
- To make the students to learn the properties of lanthanides and actinides and method of reduction of oxide ores

UNIT- I: 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

Chemistry of higher boranes: Classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9 , $B_{10}H_{14}$ and $B_nH_n^{2-}$. Carboranes and metallocarboranes.

Cyclophosphazenes, phosphazene polymers, P-O and P-S cage compounds. S-N compunds: binary sulphur nitrides - S_4N_4 , S_2N_2 and $(SN)_x$. Borazines and boron nitride.

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

UNIT-III

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

Methods of reduction of oxide ores, chemical and electrolytic reductions, Ellingham diagram, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

15 Hrs

15 Hrs

15 Hrs

References:

- 1. Symmetry and Spectroscopy of Molecules: K.Veera Reddy, 2nd Edn.,New Age Intl Publishers, 2009
- 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.
- Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3rd Edn., Wiley, 2007.
- 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.
- Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th Edn., Wiley, 2014.
- Advanced Inorganic Chemistry: Satya Prakash, G. D. Tuli, S. K. Basu, R. D. Madan, Vol. II, 4th Edn., S. Chand, 2014.
- 12. Chemistry of the Elements: N. N. Greenwood and A. Earnshaw, 2nd Edition, Pergamon Press, 1997.
- 13. 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

Rationale /Learning Objectives:

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

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, Knoevenagel condensation, Perkin reaction and Wittig reactions.

UNIT-II

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: Chemistry of Heterocyclic Compounds

Introduction, saturated and unsaturated heterocycles, three membered heterocycles structure, reactivity, synthesis and reactions of aziridines, epoxides, episulfides, diaziridines, oxaziranes and diazirines. Five membered simple and fused heterocyclessynthesis & reactions of derivatives of furan, pyrrole & thiophene. Six membered heterocycles- synthesis & reactions of derivatives of pyridine. Biologically important heterocycles. FusedHeterocycles-Indole, Benzofuran, Quinolines, Isoquinolines and Cumarines



15 Hrs

15 Hrs

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.

10. Advanced Organic Chemistry: Carey and Sundberg, Part A & B, 3rd edition, Plenum Press, New York, 1990.

- 11. Organic Chemistry: I. L. Finar, ELBS Longmann, Vol. I, 1984.
- 12. Advanced General Organic Chemistry: S. K. Ghosh, Book and Alleied (P) Ltd., 1998.
- 13. An Introduction to the Chemistry of Heterocyclic Compounds: Acheson, Wiley Eastern, 1987.
- 14. Heterocyclic Chemistry: J. Joule & G. Smith, Van-Nostrand, ELBS, 1978.



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Rationale /Learning Objectives:

application of HMO theory of linear conjugated systems and aromatic systems

of partition function and the irreversible system

Unit I: Statistical and Irreversible thermodynamics15 Hrs

OC H 453: ADVANCED PHYSICAL CHEMISTRY

Teaching Hours: 3 hrs per week

To study the significance of partition function, thermodynamics properties in terms

To understand ion-solvent interaction, different application of electrochemistry To learn approximate methods in quantum chemistry, their application and

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: Electrochemistry

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. Spectroscpic and thermochemical approach to ion-solvent interaction. Solvation number – Introduction, methods of determination.

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

UNIT-III: 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



15 Hrs ffect on

15 Hrs

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, 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. 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. Instrumental Methods of Chemical Analysis, Kudesia Sawhney, Pragati Prakasha (Meerut).
- 11. Introductory Quantum Chemistry: A. K. Chandra, 4th Edn., Tata McGraw Hill, 2009.
- 12. Quantum Chemistry: Ira N. Levine, 7th Edn., Prentice Hall, 2013.
- 13. Quantum Chemistry: R. K. Prasad, 4th Edn., New Age International Publications, 2012.
- Quantum Chemistry: Donald Allan McQuarrie, 5th Edn., University Science Books, 2013.



OC S 454: SPECTROSCOPY AND ANALYTICAL TECHNIQUES Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- 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
- To learn the principle, instrumentation and application of atomic absorption and emission spectrometer, molecular luminescence and nephelo & turbidometers
- To know the basic principle of mass spectrometry and application of mass spectroscopic techniques in structural elucidation of organic molecules

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, fluorimetry in quantitative analysis, instruments, fluorescence and structure, fluorescence quenching, 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. Activation analysis.

UNIT-III: Mass Spectrometry

12 Hrs

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, ¹H and ¹³C 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.
- 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.
- 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

Rationale /Learning Objectives:

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

UNIT I

12 Hrs

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intra ellular organelles and their functions, comparison of animal and plant cells. Overview of metabolic processes - catabolism and anabolism. ATP- the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems. Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

Lipoprotiens: composition and function, role in atherosclerosis, properties of lipid aggregates, micelles, bilavers, liposomes and their biological functions. Biological membranes- Fluid mosaic model of membrane structure. Lipid metabolism(
-oxidation of fatty acids).

Unit II: 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, a- 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 III: Carbohydrates

12 Hrs

12 Hrs

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.

References:

1. Principles of Biochemistry – A L Lehninger, Worth Publishers.

- 2. Nelson & Cox., Lehninger's Principles of Biochemistry.
- 3. Harper, Harper's Illustrated Biochemistry
- 4. Hermann Dugas, Bioorganic Chemistry.



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- 5. J. L. Jain, Fundamentals of Biochemistry, S. Vhand & Company Ltd.
- 6. Amino acids and Peptides- G. C. barret and D T Elmore (Cambridge university press) 1998.
- 7. The Carbohydrates Vol. IA I B IIA and IIB W. Pigman and D. Horton (Academic Press) 1970.
- 8. Bioorganic chemistry A chemical approach to enzyme action Herman Dugas and Christopher Penney.
- 9. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.



Open Elective papers

CH E 456: CHEMISTRY OF LIFE

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To learn formulation and manufacture of cosmetics, analysis of oils, fats and detergents
- To give an detailed account on food nutritional aspects, artificial food preservatives and colourants
- To learn basic concepts of dyes and fertilizers

Unit I: Cosmetics, Perfumery, Fats, Oils, Soaps and Detergents12 Hrs

Cosmetics: Formulations and manufacturing of cream and lotions, lipstick and nail polish, shampoos, hair dyes and tooth pastes.

Perfumery: Introduction, Compounds used in perfumery and their classification, methods of preparation and importance of phenyl ethanol, musk xylene, phenyl acetic acid and its esters, benzyl acetate, synthetic musks and jasmine.

Fats, Oils, Soaps and Detergents: Introduction, composition, properties, vegetable oils, animal oils, waxes, Classification, Analysis of oils, fats and waxes-acid value, saponification value, Iodine value, hydrogenation of oils, manufacture of soap, cleansing action of soap, synthetic detergents, surfactants.

Unit II: Food and its nutritional aspects

Introduction, definition of food and nutrition, classification of foods- vitamins, proteins and carbohydrates. Basic food science, basic knowledge of important nutrients, basic five food groups. Balanced diet- recommended dietary allowances, food list, planning the menu, food adulteration- common adulteration in food, contamination of food stuffs, microscopic examination of foods for adulterants. Food additives, food preservatives like benzoates, propionates, sorbates, bisulphites. Artificial sweeteners like saccharin, dulcin and sodium cyclamate. Artificial food colourants- coal tar dyes and non-permitted colours and metallic salts. Flavours-Vanillin, esters (fruit flavours) and monosodium glutamate.

Unit III: Dyes and Agrochemicals

Dyes: Introduction, organic dyes, classification, dyeing methods, application and evaluation of dyes, Natural dyes.

Fertilizers: Classification of fertilizers, prospective developments in mineral fertilizers manufacturing, Future process technologies in fertilizer industries-Ammonia technologies, urea technologies, phosphatic technologies

Insecticides and Pesticides: Introduction, Types-organic insecticides, inorganic insecticides, properties, uses, hazards, Fumigants, Fungicides



12 Hrs

12 Hrs

References:

- 1. Analysis of Foods H.E. Cox
- 2. Chemical analysis of Foods H.E Cox
- 3. Foods: Facts and Principles N Shakuntala Many & S. Swamy, 4th Edn. New Age International (1998).
- 4. Synthetic organic chemistry, G R Chatwal, Himalaya publishing house.
- 5. A formulary of paints and other coatings, M Ash & I Ash
- 6. Encyclopedia of Chemical Technology, Kiik & others.
- 7. Perfumary Technology, B. Billot and F. V. Wells
- 8. Synthetic Dyes Vol-I- Venkataraman, 1999.
- 9. A Text Book of Fertilizers, Ranjan Kumar Basak.
- 10. Agronomy Theory & Digest, Bidhan Chandra, Krishi Vishwavidyalaya, Mohanpur.
- Fertilizers, Organic Manures & Biofertilizers–A Product Quality Guide for Major & Micronutrients, HLS Tandon, Fertilizer Development and Consultation Organisation, New Delhi.
- 12. Handbook on Fertilizer Technology, Bham Swaminathan & Manish Goswami, The Fertilizer Association of India, New Delhi
- 13. Engineering Chemistry, M. M. Uppal, Khanna Publishers



CH E 457: ENVIRONMENTAL CHEMISTRY

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To give an awareness on major air pollutants, their effects and methods of control
- To render knowledge on waste water treatment, water analysis and desalination •
- To introduce toxicity of heavy metals, biochemical effects and major soil • pollutants and their control

UNIT-I

Air Pollution, Analysis & Control Methods: Qualitative study of environmental segments, air pollutants, sources, prevention & control, Green house gases & acid rain. Carbon monoxide, industrial sources & tranportation sources. Ozone hole & CFC's, global warming. Photochemical smog & PAN. Catalytic converters for mobile sources, Air quality analysis, Bhopal gas tragedy. Analysis of air pollutants, Dispersion of air pollutants-weather, wind speed and acidity.

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

UNIT-II

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. Public health significance & measurement of colour, turbidity, total solids, acidity, fluoride, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate & different forms of nitrogen in natural & polluted water. Significance of DO, BOD, COD & TOC. Water purification for drinking & industrial purposes, disinfection techniques, demineralization, sewage analysis, desalination processes & reverse osmosis.

UNIT-III

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.

Solid pollutants: Treatment and disposal. Treatment of industrial liquid wastes. Sewage and industrial effluent treatment. Radioactive wastes and its control. Composition of soilinorganic and organic components

Soil pollution: Classification of pollutants and their characteristics, sources, prevention and control, sampling and monitoring techniques.



12 Hrs

12 Hrs

12 Hrs

References:

- 1. Environmental Chemistry: A. K. De, 7th Edn., New Age, 2013
- 2. Environmental Chemistry, S. K. Banerji, Prentice Hall India, 1993.
- 3. Chemistry of Water Treatment, S. D. Faust and O.M. Aly, Butterworths, 1983.
- 4. Chemistry for Environmental Engineering, Sawyer and McCarty, McGraw Hill, 1978.
- 5. Environmental Chemistry, I. Williams, John Wiley, 2001.



OC P 458: 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 be 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. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
- 7. Hardness of water
- 8. Analysis of Halide Mixture Iodide by KIO₃ and total halide by gravimetrically.
- 9. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
- 10. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
- 11. Statistical Analysis of Data.

Reference:

1. Vogel's Text Book of Quantitative Chemical Analysis(5th Ed), G.H.Jeffrey, J. Bassette, J.Mendham and R.C.Denny, Longman, 1999.

OC P 459: 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 etal 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 460: 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 using water and benzene as solvents.

2. Detn.of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.

- 3. Heat of solution of substances by solubility method.
- 4. Phase diagram of two component systems by thermal analysis.
- 5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order



and rate constant, (b) Relative strength of two acids and c) Energy of activation.

- 6. First and second order kinetics of reaction between potassium persulphate and KI.
- 7. Kinetics of (a) inversion of cane sugar, (b)sodium formate-iodine reaction .
- 8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically. Thermometric titration of an acid with a base.

9. Detn.of association constants carboxylic acids in organic solvents by distribution method.

- 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. To compare the cleaning powers of two samples of detergents.

References:

- 1. Findlay's Practical Physical Chemistry: B. P. Levitt, 9th Edn., Longman, London, 1973.
- 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 Experiments in Physical Chemistry: 1st Edn., J.C.Ghosh, Bharathi Bhavan, 1974.
- 5 Practical Physical Chemistry: 2nd Edn., B. Vishwanathan, P.S. Raghavan, Viva Books, 2012.
- 6 Experimental Physical Chemistry: 1st Edn., V. D. Athawale, Parul Mathur, New age International, 2012.



III SEMESTER



OC H 501: REACTION MECHANISMS

Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit-I: Organic Name Reactions-I:

Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith Cycloproponation reaction, Stork Enamine reactions, Suzuki coupling, Heck reaction, Bucherer reaction, Wittig reaction and Mitsunobu reaction.

Unit-II: Molecular Rearrangements

Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baeyer-Villiger, Beckmann, Hofmann, Lossen, Curtius, Schmidt rearrangement, Stevens, Shapiro, Baker-Venkatraman, Smiles rearrangement, Sommelet-Houser rearrangement, and Amadori rearrangement.

Unit-III: Organic Name Reactions-II

Alagar-Flynn-Oyamada reaction, Auwers synthesis of Flavones, Baeyer-Drewson Indigo synthesis, Barton-olefin synthesis, Bayil-Hillman reaction, Corey-Kim reaction, Swern oxidation, Oppenauer oxidation, Yamada reaction, Dakin reaction, Houben-Hoesch reaction, Japp-Klingmen reaction, Staudinger reaction, Hell-Volhard Zelinsky reaction.

References:

1. Advanced Organic Chemistry-Part A & B: Francis A Carey and R. J. Sundberg, 5th Edn., Springer, 2007.

2. Organic Reactions Mechanisms: P. S. Kalsi and R. K. Parashar, Narosa Publishing House, 2011.

3. Synthetic Organic Chemistry: G. R. Chatwal, Himalaya, Bombay, 1994.

4. Organic Chemistry, Vol. I-II: I. L. Finar, Longmann ELBS, London, 2000.

5. Advanced Organic Chemistry-Reaction Mechanisms: Reinhard Bruckner, Academic, 2005.

6. Organic Synthesis: Jagadamba Singh and L. D. S. Yadav, Pragathi Prakashan, 2014.

7. Reactions, Rearrangements and Reagents: S. N. Sanyal, 4th Edn., Bharati Bhawan (P&D), 2013.

8. Name Reactions for Functional Group Transformations: Jie Jack Li and E. J. Corey, Wiley-Interscience, 2007.



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15 Hours

15 Hours

15 Hours

- 9. Organic synthesis Based on Name Reactions: A. Hassner and I. N. N. Namboothiri, 3rd Edn., Elsevier, 2012.
- 10. Name Reactions- A Collection of Detailed Reaction Mechanism: Jie Jack Li, 3rd Edn., Springer, 2006.

11. 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

Rationale /Learning Objectives:

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

Unit-I:

15 Hours

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: Reduction Reactions and Safety measurements (MSDS)15 Hours

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 LiAlH₄ & NaBH₄, 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-II: Activating, Protecting and Miscellaneous Reagents15 HoursActivating group: DCC, EDC, HATU, TBTU, CDI, BOP, T3P

Protection of NH Groups: Benzylchloroformate, Ethyl chloroformate, F-moc, Benzyl, Cbz and Boc-anhydride.

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

Protection of OH Group: Benzyl chloromethyl ether, Chkoromethyl methy ether, 3,4-Dihydro-2H-pyran, Tosylation, Ethyl vinyl ether and Trimethyl chlorosilane.

Protection of Aldehydes and Ketones: 1,2-ethane dithiol and Ethylene glycol Protection of diols, Protection of double bonds and triple bonds.

Miscellaneous Reagents: Lawesson reagent, Triphosgene, DMF-DMA, Sodamide and 1,3-propanedithiol.



References:

1. Modern Organic Reactions: H. O. House, W. A. Benjamin, 1972.

2. Organic Synthesis: R. E. Ireland, Prentice Hall India, 1969.

2. Art in Organic Synthesis: Anand, Bindra & Ranganathan, Wiley, 1970.

3. Advanced Organic Chemistry-Part A & B: F. A. Carrey & R. J. Sundberg, 4th Edn., Springer, 2007.

4. Modern Methods of Organic Synthesis: N. Carruthers and I. Coldham, Cambridge University, 2004.

5. Modern Reduction Methods: P. G. Anderson and I. J. Munslow, Wiley-VCH, 2008.

6. Protecting groups in Organic synthesis: T. W. Greene and P. G. M. Wuts, 3rd Edn., Willey, 1998.

7. Organic Synthesis: J. Singh and L. D. S. Yadav, 10th Edn., Pragathi Prakashan, 2014.

8. Modern organic Synthesis: An Introduction: G. S. Zweifel and M. H. Nantz, W. H. Freemen & Co. NY, 2006.

9. Advanced Organic Synthesis-Methods and Techniques: Richard S. Monson, Rhadon Academic Press, NY & London, 1971.



OC H 503: ADVANCED HETEROCYCLIC CHEMISTRY Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit-I: Heterocyclic Chemistry-I

Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Structure, reactivity, synthesis and reaction of the following: Four membered heterocycles-Oxitanes, Azetidines and Thietanes; Five membered heterocycles- 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.

Unit-II: Heterocyclic Chemistry-II

Mesoionic compounds: Introduction, Synthesis and reaction of sydnones, mesoionic oxadiazolium and thiadiazolium compounds. **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 Uracil, Thymine and Cytosine. Synthesis and classical structure of proof of Adenine and Guanine. Structural elucidation and synthesis of Uric acid, Caffeine, Pyrazine. Alloxazine and Isoalloxazine. **Heterocycles in functional group and ring transformation:** Alkanes from thiophenes, cycloalkanes from pyrazolines, dienes from pyrroles, alcohols from isooxazolines, acetylene from selenadiazoles, coumarin to benzofuran, sydnone to pyrazole, chromones to pyrazoles, furans to pyridines, pyrroles to pyrimidines.

Unit-III: Name Reactions in Heterocyclic Chemistry

Corey-Chaykovsky reaction, Hoch-Cambell aziridine synthesis, Jacobsen-Katsuki epoxidation, Wenker aziridine synthesis, Hoffmann Loffler-Freytag reaction, Gassman indole synthesis, Bucherer carbazole synthesis, Grabe-Ullmann carbazole synthesis, Schweizer allenyl azide rearrangement, Dimroth triazole synthesis, Fiesselmann thiophen, Erlenmeyer- Plochl azlactone synthesis, Cornforth rearrangement, Bockiheide reaction, Ciamician Dennstratt reaction, Gabriel-Colman rearrangement, Gould-Jacobs reaction.

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.



15 Hours

15 Hours

15 Hours

- 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.
- 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.



OC S 504: CHEMISTRY OF SYNTHETIC DRUGS Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To have an brief introduction to drugs and common terms used in medicinal chemistry, to understand the theories behind drug action, concepts of drug design, factors governing ability of drugs, synthesis of general and local anaesthetics, mode of action of general anaesthetics and local anaesthetics.
- To study the classification and structure of antibiotics, analgesics, antiinflammatory and cardiovascular agents, to understand their mode of action.
- To learn about CNS drugs, antihistamines and antimalarials. To understand their mode of action.

Unit I:

12 Hours

Drugs : Introduction to drugs, classification and nomenclature of drugs. Theories of drug action, analogs and prodrugs. Drug design- factors governing drug design, rational approach to drug design, tailoring of drugs, various methods of drug design, physico-chemical factors and biological activities. Factors governing ability of drugs.

General anaesthetics: introduction and classification. Synthesis of Halothane, Methoxyflurane and Methohexital sodium, Thiamylal sodium, mode of action.

Local anaesthetics: Introduction and classification. Synthesis of anaesthetics like Benzocaine, Butamben, Procaine Hydrochloride, Tetracaine hydrochloride, Butacaine sulphate, α -Eucaine, Benzamine hydrochloride, Prilocaine & Mepivacaine. Mode of action of Benzocaine, Butacaine sulphate, Mepivacaine, Procaine Hydrochloride,

Unit II:

12 Hours

Antibiotics: Introduction, classification, β -lactum antibiotics-Penicillin, cephalosporins. Mechanism of action of following antibiotics, Penicilin- Stereochemistry & Synthesis of Penicillin G, chemical degradation and bacterial resistance, mechanism of action Cephalosporians- Nomenclature, Classificfation, Degradation and 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 Hours

CNS depressants: Sedative and Hypnotic agents: Introduction, Classification. Synthesis of Barbitone, Methylphenobarbital, Butobarbitone, Chloradiazepoxide, Diazepam, and Phenobarbital.

Anticonvulsant: Synthesis of Phenytoin sodium, Trimethadione and Carbamazepine **CNS stimulants**: Introduction and classification. Synthesis and mechanism of action of Caffeine, Nikethamide, Phetermine, Methylphenidate.



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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, 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. Medicinal-Chemistry of Anticancer-Drugs: Carmen Avendano & J. C Menedez, Elsevier B.V, 2008.

5. The organic chemistry of drug synthesis Vol. III: Daniel Lednicer, John Wiley & Sons Inc., 1984

6. Medicinal Chemistry, a Molecular & Biochemical Approach: Thomas Nogrady & Donald F Weaver, 3rd Edn., Oxford University Press, 2005.

7. Advanced Practical Medicinal Chemistry: Ashutosh Kar, New Age International Pvt. Ltd., 2004.

8. Textbook of Organic Medicinal & Pharmaceutical Chemistry: Wilson, Giswold & Doerge 7th Edn., Lippincott Company, 1977.

9. Pharmacology & Pharmacotherapeutics-Part I and II: Satoskar and Bhandarkar 10th Edn., Bombay Popular Prakashan, 1986.

10. Principles of Medicinal Chemistry: Foye: 3rd Edn., Varghese Publishing House, 2008.

11. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi, 1996.

12. Burger's Medicinal Chemistry-Part-I-III: 4th Edn., Wolff, Wiley Eastern, NewYork, 1980.

13. Organic Chemistry-Vol. I and II: I. L. Finar, 6th Edn., Longman-ELBS, London, 2009.

14. Synthesis of Essential Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2006.



OC S 505: BIOORGANIC CHEMISTRY Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To understand the general structure, properties, classification of amino acids and general methods of synthesis of amino acids and to understand the structure and conformation of peptide bond
- To learn about nucleic acids and chemical synthesis of nucleosides and their functions
- To learn introduction, classification nomenclature, source and deficiency diseases of vitamins and to learn biological functions of vitamins

Unit-I:

Amino acids and Peptides: Introduction and synthesis of amino acids, Structure and conformation of peptide bond, N-terminal, C-terminal determination of peptides, enzymic cleavage of peptides, reagents for selective cleavage of polypeptide bonds. Peptide synthesis: Solution phase and Merrifield's solid phase synthesis, solution phase synthesis of oxytocin and vasopressin.

Proteins: Classification, Structure determination: primary, secondary, tertiary and quartenary structure determination. Stereochemistry of peptide chains, chemical bond involved in protein structure. Protein configuration: α helix, aminoacids effecting α helix, Rigid and planar peptide bond, Ramachandran plot, β – pleated sheets, structure of silk fibroin, random coil structure of proteins, triple helical structure collagen, similarity in 3D structure of haemoglobin and myoglobin.

Unit-II:

Nucleic acids: Introduction, nucleosides and nucleotides, structure of nucleosides, chemical synthesis of nucleosides- Adenosine , Guanosine (purine nucleosides), structure of nucleotides, synthesis of nucleotides(AMP). DNA (Watson & Crick model of double stranded DNA) & RNA. Functions of nucleic acids, Replication, Transcriptions, Translation, Protein synthesis, Flow of Genetic Information, Genetic code.

Unit- III:

Vitamins: Introduction, Classification and Nomenclature-Source and Deficiency diseases-Biological, functions of Vitamins- Study of the following Vitamins: Vitamin $A_1 \& A_2$, Vitamin B_6 and B_{12} , Vitamin C, Vitamin K_1 and K_2 , Pantothenic acid, folic acid.

Lipids: Introduction, classification of lipids, synthesis of fatty acids. Compound lipids-Phopholipids, Glycospingo lipids and derived lipids.

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. Essentials of Chemistry and Bio-Chemistry: Monique Laberge, Chelsor House Publishers, 2008.



12 Hours

12 Hours

12 Hours

CH E 506: MEDICINES IN DAILY LIFE Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To have brief introduction to drugs and common terms used in medicinal chemistry, mode of action of common drugs used in daily life and role of trance elements in human life.
- To study common drugs used as antibiotics, anti-inflammatory drugs, antineoplastic agents the classification and structure of antibiotics, analgesics, anti-inflammatory CNS agents and cardiovascular agents.
- To learn about ayurvedic medicines, medicinal plants, plant extraction and method of purification.

Unit I:

Introduction to drugs, chemotherapy, pharmacokinetics and pharmacodynamics, metabolites and antimetabolites. Prodrugs and analogs, agonists and antagonists. Concept of drug receptor, generic drugs. Introduction to common drugs used and their mode of action, classes of drugs, their role in curing the diseases, 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 II: Synthetic Drugs

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, Cis-platin and uracil mustards. Anti-virals-Acyclovir, Amantadine. Cardiovascular drugs- Amyl nitrite, sobitite, Guanidine, Methyldopa. Local anti-infective drugs-Sulfonamides, Ciprofloxacin, linezolid, Isoniazid, Chloroquin and primaquin. Natural Psychoactive drugs- the chemotherapy of the mind- Phenobarbital, phenytoin, barbiturates, thiopental sodium and caffeine.

Unit-III: Ayurvedic Medicines

Introduction, classification, identification of biological activity of plants, plant products, bhasmas-formulations-method of formulations and analysis of active ingradient.

Medicinal plants-survey of medicinal plants, identification of their occurrence, collection, method of storage, different techniques of extraction of the constituents. Phtocheical screening methods, semi purifications for active constituents. Isolation and identification of active molecules from medicinal plants. Chromatographic methods adopted for purification of active ingredients.

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. Medicinal-Chemistry of Anticancer-Drugs: Carmen Avendano & J. C Menedez, Elsevier B.V, 2008.



12 Hours

12 Hours

12 Hours

5. The organic chemistry of drug synthesis Vol. III: Daniel Lednicer, John Wiley & Sons Inc., 1984

6. Medicinal Chemistry, a Molecular & Biochemical Approach: Thomas Nogrady & Donald F Weaver, 3rd Edn., Oxford University Press, 2005.

7. Advanced Practical Medicinal Chemistry: Ashutosh Kar, New Age International Pvt. Ltd., 2004.

8. Textbook of Organic Medicinal & Pharmaceutical Chemistry: Wilson, Giswold & Doerge 7th Edn., Lippincott Company, 1977.

9. Pharmacology & Pharmacotherapeutics-Part I and II: Satoskar and Bhandarkar 10th Edn., Bombay Popular Prakashan, 1986.

10. Principles of Medicinal Chemistry: Foye: 3rd Edn., Varghese Publishing House, 2008.

11. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi, 1996.

12. Burger's Medicinal Chemistry-Part-I-III: 4th Edn., Wolff, Wiley Eastern, NewYork, 1980.

13. Organic Chemistry-Vol. I and II: I. L. Finar, 6th Edn., Longman-ELBS, London, 2009.

14. Synthesis of Essential Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2006.



CH E 507: CHEMISTRY OF MATERIALS Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To have brief knowledge on cement, glass lubricants, paints, pigments, metal finishing and chemistry behind these materials.
- To understand the concept of catalysis, to study different types of corrosion, chemical energy sources
- To have sound knowledge on polymers and polymer composites. .

Unit I:

12 Hours

Cement: Types, Manufacture, Additives, Setting, Properties & Testing of cement.

Glass: Manufacture, Properties, Types, Shaping of sheets & plate glasses. Annealing, Finishing, Special glasses.

Lubricants: Theories (mechanisms) of lubrication, Classification of lubricants, Properties of lubricants, Choice of lubricants.

Paints and Pigments: White pigments (white lead, ZnO, lithopone, titanium dioxide),Colour pigments (Blue, red, yellow and green pigments). Paints and distempers:Requirements of a good paint, Emulsion, Latex, Luminescent paints, Fire retardant paints,Varnishes,Enamels,Lacquers,SolventsandThinners.

Metal Finishing: Characteristics of a good deposit, Factors influencing the nature of deposit, Methods of cleaning the metal surface to be coated, Electroplating: Requirements of an electrolyte solution for electroplating, Applications of electroplating: Electroplating of Copper, Nickel, Chromium, Electroless Plating: Electroless plating of Nickel and Copper.

Unit II:

12 Hours

12 Hours

Catalysis: Introduction, action of a catalyst, characteristics of catalytic reactions, types of catalysis, catalytic promoters, catalytic poisons. Surface of a catalyst and its role on catalytic reaction. Some industrial processes using catalysts, criteria for choosing a catalyst for industrial application.

Corrosion: Introduction, Definition, Dry corrosion, Electrochemical theory of Corrosion, Factors influencing the Corrosion rate, Types of Corrosion, Corrosion Control.

Chemical energy system and limitations, principles and applications of primary & secondary batteries and fuel cells. Basics of solar energy, future energy storer.

Unit III:

Polymers: Introduction, some basic definitions, classification of polymers. Types of polymerization, methods of polymerization, glass transition temperature, structure-property relationship, resins and plastics, moulding of plastics into articles, some commercial polymers-Polyethylene, Teflon, Polyurethanes. Elastomers, synthetic rubbers, adhesives.

Polymer composites- Synthesis, properties and uses. **Conducting polymers**: Synthesis and applications. Problems of plastic waste management. Strategies for development of environmental friendly polymers.



References:

1. Introduction to Industrial Chemistry: B. K. Sharma, 10th Edn., Goel Publishing, Meerut, 1998

2. Engineering Chemistry: R. V. Gadag and A. Nityananda Shetty, IK International Publishing House Pvt. Ltd., Bangalore, 2006.

3. Text Book of Engineering Chemistry: R. Gopalan, D. Venkappayya and Sulochana Nagarajan, 4th Edn., Vikas Publishing House Pvt. Ltd., New Delhi, 2006.

4. Atkin's Physical Chemistry: P. Atkins and J. de Paula, 8th Ed., Oxford University Press, 2008.

5. Polymer Science and Technology: J. R. Fried, 3rd Edn., Prentice Hall. 2014.

6. Advanced Physical Chemistry: Gurudeep R Chatwal, 35th Edn., Goel Publishing, Meetut, 2009

7. A Text Book of Engineering Chemistry: S. S. Dara, 2nd Edn., S. Chand and Company Ltd., 2007.

8. Engineering Chemistry: M. M. Uppal, 7th Ed., Khanna Publishers, 2011.



OC P 508: 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 509: 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.

4. Laboratory Experiments in Organic Chemistry: Adam, Johnson & Wicon, McMillan, London, 1979.

5. Experimental Organic Chemistry: H. D. Durst & G. E. Goke, McGraw-Hill, 1980

OC P 510: PROJECT WORK AND DISSERTATION

8 Hours per week



IV SEMESTER



OC H 551: ORGANOMETALLIC CHEMISTRY Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit-I:

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

Unit- II: 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: Reagents in Organic Synthesis-II

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

References :

1. Principles and Applications of Organotransition Metal Chemistry: J. P. Collman, L. S. Hegedus, J. R. Norton and R. G. Finke, University Science Books, 1987.

- 2. Organometallic Chemistry: R. C. Mehrotra and A. Singh, New Age International, 1999.
- 3. Organometallic Chemistry of Transition Metals: R. H. Crabtree, Wiley , 1999.
- 4. Advanced Inorganic Chemistry: F. A. Cotton and G. Wilkinson, Wiley, 1991.

3. Organic Name Reactions and Molecular Rearrangements: Gurudeep Raj, 3rd Edn., Krishna Prakashan Media (P) Ltd., 2011.

4. Organic Synthesis: Jagadamba Singh and L. D. S. Yadav, 10th Edn., Pragathi Prakashan, 2014.



15 Hours

15 Hours

15 Hours

OC H 552: ORGANIC SYNTHETIC DESIGN AND GREEN TECHNIQUES Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

- To learn about synthetic design, planning of organic synthesis and functionality of • groups.
- 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
- 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

Unit-I

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. **15 Hours**

Unit-II

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, Benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxyindole-3-acetic acid, 6-methyl quinoline and 1-phenyl-4-p-methoxyphenyl-1,3-butadiene. Illustrative Synthesis: Juvabione, Longifolene, Prelog-Djerassi Lactone, Taxol, Epothilone.

Unit-III:

Green Chemistry Techniques:

Introduction, Principles, Concept of atom economy in chemical synthesis, techniques and direction in practicing green chemistry: Applications of microwave irradiation and ultrasound in chemical processes. Use of renewable feedstock and biosynthesis-Solvent free organic reactions, use of safer reagents, greener solvents and greener catalysts.

Green Chemistry in action: Greener synthesis of adipic acid, catechol, paracetamol, caprolactum, furfural, citral, multicomponent synthesis, Green chemistry in manufacture of drugs

References



15 Hours

15 Hours

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.



OC H 553: PHOTOCHEMISTRY AND ASYMMETRIC SYNTHESIS Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit I:

15 Hours Organic Photochemistry: Bonding and antibonding orbital, σ and π orbitals, σ^* and π^* orbitals, singlet and triplet states, relative energies and excited states, Chemistry of excited states of organic molecules, Jablonski diagram and quantum yield, Photodissociation, Photoreduction, Photochemical isomerisation, Photocyclisation and related reactions. Norrish Type-I and Type-II reactions, Di-pi methane rearrangement, Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction, Photochemistry of alkenes, benzenes, photochemistry of substituted cyclohexanes, Yang cyclisation. Photochemistry of vision, Introduction to Photochemical cells, energy conversion and storage

Unit II:

Pericyclic Reactions: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. 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.

Cycloaddition Reaction: Suprafacial and Antarafacial addition, 4n and 4n+2 systems, 1,3-dipolar cyclo additions.

Sigmatropic Reactions: Suprafacial and Antrafacial shift of H, [1,3], [1,5], [1,7] and [3,3]-sigmatropic shifts. Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

UNIT III:

15 Hours

15 Hours

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

Rationale /Learning Objectives:

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

Unit I:

Anti-neoplastic agents: Introduction, Classification. Carcinogenesis-initiation, promotion, progression of cancer cells. Types of cancer-solid tumors, hematological malignancies. Treatment of cancer-surgery, photoradiation therapy, radiation therapy) immunotherapy, chemotherapy, combined chemotherapy, adjuvant chemotherapy, gene therapy. Alkylating mechanism of action of Mechlorethamine HCl, agents-classification, structure and Chlorambucil and cyclophosphamide.

Antimetabolites- Folic acid Antagonists-Leucovorin Rescue. Purine Antagonists: 6-Mercaptopurine (6MP) and 6-thioguanine (6TG).

Cardiovascular agents: Introduction and classification.

Antiarrythmic agents- Introduction, Mechanism of action, Synthesis of Verapamil

Unit II:

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, Cefixin 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 and Aliskiren. Proton pump inhibitors: Synthesis of Rabeprazole and Ranitidine. Mode of action of Rabeprazole. Quinolone Antibacterials: Synthesis of Nalidixic acids and Ciprofloxacin. Mode of action of Ciprofloxacin.

Unit III:

Industrial Pharmacy: Introduction to industrial processing, extraction-methods of extraction, continuous extraction. Distillation-theory of distillation, methods of distillation, azeotropic. steam. extractive distillation. Techniques of Crystallization-cooling crystallization, seeding crystallization and anti-solvent crystallization. Drying-classification and types of dryers-tray dryer, fluidized dryer, freeze dryer, spray dryer, factors affecting drying.

Technology of drug delivery system: Manufacturing, quality control, standard operating procedure, labeling, packing and storage of formulations belonging to categories of solid(tablets capsules), liquids (syrup, emulsions, suspensions) and parental dosage forms. Brief introduction to patents.

References:



12 Hours

12 Hour

12 Hours

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.



OC S 555: CHEMISTRY OF NATURAL PRODUCTS Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit-I

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, Adrenaline, Ephedrine, Piperine, Cinchonine, Quinine, Morphine and Reserpine.

Unit-II

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

Diterpenoids: Abietic and Pimaric acid, <u>Triterpenoids</u>: Squalene. <u>Carotenoide</u>: Introduction and geometrical isomerization of Carotenes. Structre and Synthesis of β -Carotene and Lycopene.

Prostaglandins: Introduction, Nomenclature, Classification and Biological role of Prostaglandins, Structural elucidation and stereochemistry of PGE₁, PGE₂ and PGE₃. Total synthesis of PGE₁ (Corey's method)

Unit-III

12 Hours

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.



12 Hours

12 Hours

OC S 556: INDUSTRIAL ORGANIC CHEMISTRY Teaching Hours: 3 hrs per week

Rationale /Learning Objectives:

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

Unit-I

12 Hours

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 Hours

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. <u>Pigments:</u> 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:

Agrochemicals: Introduction to heterocycles in Herbicides. Inhibitor of photosynthesis: 1,3,5-triazine, 1,2,4-triazine, pyridazinones, thiadiazoles, benzothiazole, oxadiazole, pyridines and miscellaneous. **Plant growth regulators:** Indole, pyrimidine. Fungicides: Triazoles, pyrimidines, imidazoles, benzimidazoles, Sulfenyl derivatives. Dicarboximides. Heterocyclic organophosporous reagents. **Insecticides:** Organo phosphorus compounds. **Veterinary Products:** Antimicrobials, Antiprotozoals, Ectoparasiticides, Growth promotants.



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



OC P 557: ORGANIC CHEMISTRY PRACTICALS- V Teaching Hours: 6 hrs per week

Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toludine, ε -Caprolactam from cyclohexanone, p-Amionobenzoic acid from p-Nitrotoludine, s-Tribromobenzene from aniline, o-hydroxy acetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluine from p-Toludine, 2,5-Dihydroxy acetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid, 2,4-Dinitrophenol from Chlorobenzene, o-Aminobenzoic acid from Phthalic anhydride, 2-Carbethoxycyclopentanone from Adipic acid, α -Acetylamino cinnamic acid from Glycine, p-Aminoazobenzene from Aniline.

Elucidation of structure of organic compounds using UV, IR,NMR and Mass spectra.

OC P 558: ORGANIC CHEMISTRY PRACTICALS –VI

Teaching Hours: 6 hrs per week

Seperation, 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.

OC P 559: ORGANIC CHEMISTRY PRACTICALS- VII Teaching Hours: 6 hrs per week

Isolation and Charecterization 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. Charecterization 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

