MANGALORE UNIVERSITY

Department of Studies in Chemistry
Mangalagangothri-574199

M. Sc. Degree Programme

(CHOICE BASED CREDIT SYSTEM – SEMESTER SCHEME)

Syllabus for M.Sc. Degree Programme in

ORGANIC CHEMISTRY

(With effective from the Academic Year 2024-25)

MANGALORE UNIVERSITY

DEPARTMENT OF STUDIES IN CHEMISTRY
MANGALAGANGOTHRI – 574199

Two years Master Degree Programme (Four Semesters)
M.Sc. in ORGANIC CHEMISTRY
Choice Based Credit System (CBCS) Semester Scheme
(With effective from the Academic Year 2024-25)

PREAMBLE

Revision of syllabi for the two year Masters Degree (Choice Based Credit System - Semester Scheme) Programme in Organic Chemistry.

PG BOS in Chemistry/Organic Chemistry has revised and prepared the syllabi (CBCS based) for the PG programme in Organic Chemistry by giving certain guidelines to offer Hard Core, Soft Core and Open Elective courses with credits to each course amounting to 90 credits for the entire programme. The 12 theory courses (4 credits each) are assigned as Hard Core courses with total credits of 48. Students have to study 4 soft core theory courses (3 credits each) with a total of 12 credits. The choice has been given for the soft core courses. Nine practical courses will be taught as soft core courses. Three of these practical courses will be offered in each of the I and II semesters with 2 credits for each course and two practical courses in III semester and one practical course in the IV Semester with 3 credits for each course. In lieu of the second practical course in the IV Semester, students will carry out project work and dissertation for 3 credits. Total Soft core credits from practical courses amounts to 24. Board of Studies in chemistry/organic chemistry has carefully chosen two Open Elective courses (3 credits each) for the students from other disciplines, one each in II and III semesters, with total credits of 6. Therefore, grand total credits for the programme = 90. A detailed skeleton of the entire programme is being tabulated for the benefit of the aspiring post graduates. Other important aspects such as University question paper pattern, internal assessment examinations, allotment of marks and the approximate dates of the internal examinations are being tabulated with a discussion in the BOS.

Sl. No.	Semester	Hard core (H) credits	Soft core (S) credits	Open elective (E) credits	Practical / Project Report (P) credits	No. of Practical Paper/Project Work*	No. of Theory Paper	Total Credits
1	I	12	3	--	6	3(S)	3(H)+1(S)	21
2	II	12	3	3	6	3(S)	3(H)+1(S)+ 1(E)	24
3	III	12	3	3	6	2(S)	3(H)+1(S)+ 1(E)	24
4	IV	12	3	--	3+3	1+1*(Project Work)(S)	3(H)+1(S)	21
Total		48	12	6	24	--	--	90

Total Credits from all the Four Semesters: 90
Total Hard Core credits = 48 (T)/90=53.3%; Total Soft Core credits = 36/90=40.0%

Open Elective Credits = 6 /90=6.7% (Not to considered for calculating the CGPA)
H = Hard Core, S = Soft Core, P = Practical/Project Work E = Open Elective

OBJECTIVES OF THE SYLLABUS

The revised syllabus is designed to provide a flexible structure within which students can choose the topic of their interest in addition to knowledge in the fundamentals of the subject. The syllabus takes into account the requirements for higher education, namely to maintain the quality of education and student competency level on par with national and international institutions. The syllabus is structured to ensure that the students become aware of the practical applications of scientific knowledge to build careers in the scientific field.
The syllabus aims to enable students to:

- To provide knowledge and skills in the field of chemistry
- To generate manpower trained in chemistry to meet the need of industry and academia and to pursue further studies by acquiring the knowledge and understanding of chemical principles.
- To appreciate, understand and use the scientific method in the solving of problems.
- To develop the ability to disseminate chemical information effectively.
- To acquire good laboratory skills and practice safety measures when using equipment and chemicals as well as the safe disposal of chemical waste.
- To apply chemical knowledge to everyday life situations and develop inquisitiveness in order to continue the search for new ways in which the resources of our environment can be used in a sustainable way.
- To develop the personality of an individual by giving them the necessary skills.
- To offer 100% placement assistance.

SCOPE OF THE PROGRAMME

M.Sc. Organic Chemistry is a specialized post graduate course with job opportunities in industry. The Research and Development and Quality Control divisions of every industry require personnel who are trained in handling various instruments. The structure of the programme and curriculum is designed to enable the students to develop creative abilities which are very much needed by the industry. The programme is definitely at par with M.Sc. Chemistry, M.Sc. Industrial Chemistry, M.Sc. Analytical Chemistry, etc.

ELIGIBILITY

- Candidates would have studied any branch of Physical or biological science with chemistry as one of the optional / major / special subjects in the under graduate level
- Not less than 45% (40% in case of SC/ST students) marks in the aggregate excluding languages in the under graduate level.
- The students should have studied physics and Mathematics as optional / major / special / minor / subsidiary subjects either at B.Sc. or at P.U.C. / Higher Secondary level.
- B.Sc. Polymer Chemistry graduates are also eligible for admission to this programme provided they have studied Physics and Mathematics as major/subsidiary subjects at B.Sc./P.U.C./Higher Secondary level.

Detailed Structure, Credits and Scheme of Examination of the Postgraduate Courses of Chemistry under Choice Based Credit System-Semester Scheme for the entire programme

I Semester					
Description of the Course	**Hard Core/ Soft Core Course**	**Teaching Hours per Week & Sem**	**Credits**	**Hours of Examination**	**Max. Marks: Exam.+ IA = Total**
OC H 411: Inorganic Chemistry	H	4 48	4	3	70 + 30 =100
OC H 412: Organic Chemistry	H	4 48	4	3	70 + 30 =100
OC H 413: Physical Chemistry	H	4 48	4	3	70 + 30 =100
OC S 414: Inorganic Spectroscopy and Optical Methods OC S 415: Molecular Spectroscopy and Diffraction Techniques (any one of the above)	S	3 36	3	3	70 + 30 =100
OC P 416: Inorganic Chemistry Practicals-I	S	4 48	2	4	35 + 15 =50
OC P 417: Organic Chemistry Practicals-I	S	4 48	2	4	35 + 15 =50
OC P 418: Physical Chemistry Practicals-I	S	4 48	2	4	35 + 15 =50
		Total	**21**		**550**
II Semester					
Description of the Course	**Hard Core/Soft Core Course**	**Teaching Hours per Week Sem**	**Credits**	**Hours of Examination**	**Max. Marks: Exam.+ IA = Total**
OC H 461: Advanced Inorganic Chemistry	H	4 48	4	3	70 + 30 =100
OC H 462: Advanced Organic Chemistry	H	4 48	4	3	70 + 30 =100
OC H 463: Advanced Physical Chemistry	H	4 48	4	3	70 + 30 =100
OC S 464: Organic Spectroscopy OC S 465: Environmental Chemistry (any one of the above)	S	3 36	3	3	70 + 30 =100
OC E 466: Environmental, Electro and Polymer Chemistry	S	3 36	3	3	70 + 30 =100
OC P 467: Inorganic Chemistry Practicals-II	S	4 48	2	4	35 + 15 =50
OC P 468: Organic Chemistry Practicals-II	S	4 48	2	4	35 + 15 =50
OC P 469: Physical Chemistry Practicals-II	S	4 48	2	4	35 + 15 =50
		Total	**24**		**650**

III Semester					
Description of the Course	**Hard Core/ Soft Core Course**	**Teaching Hours per Week Sem**	**Credits**	**Hours of Examination**	**Max. Marks: Exam.+ IA = Total**
OC H 511: Organic Reaction Mechanism	H	4 48	4	3	70 + 30 =100
OC H 512: Reagents for Organic Synthesis	H	4 48	4	3	70 + 30 =100
OC H 513: Advanced Heterocyclic Chemistry	H	4 48	4	3	70 + 30 =100
OC S 514: Bioorganic Chemistry OC S 515: Chemistry of Biomolecules	S	3 36	3	3	70 + 30 =100
OC E 516: Analytical and Green Chemistry	S	3 36	3	3	70 + 30 =100
OC P 517: Organic Chemistry Practicals-III	S	6 72	3	6	70 + 30 =100
OC P 518: Organic Chemistry Practicals-IV	S	6 72	3	6	70 + 30 =100
		Total	**24**		**700**
IV Semester					
Description of the Course	**Hard Core/ Soft Core Course**	**Teaching Hours per Week Sem**	**Credits**	**Hours of Examination**	**Max. Marks: Exam.+ IA = Total**
OC H 561: Organic Synthetic Methods And Green Techniques	H	4 48	4	3	70 + 30 =100
OC H 562: Medicinal Chemistry And Advanced Stereochemistry	H	4 48	4	3	70 + 30 =100
OC H 563: Natural Products Chemistry	H	4 48	4	3	70 + 30 =100
OC S 564: Synthetic Polymers, Dyes And Pesticides OC S 565: Chromatographic Techniques For Organic Chemistry (Any one of the above two)	S	3 36	3	3	70 + 30 =100
OC P 566: Organic Chemistry Practicals-V	S	6 72	3	6	70 + 30 =100
OC P 567: Project work and Dissertation	S	6 72	3	-	70 + 30 =100
		Total	**21**		**600**
		Grand Total	**90**		**2500**

BASIS FOR INTERNAL ASSESSMENT: Internal assessment marks in theory papers of I, II III and IV semesters shall be based on two tests conducted for 30 marks for each course. Question Papers for Internal Assessment in the theory courses shall consist of Part A and B. For hard core theory courses-Part A shall contain eight (8) very short answer objective type questions carrying 2 marks each, out of which five (5) questions are to be answered. Part B shall contain four (4) descriptive answer questions with internal choice (a or b) carrying 5 marks each. For soft core

and open electives, Par A shall contain nine (9) very short answer objective type questions carrying 2 marks each, out of which six (6) questions are to be answered. Part B shall contain three (3) descriptive answer questions with internal choice (a or b) carrying 6 marks each. The tests may be conducted after 8 and 14 weeks from the start of the semester. Average of two test marks will be considered as internal assessment marks. Practical internal assessment marks shall be based on test and records. For I and II semesters, 10 marks for experiment and 5 marks for record to be allotted. For III and IV Semesters, 20 marks for experiment and 10 marks for record to be allotted. The practical tests may be conducted after 12 weeks from the start of the semester. Internal Assessment marks on Project work in the IV semester is based on two seminars of 45 minutes duration each carrying 15 marks. The seminars to be delivered in III Semester on the subject and in the IV Semester on the project work.

THEORY QUESTION PAPER PATTERN FOR HARD CORE, SOFT CORE AND OPEN ELECTIVE COURSES

The syllabus of each theory course shall be grouped into units of 12 teaching hours. All hard core courses will have 4 units. Soft core and open elective courses will have 3 units. Question Papers in all the theory courses shall consist of Part A and B. For hard core theory courses - Part A shall contain eight (8) very short answer objective type questions carrying 2 marks each drawn from all the four units of the syllabus (2 questions per unit) out of which five (5) questions are to be answered. Part B shall contain eight (8) brief and/or long answer questions carrying 12 marks each drawn from all the four units of the syllabus (2 questions per unit) out of which five(5) questions to be answered choosing at least one question from each unit.

For soft core and open electives, Part A shall contain nine (9) very short answer objective type questions carrying 2 marks each drawn from all the three units of the syllabus (3 questions per unit). Seven (7) questions are to be answered. Part B shall contain six (6) brief and/or long answer questions carrying 14 marks each drawn from all the three units of the syllabus (2 questions per unit). There may be a maximum of four sub-divisions per question, carrying 3 or more marks per sub-division. Four (4) out of six (6) questions to be answered choosing at least one question from each unit.

M.Sc. Organic Chemistry Hard Core Course

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

Answer any **Five** sub-divisions from **Question No. 1** in **Part-A** and **Five** questions from **Part-B**. Figures to the right indicate marks.

Part-A

1. Answer any **Five** subdivisions **(5x2=10)**

a), b) } Unit-I

c), d) } Unit-II

e), f) } Unit-III

g), h) } Unit-IV

Part-B

Answer any **FIVE** questions selecting minimum of **1 question** from each unit **(5x12=60)**

Unit – I

2. a), b) } Or 2. a), b), c) } Or 2. a), b), c), d) }

3. a), b) } Or 3. a), b), c) } Or 3. a), b), c), d) }

Unit – II

4. a), b) } Or 4. a), b), c) } Or 4. a), b), c), d) }

5. a), b) } Or 5. a), b), c) } Or 5. a), b), c), d) }

Unit – III

6. a), b) } Or 6. a), b), c) } Or 6. a), b), c), d) }

7. a), b) } Or 7. a), b), c) } Or 7. a), b), c), d) }

Unit – IV

8. a), b) } Or 8. a), b), c) } Or 8. a), b), c), d) }

9. a), b) } Or 9. a), b), c) } Or 9. a), b), c), d) }

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M.Sc. Organic Chemistry Soft Core or Open Elective Course

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

Answer any **seven** sub-divisions from **Question No. 1** in **Part-A** and **Four** questions from **Part-B**. Figures to the right indicate marks.

Part-A

1. Answer any **Five** subdivisions **(7x2=14)**

a), b), c) } Unit-I

d), e), f) } Unit-II

f), g), h) } Unit-III

Part-B

Answer any **Four** questions selecting minimum of **1 question** from each unit **(4x14=56)**

Unit – I

2. a), b) } Or 2. a), b), c) } Or 2. a), b), c), d) }

3. a), b) } Or 3. a), b), c) } Or 3. a), b), c), d) }

Unit – II

4. a), b) } Or 4. a), b), c) } Or 4. a), b), c), d) }

5. a), b) } Or 5. a), b), c) } Or 5. a), b), c), d) }

Unit – III

6. a), b) } Or 6. a), b), c) } Or 6. a), b), c), d) }

7. a), b) } Or 7. a), b), c) } Or 7. a), b), c), d) }

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PRACTICAL QUESTION PAPER PATTERN: In the Practical courses, out of 35 marks, 5 marks shall be allotted for the viva-voce and 30 marks for the experiment in I and II semesters and in III and IV semesters, out of 70 marks, 10 marks shall be allotted for the viva-voce to be conducted during practical examination and 60 marks for the experiment.

PROJECT REPORT: In the 4th semester there shall be a project work and dissertation to be carried out either in the department or in an institution or industry for 4-6 weeks and submit the report. The Project Report shall be evaluated by two examiners as in the case of theory papers for 70 marks.

PROGRAMME OUTCOMES

- Master of Science in Organic Chemistry basically aims at the training of students with a detailed knowledge base in Organic Chemistry of potential utility in academia as well as Industry through advanced course work and laboratory work in the department and a project work in industries or premier institutions.
- To qualify NET/GATE/SET/Civil Services and other competitive examinations.
- For exploring global level research support for doctoral and post-doctoral studies.
- For professional employment in different domains such as academics, industries, analytical laboratories, scientific organizations, entrepreneurship, administrative positions etc.
- For enhancing the connectivity between academic institutions and industrial organisations.

PROGRAMME SPECIFIC OUTCOMES

- Students will equip themselves with up-to-date knowledge in the field of frontier areas of chemistry.
- Attain confidence to take up R & D positions in teaching, higher education institutions, public sector & private companies.
- Get motivated to take up higher studies.
- Will be able to use their knowledge in day to day life and work for betterment of society.
- Understand the social responsibility of chemistry in educating general public about protection of environment against pollution.
- Knowledge & Confidence to clear nation level competitive examinations.
- To make use of the chemistry knowledge to analyze real samples like food samples, biological samples, pharmaceutical products and environmental samples.
- To propose/develop cost effective and novel methods of synthesis of bioactive compounds/nanomaterials and in turn to design target oriented drugs to treat different diseases.
- To develop new polymeric materials, energy storage devices and fuel cells.

M.Sc. ORGANIC CHEMISTRY
FIRST SEMESTER

OC H 411: INORGANIC CHEMISTRY

Course Outcomes

- Learn the basics of ionic and covalent bonding, lattice and hydration energy,
- Enable the students to understand VSEPR and MOT theory.
- Enlighten the students to understand HSAB concept, non-aqueous solvents and ionic liquids.
- Get the knowledge alkali/alkaline earth metal complexes, compounds of boron, carbon and silicon.
- Understanding of use of organic precipitants and extraction techniques, masking and de-masking techniques, sampling techniques and statistical treatment of errors.

UNIT-I: Structures and Energetics of Ionic Crystals and Covalent Bonds [12 Hours]

Ionic Bond: Properties of ionic compounds, crystal lattices, closed packed structures, coordination number of an ion, radius ratio rule, structures of crystal lattices-NaCl, CsCl, ZnS and rutile. Lattice energy: Born Lande equation, Born-Haber cycle, uses of Born-Haber type of calculations. Covalent character in ionic bonds, Fajan's rules, hydration energy and solubility of ionic solids. Ionic radii, factors affecting the ionic radii, radius ratio rules.

Covalent Bond: Valence bond theory, resonance, hybridization and energetics of hybridization, Bent's rule, VSEPR theory-Deduction of molecular shapes. MOT of homo and heteronuclear diatomic and triatomic molecules& MO treatment for the molecules involving delocalized π-bonding (CO_3^{2-}, NO_3^- and CO_2). M.O. correlation diagrams (Walsh) for triatomic molecules.

UNIT-II [12 Hours]

Modern concept of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard-Soft Acids and Bases, Classification and Theoretical backgrounds.

Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties), protic solvents (anhydrous H_2SO_4, HF and glacial acetic acid), aprotic solvents (liquid SO_2, BrF_3 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron. Super acids and super bases. Heterogeneous acid-base reactions.

Ionic liquids: Molten salt solvent systems, Ionic liquids at ambient temperature, Reactions in and applications of molten salt/ionic liquid media. Supercritical fluids: Properties of supercritical fluids and their uses as solvents. Supercritical fluids as media for inorganic chemistry.

UNIT-III [12 Hours]

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological importance.

Synthesis, properties and structures of boron, carbon and silicon compounds: Chemistry of higher boranes, classification, structures and MO description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9, $B_{10}H_{14}$ and $B_nH_n^{2-}$, boron nitride, borazines,

carboranes, metalloboranes, metallocarboranes; Graphite, graphene, carbon nanotubes and zeolites. Cyclophosphazenes, phosphazene polymers and S-N compounds.

UNIT-IV **[12 Hours]**

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.

Chelometric titrations: Titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

Sampling techniques and preparation of samples for analysis.

References

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2. Shriver & Atkins' Inorganic Chemistry, 5th edn., P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2010).
3. Inorganic Chemistry, 2nd edn., C. E. Housecroft and A.G. Sharpe, Pearson Prentice Hall (2005).
4. Concise Inorganic Chemistry, 5thedn., J. D. Lee, New Age International (1996).
5. Concise Inorganic Chemistry, 5th edn., J. D. Lee, Blackwell Science (2000).
6. Concepts & Models of Inorganic Chemistry, B. E. Douglas, D. McDaniel & A. Alexander, Wiley (2001).
7. Basic Inorganic Chemistry, 3rd edn., F. A. Cotton, G. Wilkinson and P. L. Gaus, John Wiley and Sons (2002).
8. Inorganic Chemistry, 3rd edn., J. E. Huheey, Harper and Row Publishers (1983).
9. Inorganic Chemistry, 5th edn., G. L. Miessler, P. J. Fischer and D. A. Tarr, Pearson (2014).
10. Inorganic Chemistry, 6th edn., D. F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
11. Inorganic Chemistry, 4th edn., C. E. Housecroft and A. G. Sharpe, Pearson Education (2012).
12. Introduction to Modern Inorganic Chemistry, K.M. Mackay and R.A. Mackay, Blackie Publication (1989).
13. Concepts and Models of Inorganic Chemistry 3rd edition. B.E. Douglas, D.H. McDaniel and Alexander, Wiley (2001).
14. Ionic liquids-Classes and Properties, Ed. Scott T. Handy, Intech Publisher (2011).

OC H 412: ORGANIC CHEMISTRY

Course Outcome

- Enable the students to learn the bonding in organic systems, various aspects of aromaticity, electronic effects, acidity and basicity of organic compounds.
- To gain knowledge on methods of determination of reaction mechanism, various reaction intermediates, aliphatic electrophilic and nucleophilic substitution reactions.
- To understand the detailed aspects of optical and geometrical isomerism.

UNIT-I **[12 Hours]**

Localized chemical bonding: Hybridization index, bonding in cyclopropane, bond distances, bond angles, bond energies, bond polarity, dipole moment and calculation of heat of reactions.

Delocalized chemical bonding: Conjugation, cross conjugation, resonance, steric inhibition of resonance, hyperconjugation, tautomerism, valence tautomerism. Bonding in fullerenes.

Bonding weaker than covalent: Hydrogen bonding, EDA complexes, inclusion compounds, Addition compounds, catenanes, rotaxanes and fluxional molecules.

Aromaticity: HMO theory and its application to simple π systems - ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl systems.

Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non benzenoid molecules - Tropones, tropolones, borazine and azulene. Annulenes & hetero-annulenes.

UNIT-II **[12 Hours]**

Organic Acids and bases: Brönsted-Lowry, Lewis concepts of organic acids and bases, pH, pKa values. Electronic (resonance, inductive and hyperconjugation), steric, hydrogen bonding and solvent effects on the strengths of acids and bases. HSAB concept.

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

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

UNIT-III **[12 Hours]**

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions-S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions. Neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions.

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

halogenation of aldehydes and ketones, aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogen, mercury exchange reactions.

UNIT-IV: Stereochemistry [12 Hours]

Optical Isomerism: Conformation and configuration. Projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations, interconversion of projection formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, chirality, molecules with more than one chiral centre, threo and erythro isomers, Psedoassymmetric centres. Racemizations and resolution methods. Stereospecific and stereoselective reactions. Asymmetric synthesis-Cram's and Prelog's rules. Optical activity in the absence of chiral carbon atom-biphenyls, allenes, spiranes, adamentanes, ansa compounds, cyclophanes, *trans*-cyclooctene, binaphthyls, catenanes, rotaxanes, and helicenes. Conformational analysis of cycloalkanes and decalins.

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 (2002).
2. Organic Reactions and Their Mechanisms: P. S. Kalsi, New Age, New Delhi (1996)
3. Stereochemistry, Conformation and Mechanism, P. S. Kalsi, Wiley Eastern (1993).
4. Stereochemistry of Carbon Compounds, E. L. Eliel, Tata McGraw Hill (1994).
5. Advanced Organic Chemistry-Reactions, mechanisms & structure, J. March, Wiley (2000).
6. Organic Chemistry: Vol.-1, 2 & 3, S. M. Mukherji, S. P. Singh and R. P. Kapoor, Wiley Eastern (1994).
7. A guide book of mechanisms in Organic Chemistry, P. Sykes, Orient- Longman (1985).
8. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall (1994).
9. Organic Chemistry, 4th edn., S. H. Pine, McGraw-Hill (1987).
10. Advanced Organic Chemistry, R. A. Carey and R. J. Sundberg, Plenum, (1990).
11. Modern Concepts of Advanced Organic Chemistry, R. P. Narein, Vikas, (1997).
12. A Text book of Organic Chemistry, K.S. Tewari, N. K. Vishnoi, S. N. Mehrotra, Vikas, (1998).
13. A Text book of Organic Chemistry, 3rd edn., R.K. Bansal, New Age (1997).
14. Organic Reaction Mechanisms: R. K. Bansal, Tata McGraw Hill, New Delhi (1978).
15. Organic Chemistry, 3rd edn., F. A. Carey, Tata McGraw Hill (1996).
16. Organic Chemistry, H. Pine, McGraw Hill (1987).
17. Organic Chemistry- Vol. I, I. L. Finar, ELBS Longmann (1984).
18. Advanced General Organic Chemistry: S. K. Ghosh, Book and Alleied (1998).

OC H 413: PHYSICAL CHEMISTRY

Course Outcome

- To understand the theoretical basis of catalysis, corrosion, various complex reactions which find relevance in biological processes and are of industrial importance and photochemical aspects of chemical reactions.
- The students are introduced to the modern techniques developed for the practical applications of these concepts in different areas of science and technology.
- This course will enable the students to handle issues related to catalytic reactions, corrosion in the day to day life and in industrial reactors; enzyme mediated reactions in biochemistry, biotechnology, pharmaceutical chemistry, electronic spectroscopy and different category of photochemical reactions etc.

UNIT-I **[12 Hours]**

Catalysis: Homogeneous Catalysis–equilibrium and steady state treatments, activation energies of catalysed reactions. Acid - base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed mechanisms–Michaelis-Menten mechanism. Effect of pH, temperature and inhibitors. Semiconductor catalysis, n- & p- type. Industrial applications of catalysis.

Surface Chemistry: A review of adsorption isotherms, Langmuir and Freundlich isotherms-derivation. Multilayer adsorption: BET equation–derivation, application in surface area determination. Harkin–Jura equation and application.

Mechanism of surface reactions. Langmuir-Hinshelwood & Langmuir Rideal mechanisms.

UNIT-II **[12 Hours]**

Composite reactions: Rate equation and derivation of rate constants simultaneous and consecutive reactions, steady state treatment, rate determining steps, Chain reactions (hydrogen-halogen reactions with comparison, derivation of rate equation for H_2-Br_2). Auto catalytic reactions (Hydrogen-Oxygen reaction), explosion limits and Oscillatory reactions.

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 (T&P jump methods).

UNIT-III **[12 Hours]**

Electrochemistry: Ionic atmosphere-introduction and its effect on conductivity. Walden`s rule. Debye-Huckel limiting law (DHL), its modification and verification. Bjerrum theory of ion association, triple ion formation and its significance.

Corrosion: Introduction, Principles, and classification. Techniques of corrosion rate measurement (instrumental and non-instrumental). Thermodynamics (Pourbaix diagram). Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), passivity of

corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).

Unit-IV **[12 Hours]**

Photochemistry: Introduction to photochemistry. Determination of quantum yield- Actinometry. Frank-Condon principle and its implications in predicting shapes of absorption and emission spectra. Effect of solute solvent interactions on electronic spectra-spectral shifts. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants. Flash photolysis technique.

Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase and in solution (Stern-Volmer equation). Photoisomerization, photo Fries rearrangement and Norrish type cleavage reactions with specific examples.

References

1. Chemical Kinetics, 3rd ed., K. J. Laidler, Pearson Education, Anand Sons (2008).
2. Fundamentals of Chemical Kinetics, M. R. Wright, Harwood Publishing, Chichesrer (1999).
3. Kinetics & Mechanisms of Chemical Transformations, J. Rajaram& J. C. Kuriacose, Macmillan (2007).
4. Chemical &Electrochemical Energy Systems, R. Narayan & B. Viswanathan, University Press (1998).
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OC S 414: INORGANIC SPECTROSCOPY AND OPTICAL METHODS

Course Outcome

- Students will learn the basic principles and applications of ESR and Mossbauer spectroscopy.
- Students can be familiarising with NQR and Photoelectron spectroscopy.
- Students will gain knowledge on Atomic Absorption Spectrometry, Emission Spectroscopy, Molecular Luminescence Spectroscopy and Light-Scattering methods for detection of metals, particles and particle size.
- Overall students can solve the problems related to above mentioned analytical techniques.

UNIT-I Electron Paramagnetic Resonance and Mössbauer Spectroscopy [12 Hours]

Electron Spin Resonance (ESR) Spectroscopy: Basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of ESR spectra, hyperfine interaction, spin–orbit coupling, Zero Field splitting and Kramer's degeneracy, rules for interpreting spectra, factors affecting the magnitude of values. Instrumentation; Applications to the study simple inorganic and organic free radicals and to inorganic complexes, biological studies and rate of electron exchange reactions.

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), structure determination of $Fe_3(CO)_{12}$, Prussian blue, oxyhemerythrin, hexacyanoferrates, nitropruside, tin halides. Detection of oxidation states and inequivalent Mössbauer atoms.

UNIT-II Nuclear Quadrupole Resonanceand Photoelectron Spectroscopy [12 Hours]

Nuclear Quadrupole Resonance (NQR) Spectroscopy: Basic concepts-Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies, Effect of magnetic field on spectra; Factors affecting the resonance signal-Line shape, position of resonance signal; Relationship between electric field gradient and molecular structure. Interpretation of NQR data, Structural information of PCl_5, $TeCl_4$, Na^+ $GaCl_4^-$, BrCN, HIO_3 and Hexahalometallates.

Photoelectron Spectroscopy: Basic principles, photoionization process, ionization energies, Koopman's theorem, Electron Spectroscopy for Chemical Analysis (ESCA)-Photoelectron spectra of simple molecules-N_2, O_2 and F_2; Photoelectron spectra for the isoelectronic sequence- Ne, HF, H_2O, NH_3 and CH_4; chemical information from ESCA.

X-ray photoelectron and Auger electron spectroscopy: Principles and applications. Auger transitions, measurement techniques. Applications.

UNIT-III Atomic Spectroscopy **[12 Hours]**

Flame Photometry: Flame Emission spectroscopy (FES) and atomic absorption spectroscopy (AAS)-Introduction, principle, flames and flame spectra, variation of emission intensity with the flame, flame temperature, chemical reactions in flame, metallic spectra in flame, flame background. Total consumption and premix burners, role of temperature on absorption, emission and fluorescence. Effect of organic solvents. Comparative study of the basic components and difference in the instrumental design for atomic absorption and flame photometry. Precision and accuracy of AAS and FES. Relationship between AAS and FES, advantages over FES, devices used for the formation of an atomic vapour, applications, determination of sodium in different samples by flame photometry. Plasma emission spectroscopy, Principle, Inductively coupled plasma emission (ICP). ICP torch, instrumentation and applications.

References

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2. Fundamental of Analytical Chemistry, 8th edn., D. A. Skoog, D.M. West, Holler and Crouch, Saunders College Publishing, New York (2005).
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5. Instrumental methods of analysis, 7th edn., H. H. Wlliard, L. L. Merrit and J. J. Dean, Wadsworth (2012).
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OC S 415: MOLECULAR SPECTROSCOPY AND DIFFRACTION TECHNIQUES

Course Outcome

- Deals with the understanding of the spectroscopic techniques which are based on the interaction of the electromagnetic radiation in the microwave, infrared and X-ray region with the molecules.
- The techniques introduced here are major characterization techniques employed to understand the chemical composition of compounds and the physical characteristics.
- The paper has multidisciplinary relevance as these techniques are used in various fields namely, chemistry, physics biology and materials science.

Unit-I **[12 Hours]**

Introduction to spectroscopy, intensity of spectral lines, Natural line width and broadening, Rotational, vibrational and electronic energy levels, selection rules.

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-CO_2 and H_2O).

UNIT–II **[12 Hours]**

Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation.

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

Unit III **[12Hours]**

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 method), powder diffractometer. Single crystal technique: Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences. Crystalline X-ray diffractometer (4 angle), X-ray scattering by 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), Structure of surfaces - (Low and high Energy Electron Diffraction, Electron microscopy (TEM & SEM): Principle and Applications.

Theory and applications of Neutron diffraction. Comparison between X-ray, electron and Neutron diffractions.

References

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4. Spectroscopy, B.K. Sharma, Goel Prakashan (2015).
5. A Basic Course in Crystallography, J. A. K. Tareen and T. R. N. Kutty, University Press (2001).
6. Essentials of Crystallography, M. A. Waheb, Narosa Publishing House (2009).
7. X-ray methods, Clive Whiston, John Wiley & Sons (1987).

OC P 416: INORGANIC CHEMISTRY PRACTICALS-I

Course Outcome

- Students will have hands on experience on the analysis of Hematite Dolomite, Pyrolusite, Solder.
- Analysis of halide mixture, Colorimetric determination and Gravimetric determinations
- To understand complexometric determination and hardness of water.
- It enables the students to learn statistical analysis of data.

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using Ce^{4+}.
2. Analysis of Dolomite - insoluble residue by gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complexometric determination of Mn, Ca, Mg, Cu, Ni and Fe-Cr mixture.
6. Hardness of water.
7. Analysis of halide mixture - Iodide by KIO_3 and total halide by gravimetrically.
8. Colorimetric determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Preparation of Chrome alum/Chrome red/Lithopone/Mohr's salt.
11. Statistical analysis of data.

References

1. Vogel's Text Book of Quantitative Chemical Analysis, 5th edn., G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, Longman (1999).
2. Quantitative Analysis, 5th edn., R. A. Day and A. L. Underwood, Prentice Hall (1998).
3. Vogel's Qualitative Inorganic Analysis, 7th edn., G. Svehla, Longman (2001).
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OC P 417: ORGANIC CHEMISTRY PRACTICALS–I

(**Any twelve preparations are to be carried out)**

Course Outcome

- Student will learn the setting up of reaction and handling of glassware and reagents
- Enlighten the students to understand the method of organic preparation by utilizing various kinds of organic reactions.
- Explain the principle and mechanistic aspects of various basic organic reactions.
- Learn the isolation and purification of products.
- Acquire the experimental skills for the preparation of organic compounds.

Preparation of the following compounds through single step and isolation, recrystallization and determination of melting point & yield.

1. Preparations of *p*-bromoacetanilide from acetanilide, 2,4,6-tribromophenol from phenol, phenacyl bromide from acetophenone,1-bromo-2-naphthol from 2-naphthol and α,β-dibromocinnamic acid from cinnamic acid through bromination reactions.
2. Preparations of *p*-niroacetanilide from acetanilide, methyl *m*-nitrobenzoate from methyl benzoate, 2,4-dinitrochlorobenzene from chlorobenzene and 2,4-dinitroanisole from anisole through nitration reactions.
3. Preparations of *p*-nitroaniline from *p*-nitroacetanilide and *p*-bromoaniline from *p*-bromoacetanilide through hydrolysis reactions.
4. Preparations of nerolin (β-naphthyl methyl ether from β-naphthol and N-methylanthranilic acid from anthranilic acid through methylation reactions.
5. Preparations of α-and β-D-glucose penta-acetates from glucose, β-naphthyl acetate from β-naphthol and resacetophenone from resorcinol through acetylation.
6. Preparations of phenoxyacetic acid from phenol, *o*-cresyloxyacetic aid, 2,4-dichlorophenoxyacetic acid from 2,4-dichlorophenol and *p*-aminobenzoic acid from *p*-chlorobenzoic acid through nucleophilic substitution reactions.
7. Preparation of S-Benzylisothiuronium chloride from benzyl chloride through nucleophilic substitution reaction.
8. Preparation of cyclohexene from cyclohexanol and succinic anhydride from succinic acid through dehydration reactions.
9. Preparations of adipic acid from cyclohexanol and *p*-nitro benzoic acid from *p*-nitrotoluene through oxidation reactions.
10. Preparations of *p*-benzoquinone from hydroquinone and anthraquinone from anthracene by oxidation reaction.
11. Preparations of Benzhydrol from Benzophenone, azobenzene from nitrobenzene and *m*-nitroaniline from *m*-dinitrobenzene through reduction reactions.

12. Preparation of 4-Formyl-N,N-dimethyl aniline from N,N-Dimethylaniline through Vilsmeier-Haack formylation reaction.
13. Preparation of *o*-hydroxybenzophenone from phenyl benzoate via Fries rearrangement.
14. Preparation of *p*-chlorobenzoic acid from *p*-toluidine through diazotisation and Sandmeyer reaction.
15. Preparations of benzoic acid and benzyl alcohol from benzaldehyde and 4-chlorobenzoic acid and 4-chloro benzyl alcohol from 4-chlorobenzaldehyde by Cannizzaro reactions.
16. Preparations of benzalacetone and dibenzalacetone from benzaldehyde and acetone through Claisen-Schmidt condensation.
17. Preparation of cinnamic acid from benzaldehyde through Perkin condensation reaction.
18. Preparation of *o*-benzoyl benzoic acid from phthalicanhydride and benzene through Friedel-Craft's acylation.
19. Preparation of triphenylmethanol from benzoic acid through Grignard reaction.
20. Preparation of diazoamino benzene from aniline through diazotisation and coupling reactions.
21. Preparations of *p*-iodonitrobenzene and *o*-iodobenzoic acid via diazotisation and nucleophilic substitution.
22. Preparation of osazone derivatives of monosaccharides through condensation reaction.
23. Preparation of hippruic acid from glycine through condensation reaction.

References

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2. Experimental Organic Chemistry–Vol. I & II, P. R. Singh, D. S. Gupta and, K. S. Bajpai, Tata McGraw-Hill (1981).
3. Laboratory Manual in Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied (1992).
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13. Advanced Practical Organic Chemistry-Vol. II, Jag Mohan Himalaya Publishing House (1992).

OC P 418: PHYSICAL CHEMISTRY PRACTICALS - I

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

Course Outcome

- Experiments have been designed which make use of the concepts of electrochemistry, thermodynamics, and solution chemistry.
- Students get hands on experience in use of instruments such as potentiometer, conductometer, pH meter, spectrophotometer, refractometer, viscometer etc and will be able to test the theoretical concepts.

1. Verification of Nernst equation for Ag^{+}, Cu^{2+} and Zn^{2+} species and Determination of thermodynamic parameters of an electrode reaction by EMF method.
2. Determination of pK values of dibasic acids by potentiometric/pH metric method
3. Potentiometric titration of halides in mixtures (Cl^{-}, Br^{-} and I^{-}) with silver nitrate
4. Composition of zinc ferrocyanide complex by potentiometric titration.
5. Conductometric titrations of displacement and precipitation reactions.
6. Spectrophotometric determination of dissociation constant.
7. Determination of equivalent conductance and dissociation constants of weak acid and base.
8. Determination of solubility of lead iodide at different T & hence molar heat of solution
9. Determination of degree of hydrolysis of CH_3CO_2Na and NH_4Cl by conductivity method.
10. Measurements of the conductance of a weak acids (a) HOAC from strong electrolytes (NaOAc, HCl and NaCl), (b) HCOOH from strong electrolytes (HCOONa, HCl and NaCl) and to calculate the ionization constant of the acid.
11. Determination of pK_a of acids by pHmetry
12. Study of variation of viscosity of a liquid with temperature
13. Determination of molecular weight of polymers by viscometric measurements.
14. Determination of the composition of a solution by S.T. measurements.
15. Determination of the Critical Micelle Concentration by surface tension/conductometric measurements.
16. Determination of vapour pressure of organic compounds by gas saturation method
17. Determination of Specific and molar refractivity of liquids and parachor value of a species by refractometric method.

Any other relevant experiments of interest.

References

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2. Practical Physical Chemistry, 3rd edn., A. M. James and F. E. Prichard, Longman Publication (1974).
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II SEMESTER

OC H 461: ADVANCED INORGANIC CHEMISTRY

Course Outcome

- Students will learn the predictions of spectral and structural properties of organic and inorganic molecules through symmetry elements and symmetry operation.
- Understand the halogen and noble gas chemistry.
- Study the chemistry of silicates and silicone polymers.
- Acquire knowledge on metallurgical aspects of oxide ores, metal oxides, nitrides, fluorides and sulphides.
- Study the chemistry of reactions in non-aqueous media.
- Learn the industrial biological applications of ceramic materials.
- Know the chemistry and applications of lanthanoids and actinoides.

UNIT-I Symmetry and Group Theory **[12 Hours]**

Symmetry elements and symmetry operations. Point groups used with Molecules: Concept of a group, definition of a point group. Classification of molecules into point groups. Subgroups. Hermann-Maugin symbols for point groups. Multiplication tables (C_{2V}, C_{2h} and C_{3V}). Matrix notation for the symmetry elements. Classes and similarity transformation. Representation of groups: The great orthogonality theorem and its consequences. Character tables (Cs, Ci, C_2, C_2v, C_{2h} and C_3v). Applications of group theory to chemical bonding (hybrid orbitals for σ-bonding in different geometries and hybrid orbitals for π-bonding. Symmetries of molecular orbitals in BF_3, C_2H_4 and B_2H_6.

UNIT-II **[12 Hours]**

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

Oxy and Peroxy acids of N, P and S.

Silicates: Structure, classification - silicates with discrete anions, silicates containing chainanion, silicates with layer structure, silicones with three-dimensional net-work and applications. **Silicones:** General methods of preparation, properties. **Silicone polymers**: silicone fluids, silicone greases, silicone resins, silicone rubbers and their applications.

UNIT-III **[12 Hours]**

Chemistry of Ti subgroup and inner transition elements

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti and Ni subgroups as examples.

Lanthanoid Chemistry: General trends, Electronic, optical and magnetic properties. Abundance and extraction, General principles: conventional, solvent extraction and ion-exchange methods. Separation from monazite. Chemistry of principal oxidation states (II, III and IV). Stability of tetrahalides, dihalides and aqua ions of simple lanthanide compounds. Redox potentials. Uses: lanthanides as shift reagents, lanthanides as probes in biological systems. High temperature super conductors.

Actinoid Chemistry: General trends and electronic spectra. Occurrence and preparation of elements, Isolation of the elements: thorium and uranium, enrichment of uranium for nuclear fuel, uranium hydrides, oxides and chlorides. Chemical reactivity and trend. Chemistry of trans-uranium elements.

UNIT-IV **[12 Hours]**

Metallurgy and redox potentials: Methods of reduction of oxide ores, chemical and electrolytic reductions, Ellingham diagram, specialized techniques for the extraction of metals- Amalgamation, Hydrometallurgy, Solvent Extraction, Ion exchange chromatography. Reduction potentials, Latimer and Frost diagrams–features and applications. Effect of complexation on potential.

Metal oxides, nitrides and fluorides: Monoxides of the 3d metals, higher oxides and complex oxides, oxide glasses, nitrides and fluorides.

Sulfides, intercalation compounds and metal rich phases: Layered MS2 compounds and intercalation, Chevrel phases.

Ceramic materials: Sol-gel process and applications of biomaterials of ceramics.

References

1. Group Theory in Chemistry, 2nd edn., M. S. Gopinathan, V. Ramakrishnan, Vishal Publishing, (2007).
2. Symmetry and Group theory in Chemistry, 1st edn., R. Ameta, New Age, (2013).
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12. Principles of Inorganic Chemistry, 31st edn., B. R. Puri, L. R. Sharma, K. C. Kalia, Vishal Publishing, (2013).
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17. Nature and Properties of Engineering Materials, Z. D. Jastrazebski, John Wiley & Sons, (1989).

OC H 462: ADVANCED ORGANIC CHEMISTRY

Course Outcome

- Students will gain an understanding of all details of aromatic electrophilic and nucleophilic substitution reactions.
- Learn about various free radical reactions and elimination reactions including pyrolytic eliminations.
- Gain an understanding of formation and hydrolysis of esters.
- Study the all types of addition to carbon-carbon and carbon-heteroatom multiple bonds.
- Know the reaction mechanism and synthetic uses of organic named reactions.

UNIT-I **[12 Hours]**

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reactions-nitration, halogenation, sulfonation, Friedel-Crafts alkylation and acylation, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Mannich reaction, Diazonium coupling, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions - S_NAr, S_N1 &aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement.

UNIT-II **[12 Hours]**

Free Radical Reactions: Mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer & Hunsidiecker reactions.

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

Pyrolytic Eliminations: Mechanisms of pyrolysis of acetates. Xanthate pyrolysis-Chugaev reaction, Hofmann degradation and Cope elimination.

UNIT-III **[12 Hours]**

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $B_{AL}1$, $B_{AL}2$, $A_{AC}1$ & $A_{AL}1$ mechanisms. Trans-esterification.

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, oxygen-epoxidation, carboxylic acids and amines. Michael addition, Addition to cyclopropanes.

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformatsky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions.

UNIT-IV **[12 Hours]**

Organic Name Reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Gattermann-Koch reaction, Duff reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Suzuki coupling, Heck reaction, Ullmann reaction, Bucherer reaction, Shapiro reaction, Mitsunobu reaction, Stephen reaction.

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OC H 463: ADVANCED PHYSICAL CHEMISTRY

Course Outcome

- It is an advanced level course which helps to understand the concepts of physics and their subsequent applications in the field of chemistry. The concepts of chemical thermodynamics help in the design of processes in chemical industries.
- The concepts of statistical thermodynamics find relevance in understanding the nature of solids and metals in specific.
- Quantum chemistry forms the basis of chemical bonding, photochemistry and spectroscopy.
- Reaction dynamics deals with advanced aspects of chemical kinetics.

UNIT-I Chemical Thermodynamics [12 Hours]

Entropy: Physical significance, entropy change in an ideal gas. Entropy change in reversible and irreversible processes. Thermodynamic equations of state.

Free energy, Maxwell's relations and significance. Gibbs – Helmholtz equation and its applications.

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

Chemical affinity and thermodynamic functions. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.

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

Fugacity: Relationship between fugacity and pressure. Determination of fugacity- graphical method and Lewis Randall rule.

Activity and activity coefficient: Determination of activity by vapour pressure method.

UNIT-II Statistical thermodynamics [12 Hours]

Thermodynamic Probability, phase space, micro and macrostates, statistical weight factor, assembly, ensemble-significance, classification and comparison. Derivation of Distribution laws, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Laws, Limit of applicability of various laws. Partition function, Significance, Relationship between partition function and thermodynamic functions -Average energy, heat capacity, free energy, chemical potential for molecular particles.

Thermodynamic quantities in terms of partition function of particles: Evaluation of Translational, vibrational, rotational, electronic partition functions. Law of equi-partition principle. Partition function and equilibrium constant. Applications of partition function to mono atomic gases, diatomic molecules.

Statistical thermodynamic properties of solids (Heat capacity): Introduction, thermal characteristics of crystalline solid, Einstein model, Debye modification equilibrium constant.

UNIT-III Quantum Chemistry **[12 Hours]**

Particle waves, its character and significance. De-Broglie concept, uncertainty principle, Formulation of Shrodinger equation- significance and characteristics of wave function, Statistical significance of ψ. Normalization and orthogonality, Acceptable wave functions.

Postulates of quantum Mechanics, Operators, Operator algebra, types and applications, operators for the dynamic variables of a system (position, linear momentum, angular momentum, kinetic energy, potential energy and total energy). Eighen values and Eighen functions. Solution of SE for particle in a box (1D & 3D), particle in a ring, H atom. Applications of quantum mechanics to chemical bonding. Covalent bond-Valence bond and molecular orbital approaches with comparison.

Unit-IV Reaction Dynamics **[12 Hours]**

Kinetics of Composite Reactions: Inorganic reaction mechanism (decomposition of N_2O_5 and phosgene). Organic reaction mechanism-decomposition of acetaldehyde, Gold-Finger, Letort-Niclause rules, combustion of hydrocarbon.

Transition state theory: Derivation of rate constant, equilibrium hypothesis, Concept of tunnelling. Applications of TST to reactions in solution & reaction between atoms, Thermodynamic formulation of transition–state theory, limitations of TST. Extension of TST.

Potential energy surfaces: Features & construction. Theoretical calculation of E_a. Features of potential energy surfaces (attractive and repulsive surfaces for exothermic reaction). A brief account of stripping and rebound mechanisms. Spectroscopy of transient species.

References

1. Thermodynamics for Chemists, S. Glasstone, East West Press, (1960).
2. Atkin's Physical Chemistry, 7th edn., P. Atkins & J. D. Paula, Oxford University Press, (2002).
3. Chemical Themodynamics, J. Rajaram and J. C. Kuriokose, East-West Press-Pearson, (2013).
4. Thermodynamics, 3rd edn., R. C. Srivastava and S. K. Saha, Prentice-Hall of India, (2007).
5. Statistical Thermodynamics, M. C. Gupta, New age International, (2007).
6. Principles of Physical Chemistry, B. R. Puri, L. R. Sharma and M. S. Pathania, Vishal Publishers, (2014).
7. Atomic Structure and Chemical Bond, Manasa Chanda, Tata McGraw Hill, (1991).
8. Quantum Chemistry, R. K. Prasad, New Age International, (1991).
9. Advanced Physical Chemistry, G. R. Chatwal, Goel Publishes, (1992).
10. Introductory Quantum Chemistry, A. K. Chandra, Tata McGraw Hill, (1994).
11. Quantum Chemistry, A. B. Sannigrahi, Book and Allied, (2013).
12. Quantum Chemistry, A. P. Donald, Viva Books, (2013).
13. Chemical Kinetics, 3rd edn., K. J. Laidler, Pearson Education, Anand Sons, (2008).
14. Fundamentals of Chemical Kinetics, M. R. Wright, Harwood Publishing, Chichesrer, (1999).
15. Kinetics & Mechanisms of Chemical Transformations, J. Rajaramand, J. C. Kuriacose, Macmillan, (2007).

OC S 464: ORGANIC SPECTROSCOPY

Course Outcome

- Enable the students to understand the principle, theory, instrumentation and applications of UV/Electronic, IR, NMR (^{1}H, ^{13}C, ^{19}F, ^{31}P) and Mass spectroscopy.
- To solve the composite problems involving the applications of UV, IR, NMR (^{1}H &^{13}C) and Mass spectroscopic techniques.
- To develop the ability to analyse the spectrum and arrive at the correct structure of the compounds.
- Overall students can get confidence in solving spectroscopic problems.

UNIT-I **[12 hours]**

UV/Electronic Spectroscopy: Basic principles, 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. Empirical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

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

UNIT-II Nuclear Magnetic Resonance Spectroscopy **[12 hours]**

Theory and principle, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling, effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nuclear Overhauser Effect. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. Use of NMR in Medical diagnostics.

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it. Decoupling-Noise decoupling & Broad band decoupling. Off-resonance proton decoupling-some representative examples. Introduction to ^{19}F & ^{31}P NMR.

UNIT-III Mass Spectrometry **[12 hours]**

Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy. Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules.

References

1. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Monnill, Wiley (1981).
2. Applications of Absorption Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall (1965).
3. Spectroscopy of Organic Compounds, 3rd edn., P. S. Kalsi, New Age, New Delhi (2000).
4. Spectroscopic Methods in Organic Chemistry, Williams and Fleming, TMH.
5. Introduction to Spectroscopy, D. L. Pavia, G. M. L. G. C. S. Kriz, 5th edn., Cengage Learning (2014).
6. Spectrometric Identification of Organic Compounds, 8th edn., R. M. Silverstein, F. X. Webster and D. J. Kiemle, Wiley (2014).
7. Organic Spectroscopy, 3rd edn., W. Kemp, Pagrave Publishers (1991).
8. Modern Spectroscopy, J. M. Hollas, 4th edn., John Wiley and sons (2004).
9. Organic Structures from Spectra, 5th edn., L. D. Field, S. Sternhell and J. R. Kalman, Wiley (2013).

OC S 465: ENVIRONMENTAL CHEMISTRY

Course Outcome

- This course enlighten the students about environmental pollutions like Air pollution, toxic chemicals in the environment.
- Hydrologic cycle, BOD, COD, radioactive waste management, sewage and industrial effluent treatment, water purification.
- Biochemical effects of Pesticides and heavy metals.
- Students learn effect of toxic chemicals in environment.

UNIT-I **[12 Hours]**

Environmental segments, evolution of earth's atmosphere. Air pollution: Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and transportation sources. SO_x- Sources, ambient concentration, test methods, control techniques-scrubbing, limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x- Sources, ambient concentration, test methods, thermodynamics and NO_x, control techniques. Particulates: Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II **[12 Hours]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD, COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

UNIT-III **[12 Hours]**

Toxic chemicals in the environment, impact of toxic chemicals on enzymes. Detergents-pollution aspects, eutrophication. Pesticides - pollution of surface water. Sewage and industrial effluent treatment, heavy metal pollution. Chemical speciation- biochemical effects of pesticides, insecticides, particulates, heavy metals (Hg, As, Pb, Se), carbon monoxide, nitrogen oxides, sulphur oxides, hydrocarbon, particulates, ozone, cyanide and PAN. Solid pollutants and its treatment and disposal. Radioactive waste management.

References

1. Environmental Chemistry, A. K. De, New Age International (2016).
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, 5th edn., C. N. Sawyer, P. L. McCarty and G. F. Parkin, McGraw Hill (2017).
5. Environmental Chemistry, I. Williams, John Wiley (2001).
6. Environmental Pollution Analysis, 2nd edn., S. M. Khopkar, New Age International (2020).

OC E 466: ENVIRONMENTAL, ELECTRO AND POLYMER CHEMISTRY

Course Outcome

- It is an elective course offered to students from disciplines other than chemistry.
- It aims at enhancing their general understanding of chemistry. Few important topics such as sources and detection of air pollution, batteries as power sources, devices of solar energy conversion.
- It enables to understand polymers used in day to day life and their medical and technical applications.
- It creates awareness of plastic pollution and technique of plastic waste management.

UNIT-I **[12 Hours]**

Environmental segments, evolution of earth's atmosphere. Air pollution: Air pollutants, prevention and control, Greenhouse gases and acid rain. Carbon monoxide, industrial sources and transportation sources. SO_x- sources, ambient concentration, test methods, control techniques - scrubbing, limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x - Sources, ambient concentration, test methods, thermodynamics and NO_x, control techniques. Particulates: Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II **[12 Hours]**

Corrosion: Introduction, consequence, type, prevention, & measurement. Conventional sources of energy, limitations, Importance of storage, Battery-Electrodes, Cell, battery Brief account of primary, secondary, lithium battery and fuel cells. Semiconductor electrodes and Solar energy system.

Introduction to bio-electrochemistry, electrochemical communication in biological organisms. Theory and applications of Electroplating and electroless plating.

Reaction Kinetics: Theory and applications of different types of reactions-Oscillatory, chain reaction, branched chain reaction. Energy of activation and thermodynamic parameters, Collision theory of reaction rates limitations and basics of transition state theory.

UNIT-III **[12 Hours]**

Polymers: Introduction-Basic concepts and classification of polymers, Molecular weight and its distribution, Chemistry of polymerization-Step, chain, Coordination, Copolymerization.

Polymerization techniques-bulk, solution, suspension, emulsion, poly-condensation, solid and gas phase polymerization. Chemical and geometrical structure of polymer molecules, Structure-property relationship-Physical, Thermal and mechanical properties.

Synthesis, properties, structural features and applications of some important commercial polymers (PE, PP, PS, PVC, PMMA, PET, Nylon-6, Nylon-6,6), Engineering polymers (Kevlar, Nomex, ABS, PC, Teflon). Applications of polymers in separations: reverse osmosis, ultra and nano-filtration.

Applications in electronics- conducting polymers and electronic shielding, Applications of polymers in medicine.

Management of plastics in environment-recycling, incineration and biodegradation.

References

1. Environmental Chemistry, A. K. De, New Age International (2016).
2. Environmental Chemistry, S. K. Banerji, Prentice Hall India (1993).
3. Chemistry for Environmental Engineering, 3rd edn., C. N. Sawyer and P. L. McCarty, McGraw Hill (1978).
4. An Introduction to metallic corrosion and its prevention, Raj Narayan, Oxford-IBH, New Delhi (1983).
5. Chemical & Electrochemical Energy Systems, R. Narayan & B. Viswanathan, University Press (1998).
6. Industrial Electrochemistry, D. Peltcher and F. C. Walsh, Chapman & Hall (1990).
7. Text book of Polymer science, 3rd edn., F. W. Billmeyer, Wiley-Interscience Publication, New York (2005).
8. Polymer Science, V. R. Gowariker, New Age International, New Delhi (2012).
9. Specialty Polymers, R. W. Dyson, Chapman and Hall, New York (1987).
10. Polymer Science and Technology, J. R. Fried, Prentice Hall of India, New Delhi (1999).
11. Polymer Science and Technology, P. Ghosh, Tata-McGraw Hill, New Delhi (1995).

OC P 467: INORGANIC CHEMISTRY PRACTICALS-II

Course Outcome

- The students will have hands on experience in the qualitative analysis of mixtures of Inorganic Salts containing 3 cations in which 1 less common metal ion and 2 anions.
- Students will learn the systematic methods of separation techniques.
- Apart from inorganic radicals they also learn the separation organic radicals.

Qualitative Analysis of mixtures of Inorganic Salts containing 3 cations and 2 anions (1 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 Text Book of Quantitative Chemical Analysis, 5th edn., G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, Longman (1999).
2. Vogel's Qualitative Inorganic Analysis, 7th edn., G. Svehla, Longman (2001).

OC P 468: ORGANIC CHEMISTRY PRACTICALS-II
(Analysis of 6 binary mixtures is to be carried out)

Course Outcome

- Student will gain the in-depth knowledge and skill in identification and separations of organic compounds from binary mixtures of organic compounds containing both mono and bi-functional groups, their purifications and systematic qualitative analyses.
- Understand the purification of the components, determination of boiling point/melting point for components and melting point of their derivatives.
- Learn the application of concepts of different organic reactions studied in theory part of organic chemistry.
- Study the complete identification of organic compound with melting point and preparation of a suitable derivative.
- Learn the use glassware, equipment and chemicals and follow experimental procedures in the laboratory.

Identification of components in the binary mixture of organic compounds and the method of separation. Systematic semi-micro qualitative analysis by the Identification of the functional group(s) present in each of the compound and preparation of one solid derivative each for their confirmation.

Demonstration of identification and method of separation of organic compounds from ternary 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, P.R. Singh, D.S. Gupta and, K.S. Bajpai, Tata McGraw-Hill (1981).
4. Semimicro Qualitative Organic Analysis-The Systematic Identification of Organic Compounds, Nicholas D. Cheronis, John B. Entrikin, Ernest M. Hodnett, Wiley-Eastern, New Delhi (1965).
5. A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, A.I. Vogel, Longman (1970).
6. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis, B. S. Furniss, P. W. Smith, A. R. Tatchell and A. R. Tatchell, Longman-ELBS, England (1978).
7. Laboratory Manual in Organic Chemistry, Dey B. B. and Sitaraman M. V, Allied (1992).
8. Modern Experimental Organic Chemistry, John H. Miller and E.F. Neugil, D. C. Heath and Company (1982).
9. Hand book of organic analysis, H. T. Clarke and J. N. Collie, E. Arnold & Co., London (1975).
10. Experiments in Organic Chemistry, 2nd edn., Louis F. Fieser, D. C. Heath & Co. (1941).
11. Organic Experiments, 8th edn., Ed. Louis F. Fieser and Kenneth L. Williamson, Houghton Mifflin (1998).
12. Practical Organic Chemistry, Ajay Kumar Manna, Books & Allied (2018).
13. Advanced Practical Organic Chemistry-Vol. II, Jag Mohan, Himalaya Publishing House (1992).

OC P 469: PHYSICAL CHEMISTRY PRACTICALS-II

(At least 12 experiments are to be carried out)

Course Outcome

- In continuation with the practical course introduced in the first semester, this course provides opportunity to students to test the concepts learnt in the basic physical chemistry course OC H 403. Experiments have been designed on thermodynamics, kinetics, surface and interface chemistry.
- With the training gained, students will be able to handle issues related to metallurgical processes, waste water treatment, energy efficient processes, action of soaps and detergents etc.
- Students will also be introduced to the use of few software packages useful to chemists.

1. Determination of cryoscopic constants of solvents and molecular weight of non-volatile substances by thermal method.
2. Heat of solution of a sparingly soluble compound in water by solubility method.
3. Phase diagram of two component systems by thermal analysis.
4. Phase diagram of three component system (a) 3 liquids with single binodal curve, and b) two liquids and one solid
5. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of Energy of activation.
6. Determination of a) Energy of activation & b) rate constant for the First and second order kinetics of reaction between potassium persulphate and potassium iodide.
7. Kinetics of sodium formate-iodine reaction.
8. Verification of Freundlich and Langmuir adsorption isotherms for acetic acid on activated charcoal.
9. Comparison of detergent action of detergents and determination of interfacial tension.
10. Study of association of benzoic acid in benzene/toluene and determination of partition coefficient.
11. Determination of partial molar volumes of (a) Salt - water and (b) alcohol - water (methanol and ethanol) systems by density method.
12. Computers in Chemistry-Use of softwares to make linear plots and calculate constants from slope and intercepts
13. Computers in Chemistry- Drawing structures using chem draw/chem sketch

Any other relevant experiments of interest.

References

1. Findlay's Practical Physical Chemistry, Alexander Findlay and B. P. Levitt, Prentice Hall Press (1973).
2. Practical Physical Chemistry, 3rd edn., A. M. James and F. E. Prichard, Longman Publication (1974).
3. Experimental Physical Chemistry, 7th edn., D. Farrington, M. J. Howard and W. J. Warren, McGraw Hill College (1970).
4. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, New Delhi (1983).
5. Advanced Practical Physical Chemistry, J. B. Yadav, Krishnaprakashan Media Publication (2016).
6. Experiments in Physical Chemistry, J. C. Ghosh, Bharathi Bhavan, New Delhi (1974).
8. Practical Physical Chemistry, B. Viswanathan and P. S. Raghavan, ViVa Books, New Delhi (2017).

III SEMESTER

OC H 511: ORGANIC REACTION MECHANISM

Course Outcome

- Students will learn about the mechanism and synthetic utility of various kinds of molecular rearrangement reactions with diverse examples.
- Students will gain knowledge on principles of photochemistry and diverse types of photochemical reactions of organic molecules with multiple examples.
- Students will learn various concepts of pericyclic reactions, diverse types of electrocyclic, cycloaddition and sigmatropic reactions with multiple examples.
- Students will learn several name reactions that involve synthesis of heterocyclic molecules with reaction mechanism and examples.

UNIT-I **[12 Hours]**

Molecular Rearrangements: General mechanistic treatment ofnucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism and synthetic utilities of Wagner-Meerwein, Dienone-Phenol, Pinacol-Pinacolone, Demyanov, Wolff, Favorskii, Neber, Benzidine, Lossen, Curtius, Schmidt, Stevens, Baker-Venkatraman and Amadori rearrangement.

UNIT-II Organic Photochemistry **[12 Hours]**

Bonding and antibonding orbitals, singlet and triplet states, relative energies, Jablonski diagram and quantum yield, Photodissociation, Photoreduction, Photochemical isomerisation and Photocyclisation. Norrish Type-I, Type-II reactions and Yang cyclisation. Barton reaction and Photo Fries rearrangement, Paterno-Buchi reaction, Photochemistry of alkenes, benzenes, Di-pi methane rearrangement, Photodegradation of polymers. Photocatalysis, Photooxidation and photoreduction reactions. Photochemical cells, energy conversion and storage. Photochemistry of vision.

UNIT-III **[12 Hours]**

Pericyclic Reactions: Characteristics and classifications of pericyclic reactions. Aromatic Transition States (ATS)/Perturbation Molecular Orbitals (PMO) approach for the interpretation of mechanism of pericyclic reactions. Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. 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, notation of cycloadditions,2+2 and 4+2 systems, 2+2 additions of ketones and chelotropic reactions. 1,3-Dipolar cycloaddition

reactions. **Sigmatropic reactions:** Suprafacial and Antarafacial shift of H, [1,3] [1,5] and [3,3]-sigmatropic shifts. Walk, Claisen, Cope, Oxy-Cope and Aza-Cope rearrangements.

UNIT-IV Name reactions in heterocyclic synthesis [12 Hours]

Corey-Chaykovsky reaction, Hoch-Cambell aziridine synthesis, Blum aziridine synthesis, Feist-Bénary furan synthesis, Hoffmann Loffler-Freytag reaction, Fiesselmann thiophene, Gewald aminothiophene synthesis, Fischer oxazole synthesis, Gassman indole synthesis, Larock indole synthesis, Grabe-Ullmann carbazole synthesis, Bockiheide reaction, Gabriel-Colman rearrangement, Gould-Jacobs reaction, Meth–Cohn quinoline synthesis, Combes quinoline synthesis, Pomeranz-Fritsch reaction and Bischler-Napieralski isoquinolines synthesis.

References

1. Advanced Organic Chemistry, Part A & B, F. A. Carey and R. J. Sandburg, Plenum, (1990)
2. Organic Chemistry, Vol 1-3, S. M. Mukherji, S. P. Singh and R. P. Kapoor, New Age, New Delhi (1985)
3. Synthetic Organic Chemistry, G. R. Chatwal, Himalaya, (1994).
4. Organic Reaction Mechanisms, V. K. Ahluwalia & R. K. Parashar, Narovasa, (2006).
5. Organic Chemistry, Vol. I-II, I. L. Finar, Longmann ELBS, (1973).
6. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic, (2005).
7. Organic Reactions and their Mechanisms, P. S. Kalsi, New Age, (1996).
8. Organic Synthesis, R. E. Ireland, Prentice Hall, (1969).
9. Name reactions in Heterocyclic Chemistry, J. J. Li, Springer, (2014).
10. Organic Photochemistry. Vol I & II. O. L. Chapman, Marcel Dekker, New York (1973).
11. Pericyclic Reactions, S. M. Mukherji, The McMillan, (1979).
12. Strategic Applications of Named Reactions in Organic Synthesis, L. Kürti and B. Czakó, Academic press, (2005).

OC H 512: REAGENTS FOR ORGANIC SYNTHESIS

Course Outcome

- Students will learn the preparation, properties, reactions and uses of organometallic reagents in organic synthesis.
- Students will know the uses of Gillman's reagent, LDA, DCC, 1,3-dithiane, TMSI, DDQ, SeO_2, Wilkinson's catalyst, PTCs, Baker's yeast, PPA, TMS-CN, Hydrosilane, Chloramines-T, Woodward-Prevost hydroxylation, Zeigler-Natta catalyst, and crown ethers in organic synthesis and functional group transformation.
- To acquire knowledge on the various reagents employed for oxidation and reduction of various kinds of organic molecules.
- To understand the various methods of halogenations of carbonyl compounds, benzylic and allylic halogenations.

UNIT-I Reagents in Organic Synthesis-I [12 Hours]

Organometallic Reagents: Preparation, properties and uses of Organolithium, organomagnesium, Organozinc, Organocadmium, Organomercury, Organoindium, Organoaluminium and Organotellurium compounds.

Silicon containing Reagents: Preparation and reactions; Peterson reaction.

Boron containing Reagents: Preparation of organoboranes-Hydroboration, 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. Barton decarboxylation reaction, Barton deoxygenation, Stelly-Kelly coupling reaction.

UNIT-II Reagents in Organic Synthesis-II [12 Hours]

Use of the following reagents in Organic synthesis and functional group transformation: Gillman's reagent, Lithium diisopropylamide (LDA), Tri-n-butyl tin hydride, Hydrosilanes, Dicyclohexyl carbodiimide (DCC), 1,3-dithiane, Trimethyl silyliodide, Trimethyl silyl cyanide, DDQ, Selenium dioxide, Baker's yeast, Polyphosphoric acid. Chloramine-T, Aluminium *iso*-propoxide. Woodward and Prevost hydroxylation.

UNIT-III [12 Hours]

Reduction Reactions: Catalytic hydrogenation-Catalysts and solvents employed, reduction of functional groups, mechanisms and stereochemistry of catalytic hydrogenations, Hydrogenolysis, homogeneous catalytic hydrogenation.

Metal hydride reduction: Reduction with $LiAlH_4$, $NaBH_4$, BH_3 and DIBAL. Stereochemistry of reduction, Reduction in Biological systems-NADH, FAD.

Dissolving Metal Reductions: Mechanisms of reduction of conjugated system and carbonylcompounds(including Birch, Benkeser, Clemmensen reductions), Bimolecular reductions of esters, Birch reduction, Reduction with hydrazine and its derivatives, Wolf-Kishner reduction,

McMurry reaction, Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenkoreactions. Reduction with arene sulphonyl derivative of hydrazine and Reaction with diimide.

UNIT-IV **[12 Hours]**

Oxidation Reactions: Oxidation with chromium salts- Jones, Sarett and Collins reagents, Oxidation with PCC & PDC; manganese salts and MnO_2. Oxidations with Ozone, Osmium tetroxide, periodic acid, Lead tetra acetate, peracids and peresters, Dess-Martin periodinane, TEMPO, Swern oxidation and their synthetic importance in functional group transformation.

Halogenation Reactions: Halogenation of carbonyl compounds, Benzylic and Allylic halogenation, Dehydrogenation with S, Se and Pd.

References

1. Advanced Organic Chemistry, M. B. Smith and J. March, John Wiley and sons (2007).
2. Organic Chemistry, J. Clayden, N. Greeves, and S. Warren, Oxford University Press, NY (2012).
3. Stereochemistry of Carbon Compounds, E. L. Eliel, Tata McGraw-Hill, New Delhi (2006).
4. Advanced Organic Chemistry, Part A& B, F. A. Carey and R. J. Sandburg, Plenum (1990).
5. Advanced General Organic Chemistry, S. K. Ghosh, Book and Allied (1998).
6. Organic Synthesis-Special Techniques, V. K. Ahluwalia and R. Agarwal, Narosa (2005).
7. Modern Organic Reactions, H. O. House, W. A. Benjamin, California (1972).
8. Organic Synthesis, R. E. Ireland, Prentice Hall India (1969).
9. Organic Synthesis a Disconnection Approach, S. Warren, P. Wyatt., Wiley (2008)
10. Selected Organic Synthesis, I. Fleming, John Wiley & Sons (1973).

OC H 513: ADVANCED HETEROCYCLIC CHEMISTRY

Course Outcome

- Students will understand the various types of systematic nomenclature of simple, fused and bridged heterocyclic compounds with one or more diverse heteroatoms.
- Students will get the sound knowledge on the structure, synthesis and reactions of various three, four, five, six and seven membered simple and fused heterocyclic compounds with one or more heteroatom
- Study the use of heterocycles in functional group and ring transformations.
- Students will acquire knowledge about the synthesis and reactions of mesoionic compounds, structure and synthesis of anthocyanins, anthocyanidins, flavones, flavonols and isoflavones.

UNIT-I Heterocyclic Chemistry-I **[12 Hours]**

Introduction, Biologically important heterocycles, Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic, fused and bridged heterocycles. Synthesis and reactions of three membered heterocycles-aziridines, oxiranes and episulfides. Synthesis and reactions of four membered heterocycles-oxetanes, azetidines and thietanes. Synthesis & reactions of five membered heterocycles-furan, pyrrole, thiophene, oxazoles, imidazoles and thiazoles.

UNIT-II Heterocyclic Chemistry-II **[12 Hours]**

Structure, synthesis and reactions of six membered heterocycles-pyridine, α- and γ-Pyrones, Pyrimidines. Synthesis and reactions of seven heterocycles-Azepines, Oxepines and Thiepines. Synthesis and reactions of fused heterocycles-benzofuran, benzothiophene & indole. Quinoline, Isoquinoline, Coumarin, Naphthyridine. **Mesoionic compounds**: Introduction, Synthesis and reactions of sydnones. **Anthocyanins and Anthocyanidins**: Introduction and general methods of synthesis.

UNIT-III Heterocyclic Chemistry-III **[12 Hours]**

Flavones, Flavonols and Isoflavones: Introduction and synthesis of flavone, flavonal andquercetin. Structural elucidation and synthesis of Uric acid, Caffeine. **Heterocycles in functional group and ring transformations:** Alkanes from thiophenes, alcohols from isooxazolines, conversion of coumarin to benzofuran, sydnone to pyrazole, chromones to pyrazoles, furans to pyridines, pyrrole to pyridines, pyrimidine to pyrazole, isatins to quinolines, indoles to quinoline. Dimroth and Cornforth rearrangements.

UNIT-IV Heterocyclic Chemistry-IV **[12 Hours]**

Synthesis of allo and myo inositols from furan, 5,6-dihydro-7-methyl-1,4-indandione from 2-merthylfuran. Quinizarine from 2-methoxy furan, trans,trans-2,4-hexadiene from 2,5-dimethylpyrrole, γ-aryl-γ-aminobutanoic acid from pyrrole, (+)-(*S*)-4-methyl-3-heptanone from (*S*)-

1-amino-2-(methoxymethyl)pyrrolidine, 3,5-dimethyl-2-(2-methylpropyl), cyclopentan-1-one from 4-(5-*tert*-butylthiophen-3-yl)-3-methylbutan-2-one, diketone from 5-substituted –furan-2-aldehyde, δ-methyl-1-hydrindanone from 2,5-dihydro-4-methoxycarbonyl-2-thiophene acetic acid methylester, 3-butenal from oxathiolane-3,3-dioxide, dimethoxy-α-methyldopa from 4-methyl-5-ethoxy-1,3-oxazole, cis-β-amino alcohol from 3-acetyl-1,3-oxazol-2(3*H*)-one. Diastereomeric mixtures of γ-aminoalcohols from 2-methyl isoxazolidine. 3,5-dimethoxy-1,2-dimethylphthalate from 4,5-dimethoxypyrone, Barrelene from 2*H*-pyran-2-one, 3-oxohept-6-enenitrile from 2-methylisoxazole.

References

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OC S 514: BIOORGANIC CHEMISTRY

Course Outcome

Students will be able to:

- Understand the configuration and conformation of monosaccharides, chemistry of important derivatives of monosaccharides, structure and synthesis of disaccharides, general methods of determination of polysaccharide structures, structure and industrial applications of polysaccharides.
- Learn, structure, classification, properties and synthesis of amino acids.
- Explain the peptide bond formation, synthetic protocol for peptides, solution and solid phase peptide synthesis, Methods of peptide structure determination, different types protein structures and their biological importances.
- Nucleosides, nucleotides, synthesis of nucleosides, nucleotides and polynucleotides, structure and functions of nucleic acids.

UNIT-I **[12 Hours]**

Carbohydrates: Introduction and classification, Monosaccharides-Introduction, general reactions (isomerization, glycoside formation, hydrazones and osazones, alditols by reduction, oxidation-aldonic, uronic, aldaric acidsand oxidative cleavage), ring size determination of monosaccharides, configuration and conformations of monosacharides, anomeric effect, Hudson's rules, epimerization and mutarotation. Synthesis and biological importance of glycosides-ethers and esters, anhydrosugars. Deoxy and amino sugars. Dissaccharides-Structure, synthesis and biological aspects of sucrose, maltose and lactose. Industrial applications of sucrose. Polysaccharides-General methods of structure elucidation, Structure and biological functions of starch and cellulose. Industrial and biological importance of glycogen, dextran, hemicellulose, pectin, agar-agar.

UNIT-II Amino acids, peptides and proteins **[12 Hours]**

Amino acids: General structure & classification of amino acids, Abbreviation of amino acids, physiological properties, essential and non-essential amino acids, isoelectric points, Acid and base properties, Methods of synthesis-Gabriel phthalimide, azalactone and Strecker synthesis.
Peptides: Classification and nomenclature, Peptide bond -Structure and conformation, Strategy of peptide synthesis: protection (protection of amino group-Boc, Z(Cbz) and Fmoc; carboxyl group (alkyl and aryl esters) and side chain functional groups), activation and coupling (DCC, EDC, T_3P, HATU and active esters) and deprotection. Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt. Structure and synthesis of oxytocin, Synthesis of vasopressin. Biological importance of insulin, adrenocorticotropic hormone (ACTH), Growth hormone (GH) and Thyroid stimulating hormone (TSH).
Proteins: Amino acid residue analysis, C- and N-terminal determination, cleavage of peptide bond by chemical and enzymatic methods, Primary structure (amino acid sequencing), secondary structure (α- helix, β-sheets and super secondary structure) of proteins-forces responsible for holding of secondary structures, Tertiary structure of protein (folding and domain structure) and quaternary structure. Denaturation and renaturation of proteins. Biological importance of proteins.

UNIT-III **[12 Hours]**

Nucleic acids: Introduction, components of nucleic acids-Chemical and enzymatic hydrolysis of nucleic acids, Structure, nomenclature and synthesis of purine and pyrimidine bases, Nucleosides

and nucleotides, Structures and functions of NADH, NADP and ATP, Protecting groups for hydroxy group in sugar, Amino group in the base and phosphate functions. Methods of formation of internucleotide bonds-DCC, phosphodiester approach, phosphitetriester and phosphoramide methods. Solution and solid phase synthesis of oligonucleotides. Primary, secondary and tertiary structure of DNA, base-pairing, types of RNA and their structures, role of nucleic acids in the biosynthesis of proteins (Replication, Transcription, Translation), Genetic code and Finger printing.

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24. Modern Methods of Organic Synthesis, 4th edn., W. Carruthers and I. Coldham, Cambridge University Press (2015).

OC S 515: CHEMISTRY OF BIOMOLECULES

Course Outcome

- Enable the students to learn about structure and functions of lipids, prostaglandins and thromboxanes.
- Enable the students to learn about structure and synthesis of Plant pigments and Antibiotics.
- To understand the importance and functions of enzymes in biological systems.

UNIT-I **[12 Hours]**

Lipids: Introduction, Classification and biological functions, Simple lipids (Oils and fats)- Introduction and properties, synthesis of mono, di and mixed glycerides. Fatty acids: Introduction, classification, essential fatty acids- ω-3 and ω-6 fatty acids; Oxidation of fatty acids analysis of oils and fats, Synthesis of oleic acid, recinoleic acid, linoleic acid and linolenic acid, total synthesis of fatty acids. Soaps and Synthetic detergents.

Phospholipids and spingolipids-Structure and biological importance.

Prostaglandins: Introduction, Nomenclature, Classification and Biological role of Prostaglandins, Structural elucidation and stereochemistry of PGE_1, PGE_2 and PGE_3. Total synthesis of PGE_1 , PGE_2 (Corey's method & Stork's synthesis) and PGE_3 (Up John's synthesis). Inhibition of prostaglandin synthesis.

Thromboxanes: Introduction, structure, synthesis and biological activities of thromboxanes (TXA and TXB).

UNIT-II **[12 Hours]**

Plant Pigments/Porphyrins: Occurrence, extraction, classification, chemical characterization and functions of anthocyanins, flavonoids, xanthophylls and porphyrins. Structure elucidation and synthesis of Kaempferol, Quercetin, Cyanidin, Genestein, Butein and Daidzein. Structrue elucidation, synthesis and biological importance of porphyrin skeleton, haemin and chlorophyll.

Antibiotics: Introduction, Classification, β-Lactum antibiotics, Structure and synthesis of Penicillin-G, Penicillin-V, Ampicillin, Amoxycillin and Chloramphenicol. Structure and biological importance of Cephalosporin, Tetracyclin and Strectomycin.

UNIT-III **[12 Hours]**

Enzymes: Introduction, nomenclature, classification with examples and their functions. The mechanistic role of the co-enzymes in the living systems-Thiamine pyrophosphate (TPP) in oxidative and non-oxidative decarboxylation of keto acids and formation of ketols; Pyridoxal phosphate in transamination, decarboxylation, dealdolization and elimination reactions of amino acids; Lipoic acid in the transfer of acyl group and oxidation reactions; Co-enzyme A in generation and ternsfer of acyl groups; Biotin in the addition of carboxyl groups to saturated carbon atoms and in transcarboxylation reactions; tetrahydrofolic acid in one carbon transfer reactions at all oxidation levels except that of CO_2; Nicotenamide and flavin coenzymes in biological oxidation-reduction reactions. Biogenesis of fatty acids, terpenoids (mono and sesquiterpenoids), steroids, amino acids, alkaloids.

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OC E 516: ANALYTICAL AND GREEN CHEMISTRY

Course Outcome

Enable the students:

- To understand the basic principles and theory of UV-Visible, Electronic, Infra-Red, Nuclear Magnetic Resonance and Mass Spectroscopy.
- To study the utility of these techniques in structure elucidation of simple organic molecules.
- To know about water cycle, water sources, water quality, significant measurements of water parameters and treatment of water for drinking and industrial purposes.
- To learn about principles and use of green chemistry in laboratory synthesis.
- To understand the basic principles and utility of sonochemistry and Microwave induced organic synthesis.

UNIT-I **[12 Hours]**

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, Factors affecting the positions of UV bands. Theoretical prediction of λmax for polyenes, α,β-unsaturated aldehydes, ketones (Woodward-Fieser rules).

IR Spectroscopy: Basic principles, Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities.

Nuclear Magnetic Resonance Spectroscopy: Basic principles, Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Applications of NMR spectroscopy in structure elucidation of simple organic molecules.

Mass Spectrometry: Basic principles, molecular ions, meta-stable ions and isotope ions. Fragmentation processes, McLafferty rearrangement. retro Diels-Alder fragmentations. Nitrogen rule.

UNIT-II **[12 Hours]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Determination and significance of DO, BOD, COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

UNIT-III **[12 Hours]**

Green Chemistry: Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solventless) reactions, photochemical reactions, enzymatic transformations & reactions in ionic liquids.

Sonochemistry: Introduction, the phenomenon of cavitation, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions.

Microwave induced organic synthesis: Introduction, atom efficiency, % atom utilisation, advantages and limitations, alkylation of active methylene compounds, N-alkylation, condensation of active methylene compounds with aldehydes, Diels-Alder reaction, Leuckardt reductive amination of ketones.

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14. Green Chemistry-Environment benign reactions, V. K. Ahluwalia, Ane Books India, (2006).

OC P 517: ORGANIC CHEMISTRY PRACTICALS–III

(Any twelve preparations are to be carried out)

Course Outcome

- Enable the students to demonstrate the methods of organic preparations using multistep synthetic protocol.
- Learn how to engage in safe laboratory practices by handling laboratory glassware, equipment, and chemical reagents appropriately.
- Understand how to dispose of chemicals in a safe and responsible manner, how to perform common laboratory techniques including reflux, distillation and isolation/separation and purification of organic compounds by various methods.
- Comprehend the applications of different reactions in the preparation of heterocycles.
- Demonstrate skills in the preparation of heterocycles.

Preparation of organic compounds through multistep synthetic protocol

(Report of the yield, melting point, cost per Kg of the product synthesized and the cost from the catalogue).

1. Preparation of *o*-aminobenzoic acid from phthalic anhydride.
2. Preparation benzilic acid from benzoin.
3. Preparations of benzanilide from benzophenone, acetanilide from acetophenone and ε-caprolactam from cyclohexanone *via* Beckmann rearrangement.
4. Preparation of p-aminoazobenzene from aniline through diazoaminobenzene.
5. Preparation of 2,4-dinitrophenylhydrazine from chlorobenzene.
6. Preparation of m-nitrobenzoic acid from benzoic acid/methyl benzoate.
7. Preparation of *p*-amionobenzoic acid from *p*-nitrotoluene.
8. 3-Bromo-4-methyl benzaldehyde from *p*-Toluidine.
9. Preparation of α-acetylaminocinnamic acid from glycine.
10. Preparation of anthraquinone from phthalicanhydride.
11. Preparation of 4-bromoaniline from acetanilide.
12. Preparation of 4-nitroaniline from acetanilide.
13. Preparation of 2,4-dinitrophenol from chlorobenzene.
14. Preparation of 1,3,5-tibromobenzene from aniline.
15. Preparation of Ethyl resorcinol from Resorcinol.
16. Preparation of 2,5-dihydroxy acetophenone from hydroquinone.
17. Preparation of adipic acid from cyclohexanol*via*cyclohexanone.
18. Preparation of o-hydroxybenzophenone from phenol *via* Fries rearrangement.
19. Preparation of p-chlorobenzoic acid from p-nitrotoluene*via*Sandmeyer reaction.
20. Preparation of m-chloroiodobenzene from m-dinitrobenzene.
21. Preparation of N-methylanthranilic acid from phthalic acid/phthalic anhydride.
22. Preparation of N-bromosuccinimide from Succinic acid/succinic anhydride.
23. Preparation of benzphenacolone from Benzophenone*via* Benzpinacol.
24. Preparation of methyl cinnamate from cinnamic acid using Perkin reaction followed by esterification.
25. Preparation of phenyl cinnamyl ether from cinnamaldehyde through cinnamyl alcohol, cinnamyl bromide followed by nucleophilic substitution reaction with phenol.
26. Preparation of 2,5-dihydroxyacetophenone from hydroquinone
27. Preparation of 2-carbethoxycyclopentanone from adipic acid.

Preparation of Heterocycles

1. Preparation of diethyl 3,5-dimethyl-pyrrole-2,4-dicarboxylate using Knorr pyrrole synthesis.
2. Preparation of 1,2,3,4–tetrahydrocarbazole from cyclohexanone through Fischer indole synthesis.
3. Preparation of 7-hydroxy-4-methyl-coumarin from resorcinol and ethyl acetoacetate *via*Pechmann reaction.
4. Preparation of 2,3-diphenylquinoxaline from benzoin through oxidation and condensation with o-phenylenediamine.
5. Preparation of 9-chloroacridine from o-chlorobenzoic acid and aniline followed by $POCl_3$ cyclization.
6. Preparation of 9-substituted acridine from diphenyl amine and carboxylic acid using $ZnCl_2$.
7. Preparation of 1-phenyl-3-methyl-5-pyrazolone from phenyl hydrazine and ethyl acetoacetate
8. Preparation of 2,5-disubstituted oxazole from acid hydrazide and carboxylic acid.
9. Preparation of 3,5-diaryl-4,5-dihydropyrazole from substituted acetophenones*via* chalcone.
10. Preparation of 4-arylthiazole-2-amine from substituted acetophenones.
11. Preparation of quinoline from aniline.
12. Preparation of 2-phenylindole from acetophenone*via*acetophenone phenyl hydrazone.
13. Preparation of 2,4,6-trimethylquinoline from p-toluidine via 4-(p-tolylamino)pent-3-ene-2-one.
14. Preparation of flavone from o-hydroxyacetophenone via o-benzoyl acetophenone and o-hydroxy-dibenzoylmethane.
15. Preparation of benzimidazole and 2-substituted benzimidazole from o-phenylenediamine.
16. Preparation of 1-amino-5-substituted-1,2,4-triazole-2-thiol from carboxylic acid and thiocarbohydrazide.

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OC P 518: ORGANIC CHEMISTRY PRACTICALS-IV

(Any twelve experiments are to be carried out)

Course Outcome

- Enable the students to learn and identify the concepts of a standard solutions, primary and secondary standards
- Understand and learn the principle of quantitative determinations of different types of organic molecules, such as carboxylic acids, amides, esters, amino acids, sugars, phenols, amines, aldehydes, ketones, acid-ester mixture, amide-ester mixture.
- Know the quantitative determination of functional groups like hydroxyl, vic-hydroxy, enol, amino, amide and nitro groups.
- Study the quantitative determination of unsaturation in unsaturated organic compounds.
- The students will apply the green chemistry protocol for the synthesis of organic compounds.

Quantitative Determinations

1. Determination of equivalent weight of acids by titrimetric method.
2. Quantitative determination of mono/di-carboxylic acids and esters by titrimetric method.
3. Quantitative determination of aromatic amines/phenols by bromide-bromate method.
4. Quantitative determination of aromatic amines/phenols by acetylation method.
5. Quantitative determination of glycine by Sornsen's formal titration method.
6. Quantitative determination of sugars by Bertrand's/Fehling's solution method.
7. Quantitative determination of acid & ester in the given mixtures.
8. Quantitative determination of acid & amide in the given mixtures.
9. Quantitative determination of ketones by haloform reaction method.
10. Quantitative determination of ketones by oxime method.
11. Quantitative determination of aldehydes and ketones by using 2,4-dinitrophenyl hydrazine method.
12. Quantitative determination of hydroxyl and vic-hydroxy groups using different methods.
13. Quantitative determination of amino, nitro and amide groups using different methods.
14. Quantitative determination of unsaturation in organic compounds by various methods.

Green Preparations

1. Green synthesis of acetanilide from aniline and acetic acid.
2. Green synthesis of dihydropyrimidinone by Beginelli method.
3. Synthesis of biodiesel from vegetable oil and determination of pH and freezing point.
4. Preparation of benzoin from benzaldehyde by thiamine catalyzed benzoin condensation.
5. Preparation of benzopinacol from benzophenone by photoreduction method.
6. Alkylation of diethyl malonate with benzyl chloride using microwave.
7. Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide using phase transfer catalyst.
8. Synthesis of Luminol from phthalic anhydride and study of chemical luminescence.

Spectroscopic Methods

9. Demonstrations of recording/predicting/downloading the UV, IR, NMR and LC-MS spectra of organic compounds from web sites.
10. Interpretation of structure of organic molecules by the joint application of UV-Vis., IR, NMR and Mass spectra provided by the instructor.
11. Locating an organic compound by reference to literature (Chemical Abstract).
12. Applications of Chem draw and Chem sketch software tools to draw the chemical structures and to write the mechanism of the reactions.

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IV SEMESTER

OC H 561: ORGANIC SYNTHETIC METHODS AND GREEN TECHNIQUES

Course Outcomes

Enable the students:

- To understand the synthetic design with diverse chemical reactions, planning of organic synthesis and functionality.
- To learn the principles and technologies used in disconnection approach, the utility of protecting group strategy in organic synthesis and retrosynthetic analysis.
- Students will acquire the knowledge of utilization of principles of green chemistry by the use of phase transfer catalysts, crown ethers and ionic liquids in organic synthesis.
- Students will gain knowledge on Sonochemical and Microwave induced organic reactions.
- Students will also learn to understand the preparation, properties and uses of polymer supported reagents in organic synthesis and mechanistic aspects of some multicomponent reactions.

UNIT- I **[12 Hours]**

Synthetic Design: Classification of carbon-carbon single bond and double bond forming reaction and their use in carbon skeleton ring formation. Ring forming and ring cleaving reactions, use of Thorpe condensation, Carbene insertion reaction, 1,3-dipolar addition and Ene reaction in ring formation.

Planning of Organic Synthesis: Selection of starting materials and key intermediates during the synthesis. Use of Robinson annulation, Dieckmann cyclisation, Arndt-Eistert synthesis, Diel's-Alder reaction in organic synthesis. Synthesis of Cubane and Iswarane.

Functionality: Synthesis of 6 and 7-methoxytetralones, biotin and penicillin-V with special reference to the introduction of functional groups.

UNIT- II **[12 Hours]**

General introduction to disconnection approach. Synthons and synthetic equivalents. Interconversion of functional groups. One group C-X and two group C-X disconnections. Use of C-C one group and C-C two group disconnections in the synthesis of 1,2; 1,3 and 1,5-difunctionalised compounds.

Protecting groups: Protection of hydroxyl, amino, carboxylic and carbonyl groups.

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds, benzocaine, *p*-methoxyacetophenone, 2-methyl-6-methoxy-indole-3-acetic acid, & 1-phenyl-4-*p*-methoxyphenyl-1,3-butadiene. Illustrative synthesis of Limonene, Benziodarone, Nitrofurazone, Warfarin, Juvabione and Longifolene.

UNIT-III **[12 Hours]**

Green Chemistry: Principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solventless) reactions, Phase transfer catalyst catalysed reactions-Quaternary ammonium salts-synthesis and applications in the alkylations, substitution reactions, esterifications, eliminations, condensations, oxidations and reductions; Crown ethers-Synthesis, applications in the alkylations, esterifications, saponifications, elimination reactions, superoxide anion and generation of carbenes.

Sonochemistry: Introduction, Phenomenon of cavitation, Sonochemical esterification, substitution, addition, oxidation, reduction and coupling reactions.

Microwave induced organic synthesis: Introduction, reaction vessel and reaction medium, atom efficiency, % atom utilisation, advantages, limitations and precautions. Applications in alkylation of active methylene compounds, N-alkylation, condensation of active methylene compounds with aldehydes, Diels-Alder reaction, Leuckardt reductive amination of ketones, ortho ester Claisen rearrangement.

Ionic Liquids: Introduction, properties, types, preparation, applications like Epoxidation, Alkene Metathesis, Oxidation, Reduction and Enzyme catalysed synthesis.

UNIT-IV **[12 Hours]**

Polymer supported reagents in organic synthesis: Introduction, properties of polymer support, advantages of polymer supported reagents and choice of polymers. Applications: Substrate covalently bound to the support, Synthesis of oligosachcharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. Synthesis of polystyryl boronic acid and use in diol protection reaction. Reagent linked to a polymeric material: Preparation of sulfonazide polymer and application in diazo transfer reaction. Synthesis of polymer bound per acid and its applications. Polymer supported catalytic reactions: Preparation of polymer supported $AlCl_3$ and application in etherification and acetal formation reactions.

Multicomponent Reactions: Studies on the mechanistic aspects and use of theUgi, Passerini,Biginelli, Hantzsch, Doebner-Miller, Jacobson, Barbier, Baylis-Hilmann and Mannich reactions.

References

1. Art in Organic Synthesis, Anand, Bindra & Ranganath, Wiley, (1970).
2. Organic Synthesis - A Disconnection Approach, S. Warren, P. Wyatt., Wiley (2008)
3. Advanced Organic Chemistry, Part A & B, F. A. Carrey & R. J. Sundberg, Plenum Press, (1990).
4. Modern Methods of Organic Synthesis, N. Carruthers, Cambridge University, (1996).
5. Selected Organic Synthesis, I. Fleming, John Wiley & Sons, (1973).
6. Organic Synthesis: Special Techniques, V. K. Ahluwalia and R. Aggarwal, Narosa,(2003).
7. Polymers as aids in Organic synthesis, N. K. Mathur, C. K. Narang and R. E. Williams, Academic Press, (1980).

OC H 562: MEDICINAL CHEMISTRY AND ADVANCED STEREOCHEMISTRY

Course Outcome

- Students will gain an understanding on the classification and nomenclature of drugs, modern theories of drug action and drug design.
- Students will able to know classification, synthesis and mode of action of antipyretic analgesis drugs, general anesthetics, local anesthetics, cardiovascular drugs, antineoplastic agents and antiviral drugs with suitable examples.
- Students will understand the classification and synthesis of various sedative, hypnotic agents, anticonvulsants, antihistaminic agents, non-steroidal hormones and prostaglandins.
- Students will acquire knowledge about nomenclature, classification and biological role of prostaglandins, Structural elucidation, stereochemistry and total synthesis of prostaglandins.
- Students will also learn advanced stereochemistry topics such as asymmetric synthesis by employing chiral pool, chiral auxiliaries, chiral reagent and chiral catalysts.

UNIT-I **[12 Hours]**

Drugs: Classification and nomenclature of drugs. Theories of drug action-Occupancy theory, Induced fit theory and Perturbation theory. Analogues and Prodrugs, Factors governing drug design. Variation method of drug designing, Physico-Chemical factors and factors governing the ability of drugs.

Antipyretic Analgesics: Introduction and classification, synthesis & mode of action of Phenacetin, Cinchophen, Phenazone and Mefenamic acid.

General Anesthetics: Introduction and classification, synthesis & mode of action of methoxyfluorane, Thiopental sodium and Fentanyl citrate.

Local anesthetics: Introduction and classification, synthesis & mode of action of benzocaine, α-Eucaine, Lignocaine hydrochloride and Dibucaine hydrochloride.

UNIT-II **[12 hours]**

Cardiovascular drugs: Introduction and classification, Synthesis & mode of action of Hydralazine, Methyldopa, Diazoxide, Procainamide, and Prenylamine.

Antimalarials: Introduction and classification, Synthesis & mode of action of Chloroquinephosphate and pyrimethanin.

Antineoplastic agents: Introduction and classification, Synthesis & mode of action of Mechlorethamine hydrochloride, Methotrexate and Flurouracil.

Antiviral drugs: Introduction and classification, Synthesis & mechanism of action of Methisazone and Amantidine hydrochloride.

UNIT-III **[12 Hours]**

Sedative and Hypnotic Agents - Introduction and classification. Synthesis of Barbitone, Pentobarbital, Triazolam.

Anticonvulsants- Synthesis of Phenytoin sodium and Trimethadione.

CNS stimulants-Introduction and classification. Synthesis and mechanism of action of Caffeine and Phetermine.

Antihistaminic agents- Synthesis of Diphenhydramine HCI and Pheniramine.

Non steroidal hormones: Study of the Oxytocin and Vasopressin.

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 & Up John's synthesis).

UNIT-IV Advanced Stereochemistry [12 Hours]

Asymmetric Synthesis: The Chiral pool; Alpha amino acids in the synthesis of Benzodiapines, Carbohydrates (Benzyl D-Mannose to Swainsonine) Preparation of tomolal from D-mannitol, Felion-Ahn model and Cram's chelation control. Enantiomeric excess and its determination.

Chiral Auxiliaries: Oxazolidinones, Chiral sulfoxides in controlling the reduction ofketones, Use of chiral Auxillaries in Diels-Alder and aldol reactions.

Chiral Reagents: BINOL, DIBAL, Tartarates, Lithium diamides.

Chiral Catalysts: Rhodium and Ruthenium catalysts with Chiral phosphine ligands like (R)-BINAP, (R,R)-DIOP.

Asymmetric amplification and autocatalysis.

References

1. Medicinal Chemistry, A. Kar, New Age, (2005).
2. Medicinal Chemistry, G. R. Chatwal, Himalaya, (2002).
3. Principles of Drug Action-The Basis of Pharmacology, A. Goldstein, W. B. Pratt, P. Taylor, Churchill Livingstone, NY (1990).
4. Organic Chemistry, Vol II, I. L. Finar, Longmann ELBS, (1973).
5. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International, (1991).
6. Stereochemistry of Organic Compounds, P. S. Kalsi, Wiley Eastern, (1994).
7. Stereochemistry of Carbon Compounds, E. L. Eliel, John Wiley, (1990).

OC H 563: NATURAL PRODUCTS CHEMISTRY

Course Outcomes

- Students will get a good understanding of isolation, classification natural products,
- To learn methods of structure elucidation and synthesis of various types of alkaloids, terpenoids, carotenoids, steroids and steroidal hormones with representative examples, transformations in steroids and hormones.
- To study steroidal oral contraceptives.
- Students will also learn the chemistry of Vitamins and Antibiotics.

UNIT-I **[12 Hours]**

Alkaloids: Definition, Classification and isolation, general methods of structural determination, structural elucidation, stereochemistry, rearrangement, synthesis of Adrenaline, Ephedrine, Nicotine, Cocaine, Papaverine, Piperine, Cinchonine, Quinine, Morphineand Reserpine.

UNIT-II **[12 Hours]**

Terpenoids: Classification, isoprene and special isoprene rules, general methods of structure determination. Structure& synthesis of α-Pinene, Camphor, Farnesol, Zingiberene, α-Santonin, Vetivones, Caryophylene, Abietic acidand Squalene.

Carotenoides: Introduction and geometrical isomerism. Structure and synthesis of β-Carotene and Lycopene.

UNIT-III **[12 Hours]**

Steroids: Introduction and Nomenclature, Blanc's rule, Diel's hydrocarbon, Chemistry of Cholesterol, Ergosterol, Vitamin-D, Stigmasterol & bile acids.

Steroidal hormones: Chemistry of Oestrone, estradiol, estriol and their chemical relationship. Progesterone, androsterone and testosterone. Steroidal oral contraceptives.

UNIT-IV **[12 Hours]**

Vitamins: Classification, Sources and Deficiency diseases, Biological functions of Vitamins, Study of Vitamin A1and A_2, Vitamin B1, B2 B_6 and B_9, Vitamin H, Vitamin C, Vitamin E, Vitamin K.

Antibiotics: Introduction, Classification, Chemistry of Pencillin V, Cephalosporine C, Streptomycin, Chloramphenicol and Tetracyclin.

References

1. Natural Products Chemistry, VolI & II, G. R. Chatwal, Himalaya,(1990).
2. Chemistry of Natural Products, VolI & II, O. P. Agarwal, Goel, (1985).
3. Organic Chemistry, VolI & II, I. L. Finar, Longmann ELBS, (2000).
4. Chemistry of Natural Products-A Unified Approach, N. R. Krishnaswamy, University Press,(1999).
5. Chemistry of Natural Products, S. V. Bhat, B.A. Nagasampagi, M. Sivakumar, Springer-Narosa, (2005).

OC S 564: SYNTHETIC POLYMERS, DYES AND PESTICIDES

Course Outcome

Enable the students

- To acquire detailed knowledge in classification and nomenclature of polymers, methods of polymerization, mechanism and stereochemistry, properties, structure, synthesis and applications of synthetic polymers, polyesters, polyamides, phenol-formaldehyde, urea-formaldehyde and epoxy resins, polyurethanes, polycarbonates, synthetic rubber, manufacture and structural features of natural rubber and regenerated cellulose.
- To understand the modern theories of colour and constitution, classification of dyes, methods of applying dyes to the fabrics, Synthesis and applications of various types of azo dyes, triphenyl methane dyes, cyanin dyes, reactive dyes, optical brighteners and pigments.
- To gain knowledge about classification, mode of action and synthesis ofseveral organophosphorous and organochlorine insecticides, natural pyrethroid insecticides, isolation and structure of natural pyrethrins, synthetic pyrethroids.
- To study the Synthesis and uses of insect pheromones in pest control, fungicides and herbicides, fumigants and repellants, mechanism of action and toxicities of insecticides, fungicides and herbicides.

UNIT-I **[12 Hours]**

Synthetic polymers: Methods of polymerization, Mechanism and Stereochemistry, Addition polymerization (Anionic, Cationic and Free radical process), Condensation and Stepwise polymerization, Coordination polymerization, Use of Ziegler-Natta catalyst in polymerisation. Ring opening polymerization. Mechanism of co-polymerization. Properties, Structure and applications of Polythene, Polypropylene, PVC, Polystyrene & Acrylic polymers, Teflon, polyesters, polyamides, Phenol-Formaldehyde resins, Epoxy resins, Polyurethanes, Polycarbonates. Structural features and manufacture of natural rubber, Regenerated cellulose.

UNIT-II **[12 Hours]**

Dyes: Introduction, modern theories of colour and chemical constitution. Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes- Orange–II, rosanthrene O, Naphthol blue black 6B, Mordant brown, Congo red, Methyl orange, Chrysoidin G, Bismark brown. Triphenylmethane dyes - Malachite green, Rosaniline, Crystal violet; Phenolphthalein; Cyanin dyes- Ethyl Red and Cyanin blue. Reactive dyes, Optical brighteners - Tinapal and Blankophor. Pigments: Lake red and Orange R.

UNIT-III **[12 Hours]**

Insecticides: Introduction, classification and Historical importance. Mode of action and synthesis of organochlorines (Diazenon, DDT, Heptachlor, Chlordane), organophosphates (Monocrotophos, parathion, chlorpyrifos) and carbamates (Carbaryl, Carbofuran, Aldicarb). Naturally occurring insecticides-pyrethroids-natural pyrethrins-isolation and structures, synthetic pyrethroids.

Insect Pheromones: Introduction, Classification and use in insect pest control. Synthesis of disparlure, grandisol, Periplanone-A & B and bomykol.

Fungicides: Introduction, Systemic fungicides-types & examples.

Herbicides: Introduction, study of sulfonyl ureas and heterocyclic sulphonamides. Fumigants and repellants. Mechanism of action and toxicities of insecticides, fungicides and herbicides.

References:

1. Polymer Science, V. R. Gowariker, N. V. Vishwanathan & T. Shridhar, Wiley Eastern,(2008).
2. Textbook of Polymer Science, F. W. Billmeyer, Wiley, (1984).
3. A Textbook of Dyes, O. D. Tyagi & M. Yadav, Anmol Publications,(2002).
4. Textbook of Dyes, A. Arora, Sonali Publications, (2009).
5. Synthetic Dyes, Vol. I, Venkataraman, (1999).
6. Synthesis and Chemistry of Agrochemicals, Vol I & II, ACS, Wahington.
7. Chemicals for Crop Protection and Pest Managements, M. B. Green, G.S. Hartley and West, Pergamon.
8. Chemistry of Insecticides and Fungicides, S. Ramulu, Oxford & IBH, (1985).

OC S 565: CHROMATOGRAPHIC TECHNIQUES FOR ORGANIC CHEMISTRY

Course Outcome

- The students will explain the fundamentals of chromatography.
- Acquire a critical knowledge of principle, analytical and applications of paper and thin layer chromatography in organic chemistry.
- Learn the principles, separation mechanisms and applications of column chromatography.
- Understand the theory, instrumentation and applications of GC and HPLC.
- Learn column chromatography, paper chromatography, thin layer chromatography, gas chromatography and High performance liquid chromatography.
- Illustrate the principles, separation mechanisms and applications of affinity chromatography.
- Demonstrate the principle of GFC techniques used in isolation, purification, identification and analysis of macromolecules.

UNIT-I **[12 Hours]**

Fundamentals of chromatography: Introduction, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of stationary and mobile phase-nature of adsorbents, factors influencing the adsorbents, nature and types of mobile phases and stationary phases.

Paper Chromatography (PC): Definitions, theory and principle, techniques; one, two-dimensional and circular PC, mechanism of separation, structure of cellulose and types of paper, methodology, preparation of sample, choice of solvents, location of spots and measurements of RF value, factors affecting RF values, advantages and applications, Separation of amino acids and carbohydrates.

Thin Layer Chromatography (TLC): Definition, mechanism, efficiency of TL plates, methodology, selection of stationary and mobile phases, preparation of plates. Spotting, development, identification and detection, reproducibility of RF values, comparison of TLC with high performance thin-layer chromatography, paper chromatography and column chromatography. Qualitative and quantitative analysis.

UNIT-II **[12 Hours]**

Column Chromatography (CC): Construction and operation of column, choice of adsorbents and eluents, techniques of elution, methods of detection, analytical and industrial applications.

Gas chromatography (GC): Principle, comparison of GSC and GLC, instrumentation, columns pack and tubular, study of detectors-thermal conductivity. Flame ionization, electron capture and mass spectrometry. Factors affecting the separation, retention volume, retention time, applications.

High Pressure Liquid Chromatography (HPLC): Apparatus, pumps, column packing, characteristics of liquid chromatographic detectors-UV, IR, refractometer and fluorescences detectors, advantages and applications.

UNIT-III **[12 Hours]**

Ion Exchange Chromatography (IEC): Definitions, principle, requirements for ion exchange resin and its synthesis, types of ion-exchange resins, basic features of ion-exchange reactions, resin properties-ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery processes.

Gel Permiation Chromatography: size exclusion chromatography (Gel filtration) with special reference to separation of protein, carbohydrates and nucleic acids. Preparation of medium, column, determination of void volume, sample application, detectors. Affinity chromatography: Chromatographic matrix, ligand selection, linkage of ligands, absorbant derivatives. LC/MS, LC/MS-MS, GC/MS, GC/MS-MS for organic compound analysis.

References

1. Chromatography, Part A and B, 5th edn., E. Heftman, Elsevier (1992).
2. Chromatography Today, D. F. Poole and S. K. Poole, Elsevier (1991).
3. Principles of Instrumental Analysis, 7th ed., D. A. Skoog, F. J. Holler and S. R. Crouch, Cengage India Pvt. Ltd., (2020).
4. Principles of Instrumental Analysis, 4th ed., D. A. Skoog and D. M. West, Saunders College Pub.(1992).
5. Quantitative Analysis, 5th edn., R. A. Dayand A. L. Underwood, Prentice-Hall (1998).
6. Analytical Chemistry, 5th edn., G. D. Christian, John Wiley & Sons (2001).
7. Instrumental Methods of Analysis, 7th edn., H. H. Willard, L. L. Merritt and J. A. Dean, CBS Publishers, New Delhi (1988).
8. Instrumental Methods of Chemical Analysis, 19th edn., B. K. Sharma, Goel, 2000.
9. Vogel's Textbook of Quantitative Chemical Analysis, 6th edn., J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas, Pearson Education, New Delhi (2004).
10. Analytical Chemistry Principles, 2nd edn., John H. Kennedy, Saunders College Publishing, California (1990).

OC P 566: ORGANIC CHEMISTRY PRACTICALS-V
(Any twelve experiments are to be carried out)

Course Outcome

- Enable the students to gain the knowledge about the isolation, purification and characterization of various kinds of natural products.
- Learn the extraction of groundnut oil and coconut oil from their natural sources.
- Understand the characterization of natural products through derivatization and quantitative determination.
- Understand and learn the quantitative determinations of natural products, dyes, drugs, amino acids and sugars.
- Demonstrate the separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, steam distillation, paper, thin layer and column chromatography.
- Study the determination of order of reactions, salt effect and effect of acidity on reaction rates.
- Understand the recording of various spectra of the organic compounds.
- Enable the students to identify the importance of reagents used in the synthesis of drugs, dyes and polymers.
- Comprehend the applications of different reactions in the preparation of drugs, dyes and polymers.
- Demonstrate skills in the preparation of drugs, dyes and polymers.

Extraction of Organic Compounds from Natural Sources

1. Isolation of Caffeine from Tea Leaves
2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins).
3. Isolation of Nicotine dipicrate from tobacco
4. Isolation of piperine from black pepper Isolation of piperine from pepper.
5. Isolation of Lycopene from tomatoes
6. Isolation of β-carotene from carrots
7. Isolation of hesperidiene from orange peal.
8. Isolation of glutamine from red beet.
9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
10. Isolation of limonene from lemon peel (Citrus rinds).
11. Isolation of Eugenol from cloves.
12. Isolation of cinchonine from cinchona bark.
13. Isolation of azeleic acid from castor oil.
14. Isolation of cincole from eucalyptus leaves.
15. Extraction of DNA from onion peels.

16. Isolation of essential oils from cumin and rose petals.
17. Isolation of curcuminoids from turmeric powder.
18. Isolation and separation of pigments chlorophyll and B-carotene from spinach.
19. Isolation of cysteine from hair
20. Separation of caffeine from tannins by sublimation.
21. Isolation of lactose from milk (purity of sugar should be checked by LC and PC and Rf values reported).
22. Isolation of lipids from egg yolks
23. Isolation of enzymes-Lipase and Sucrase.
24. Extraction of groundnut and coconut oils.

Methods of Separation

1. Separation of mixture of cyclohexane and toluene and mixture of benzene and toluene by fractional distillation.
2. Preparation of o- and p-nitro-phenols and their separation by steam distillation/column chromatography/fractional crystallization.
3. Preparation of 6- and 8-nitro-7-hydroxy-4-methyl coumarins from 7-hydroxy-4-methyl-coumarins and their separation by fractional crystallization.
4. Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.
5. Separation and identification of amino acids/sugars by paper chromatography and determination of Rf values.
6. Separation and identification of amino acids/sugar/dyes by thin layer chromatography and determination of Rf values.
7. Separation of a mixture of ortho and para nitroanilines by thin layer chromatography using chloroform as the eluent.
8. Separation and identification of analgesic drugs-acetaminophen, aspirin, caffeine, ibuprofen and salicylamide by thin layer chromatography.
9. Separation of plant pigments of spinach extract using thin layer chromatography.
10. Separation of spinach leaf pigments/dyes by column chromatography.
11. Separation of o- and p-nitro-anilines by column chromatography using alumina column.

Quantitative Determinations

1. Determination of iodine value of an oil and fat by chloramine-T and by other methods.
2. Determination of saponification value of an oil or fat.
3. Determination of acid value of an oil or fat.
4. Preparation of carboxylic acid derivatives of natural products containing alkyl side chain in their aromatic rings and determination of their equivalent weight.

5. Preparation of aryloxy acetic acid derivatives of phenolic natural products and determination of their equivalent weight.
6. Preparation of anilinoacetic acid derivatives of natural products containing amino group and determination of their molecular weight.
7. Determination of equivalent weight of carboxylic acid by silver salt method
8. Determination of enol content by Meyer's method.
9. Determination of sucrose by Fehling's method.
10. Quantitative determination of urea by hypobromite method.
11. Quantitative determination of Vitamin C by iodometric titration.
12. Verification of the Beer-Lambert's Law and determination of the concentration of given dye solution colorimetrically.
13. Quantitative determination of uric acid and creatinine in urine.
14. Quantitative determination of pharmaceutical tablet ascorbic acid / aspirin / ibuprofen / paracetamol lbruprofen / analgin.
15. UV/VIS spectrophotometric determinations of amino acids / proteins / carbohydrates / aspirin / cholesterol / ascorbic acid / caffeine.
16. Determination of COD of water sample.
17. Determination of order of reactions-S_N1 and S_N2 reactions, salt effect and effect of acidity on reaction rates by using n-butyl bromide and *t*-butylchloride.

Preparation of Drugs

1. Preparation of sulfanilamide from acetanilide through p-acetamidobenzenesulfonyl chloride and p-acetamidobenzenesulfonamide.
2. Preparation of paracetamol from p-nitrophenol*via* reduction and acetylation.
3. Preparation of benzoccaine(p-amino ethyl benzoate) from p-nitrotoluene via oxidation, reduction and esterification reactions.
4. Preparation of phenacetin from p-nitro phenol via reduction, acetylation and ethylation.
5. Preparation of aspirin from methyl salicylate/salicylic acid.
6. Preparation of phenazone (*1,5-dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one)*from phenyl hydrazine and ethyl acetoacetate using condensation and methylation reactions.
7. Preparation of phenytoin (5,5-diphenylhydantoin) and thiophenytoin (5,5-thiohydantoin) from benzoin *via*benzil using urea/thiourea.

Preparation of Dyes

1. Preparation of benzeneazo-2-naphthol from aniline *via* diazotisation and coupling.
2. Preparations of para red, methyl red, methyl orange and orange-IIthrough diazotisation and coupling reactions.
3. Preparations of phenolphthalein, fluorescein and eosin.
4. Preparation of malachite green from N,N-dimethyl aniline and benzaldehyde.
5. Preparation of indigo from anthranilic acid/o-nitrobenzaldehyde and acetone.

Preparation of Polymers

1. Preparation of caprolactam from cyclohexanone and conversion to Nylon-6.
2. Preparation of Nylon-6,6 from hexamethylenediamine and adipic acid.
3. Preparation of urea-formaldehyde resin (bakelite) from urea and formaldehyde.
4. Preparation of phenol-formaldehyde resin (novolac and resole) from phenol and formaldehyde.
5. Preparations of polystyrene and polyacrylamide from styrene and acrylamide.

References

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2. Laboratory Manual in Organic Chemistry, 3rd edn., R. K. Bansal, New Age (1996).
3. Experimental Organic Chemistry-Vol. I & II, P. R. Singh, D. S. Gupta and, K. S. Bajpai, Tata McGraw-Hill (1981).
4. An Introduction to Natural Products Isolation-Method and Protocols, 3rd edn., Satyajit D. Sarker and Lutfun Nahar, Humana Press Inc., NJ, (2012).
5. Natural Products Isolation-Vol. 20, 2nd edn., S. D. Sarker, Z. Latif and A. I. Gray, Humana Press Inc., NJ (2006).
6. Natural Products Isolation-Volume 4, Richard J. Cannell, Humana Press, NJ (2008).
7. Experimental Organic Chemistry, H. D. Durst and G. W. Gokel, McGraw Hill Book Co., New York (1980).
8. Laboratory Experiments in Organic Chemistry, R. Adams, J. R. Johnson and C. F. Wicox, McMillan (1979).
9. Experimental Organic Chemistry, H. D. Durst and G. E. Goke, McGraw-Hill (1980). Experimental Organic Chemistry-Vol. I & II, P. R. Singh, Tata McGraw-Hill (1981).
10. Laboratory Manual in Organic Chemistry, B. B. Dey and M. V. *Sitaraman*, Books &Allied (1992).
11. Vogel's Text Book of Practical Organic Chemistry, 5thedn., B. S. Furniss, A. J. Hannaford, P. W. Smith and A. R. Tatchell, Longman-ELBS (2005).
12. A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, A.I. Vogel, Longman (1970).
13. Practical Organic Chemistry, F. G. Mann and B. C. Saunders, Orient Longman (2004).
14. Advanced Practical Organic Chemistry, J. Leonard, B. Lygo and G. Proctor, CRC Press (2013).
15. Comprehensive Practical Organic Chemistry-Preparation and Qualitative Analysis, V. K. Ahluwalia and Renu Aggarwal, Sangam Books (2001).
16. An Advanced Course in Practical Chemistry, 3rdedn., A. K. Nad, B. Mahapatra and A. Ghoshal, New Central Book Agency (2011).
17. Advanced Practical Organic Chemistry, 3rdedn., N. K. Vaishnoi, Vikas Publishing House (2009).
18. Practical Organic Chemistry, Ajay Kumar Manna, Books & Allied (2018).
19. Advanced Practical Organic Chemistry-Vol. II, Jag Mohan, Himalaya Publishing House (1992).

20. Elementary Practical Organic Chemistry-Vol. III, Quantitative Organic Analysis, A. I. Vogel, Pearson (2011).
21. Vogel's Text Book of Quantitative Chemical Analysis, 4th & 6th edn., J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, Pearson Education (2009).
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28. Semimicro Qualitative Organic Analysis, 3rd edn., Nicholas D. *Cheronis*, John B. Entrikin and Ernest M. Hodnett, Wiley-Eastern, New Delhi (1964).
29. Pharmaceutical drug analysis, 2ndedn., Ashutosh Kar, New Age International (2005).
30. Quantitative analysis of drugs in pharmaceutical formulations, 3rd edn., P. D. Sethi, CBS (2019).
31. Natural Product-A Laboratory Guide, 2nd edn., Raphael Ikan, Academic Press, New York (1991).
32. Practical Pharmaceutical Chemistry:Part-1 and Part-2, 4th edn., Ed., A. H.Beekett and J. B. Stenlake, Anthlone Press (1988).

OC P 567: PROJECT WORK AND DISSERTATION

Course Outcome

Enable the students:

- To design the project by collecting required background material by referring the literature
- To understand the functioning and safety features in the industry.
- To improve the experimental and soft skills.
- To learn various analytical and instrumental techniques and interpretation of analytical data.

The student shall carry out a project work either in the department or in an institution or industry for 4-6 weeks and prepare dissertation on the work carried out.