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

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 CHEMISTRY
Choice Based Credit System (CBCS) Semester Scheme
(With effective from the Academic Year 2024-25)
PREAMBLE

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

PG BOS in Chemistry has revised and prepared the syllabi (CBCS based) for the PG programme in 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 & 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. 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. Organic 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**
CH H 411: Inorganic Chemistry	H	4 48	4	3	70 + 30 =100
CH H 412: Organic Chemistry	H	4 48	4	3	70 + 30 =100
CH H 413: Physical Chemistry	H	4 48	4	3	70 + 30 =100
CH S 414: Inorganic Spectroscopy and Optical Methods CH S 415: Molecular Spectroscopy and Diffraction Techniques (any one of the above)	S	3 36	3	3	70 + 30 =100
CH P 416: Inorganic Chemistry Practicals-I	S	4 48	2	4	35 + 15 =50
CH P 417: Organic Chemistry Practicals-I	S	4 48	2	4	35 + 15 =50
CH 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**
CH H 461: Advanced Inorganic Chemistry	H	4 48	4	3	70 + 30 =100
CH H 462: Advanced Organic Chemistry	H	4 48	4	3	70 + 30 =100
CH H 463: Advanced Physical Chemistry	H	4 48	4	3	70 + 30 =100
CH S 464: Organic Spectroscopy CH S 465: Environmental Chemistry (any one of the above)	S	3 36	3	3	70 + 30 =100
CH E 466: Environmental, Electro and Polymer Chemistry	S	3 36	3	3	70 + 30 =100
CH P 467: Inorganic Chemistry Practicals-II	S	4 48	2	4	35 + 15 =50
CH P 468: Organic Chemistry Practicals-II	S	4 48	2	4	35 + 15 =50
CH 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**
CH H 511: Coordination Chemistry	H	4 48	4	3	70 + 30 =100
CH H 512: Reagents in Organic Synthesis and Reaction Mechanism	H	4 48	4	3	70 + 30 =100
CH H 513: Solid State Chemistry	H	4 48	4	3	70 + 30 =100
CH S 514: Medicinal and Natural Products Chemistry CH S 515: Chemistry of Biomolecules	S	3 36	3	3	70 + 30 =100
CH E 516: Analytical and Green Chemistry	S	3 36	3	3	70 + 30 =100
CH P 517: Inorganic Chemistry Practicals-III	S	6 72	3	6	70 + 30 =100
CH P 518: Organic Chemistry Practicals-III	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**
CH H 561: Organometallic Chemistry	H	4 48	4	3	70 + 30 =100
CH H 562: Organic Synthetic Methods	H	4 48	4	3	70 + 30 =100
CH H 563: Advanced Electrochemistry	H	4 48	4	3	70 + 30 =100
CH S 564: Bioinorganic Chemistry CH S 565: Polymer Chemistry (Any one of the above two)	S	3 36	3	3	70 + 30 =100
CH P 566: Physical Chemistry Practicals-III	S	6 72	3	6	70 + 30 =100
CH 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. 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. 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 Seven 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 & 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 Chemistry basically aims at the training of students with a detailed knowledge base in 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 organizations.

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 national 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. CHEMISTRY
FIRST SEMESTER

CH 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, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

References

1. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edn., J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, Pearson Education (2009).
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).

CH 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, 4^{th} 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).

CH 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).
5. Industrial Electrochemistry, D. Peltcherand, F. C. Walsh, Chapman & Hall (1990).
6. Principles and Applications of Electrochemistry, D. R. Crow, Chapman Hall (2014).
7. An Introduction to metallic corrosion and its prevention, Raj Narayan, Oxford-IBH (1983).
8. Electrochemistry and Corrosion Science, Nebtor Ferez, Springer (2010).
9. Instrumental Methods of Chemical Analysis, H. Kaur, Pragati Prakashana (2018).
10. Fundamentals of Photochemistry, K. K. Rohatgi-Mukherjee, New Age Bangalore (2000).
11. Physical Chemistry, 7th edn., P. W. Atkins, Oxford University Press (2002).
12. Photochemistry, 2nd edn., Gurdeep Raj, Goel Publishing House (1991).
13. Photochemistry, Carol E. Wayne and Richard P. Wayne, Oxford University Press (1996).

CH 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

1. Instrumental Analysis, D. A. Skoog, F. J. Holler and S. R. Crouch, Cengage Learning (2007).
2. Fundamental of Analytical Chemistry, 8th edn., D. A. Skoog, D.M. West, Holler and Crouch, Saunders College Publishing, New York (2005).
3. Analytical Chemistry, 6th edn., G.D. Christian, Wiley-India (2015).
4. Analytical Chemistry, 4th edn., G.D. Christian, John Wiley & Sons (1986).
5. Instrumental methods of analysis, 7th edn., H. H. Wlliard, L. L. Merrit and J. J. Dean, Wadsworth (2012).
6. Instrumental Methods of Chemical Analysis, B. K. Sharma, Goel (2000).
7. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Ranklin and S. Cradock, Blackwell Scientific (1991).
8. Spectroscopy in Inorganic Chemistry: Vol I & II, C. N. R. Rao and J. R. Ferraro, Academic (1970).
9. Spectroscopy-Vol.2, B. P. Straughan and S. Salker, John Wiley and Sons (1976).
10. Basic concepts of Analytical Chemistry, 3rd edn., S. M. Kopkar, New Age International (2009).
11. Principles of Instrumental Analysis, 8th edn., D. A. Skoog, F. J. Holler and T. A. Nieman, Cengage Learning (2012).
12. Analytical Chemistry: Principles, 2nd edn., J. H. Kennedy, Cengage (2011).
13. Chemical Analysis: An Instrumental Approach, 4th edn., Srivastava & Jain, S.Chand (201).
14. Instrumental methods of Chemical Analysis, 5th edn., Gurdeep R. Chatwal, Himalaya Publishing House (2015).
15. Fundamentals of Photochemistry, K. K. Rohatgi and Mukherjee, New Age (2014).

CH 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.

Rotational 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

1. Fundamentals of Molecular Spectroscopy, 4th edn., C. N. Banwell & E. M. McCash, Tata McGraw Hill (2017).
2. Spectroscopy, H. Kaur, Pragathi Prakashana (2017).
3. Introduction to Spectroscopy, D. L. Pavia, G. M. Lampmam, G. S. Kriz & J. A. Vyvyan, Cengage learning (2014).
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).

CH 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, 5^{th} edn., G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, Longman (1999).
2. Quantitative Analysis, 5^{th} edn., R. A. Day and A. L. Underwood, Prentice Hall (1998).
3. Vogel's Qualitative Inorganic Analysis, 7^{th} edn., G. Svehla, Longman (2001).
4. Advanced Practical Inorganic Chemistry, 28^{th} edn., G. Raj, Goel Publishing House (2019).
5. Practical Inorganic Chemistry, Shika N Gulati, J L Sharma and Shagun Manocha, CBS Publishers & Distributors (2017).

CH 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

1. Laboratory Manual in Organic Chemistry, 3rd edn., R. K. Bansal, New Age (1996).
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).
4. Vogel's Text Book of Practical Organic Chemistry, 5thedn., B. S. Furniss, P. W. Smith, A. R. Tatchell and A. R. Tatchell, Longman-ELBS (2005).
5. A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, A.I. Vogel, Longman (1970).
6. Practical Organic Chemistry, F. G. Mann & B. C. Saunders, Orient Longmann (2004).
7. Vogel's Text Book of Quantitative Chemical Analysis, 4th& 6thedn., J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, Pearson Education Asia (2009).
8. Advanced Practical Organic Chemistry, J. Leonard, B. Lygo and G. Proctor, CRC Press (2013).
9. Techniques and Experiments for Organic Chemistry, 6thedn., Addison Ault, University Science Book (1998).
10. Comprehensive Practical Organic Chemistry-Preparation and Qualitative Analysis, V. K. Ahluwalia and R. Aggarwal, Sangam Books Ltd. (2001).
11. An Advanced Course in Practical Chemistry, 3rd edn., A. K. Nad, B. Mahapatra and A. Ghoshal, New Central Book Agency (2011).
12. Practical Organic Chemistry, Ajay Kumar Manna, Books & Allied (2018).
13. Advanced Practical Organic Chemistry-Vol. II, Jag Mohan Himalaya Publishing House (1992).

CH 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

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., Daniels and Farrington, McGraw Hill College, (1970).
4. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill, (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).
7. Practical Physical Chemistry, B. Viswanathan and P. S. Raghavan, ViVa Books, (2017)

II SEMESTER

CH 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, xenon oxides and fluorides.

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.

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

UNIT-III [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).
3. Chemical Applications of Group Theory, 3rd edn., F. A. Cotton, John Wiley & Sons, (1990).
4. Symmetry and Spectroscopy of Molecules, 2nd edn., K. Veera Reddy, New Age International, (2009).
5. Inorganic Chemistry, 4th edn., P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press, (2006).
6. Inorganic Chemistry, 4th edn., J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, Pearson Education, (2013).
7. Concepts & Models of Inorganic Chemistry, 3rd edn., B. E. Douglas, D. McDaniel & A. Alexander, Wiley, (2007).
8. Inorganic Chemistry, 2nd edn., C. E. Housecroft and A. G. Sharpe, Pearson Prentice Hall, (2005).
9. Inorganic Chemistry: A Unified Approach, 2nd edn., W. W. Porterfield, Elsevier, (2005).
10. Advanced Inorganic Chemistry, 6th edn., F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, Wiley, (2014).
11. Advanced Inorganic Chemistry-Vol. II, 4th edn., Satya Prakash, G. D. Tuli, S. K. Basu, R. D. Madan, S. Chand, (2014).
12. Principles of Inorganic Chemistry, 31st edn., B. R. Puri, L. R. Sharma, K. C. Kalia, Vishal Publishing, (2013).
13. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley and Sons, (2006).
14. Inorganic Chemistry: A Unified Approach, W. W. Porterfield: Elsevier, (2005).
15. Chemistry of the Elements, 2nd edn., N. N. Greenwood and A. Earnshaw, Butterworth, (2005).
16. Essential of Materials Science and Engineering, Donald R. Askeland, Pradeep P. Fulay, 2nd edn., Cengage learning, (2009).
17. Nature and Properties of Engineering Materials, Z. D. Jastrazebski, John Wiley & Sons, (1989).

CH 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, Ullmann & 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.

References

1. Organic Reactions and Their Mechanisms, P. S. Kalsi, New Age, (1996).
2. Advanced Organic Chemistry, 4th edn., J. March, Wiley, (2000).
3. Organic Chemistry: Vol.-1,2 & 3, S. M. Mukherji, S. P. Singh and R. P. Kapoor, Wiley Eastern, (1994).
4. Mechanism and Theory in Organic Chemistry, Lowry T. H., Richardson K. S., Harper and Row, (1987).
5. Reaction Mechanisms in Organic Chemistry, S. M. Mukherji, S. P. Singh and R. P. Kapoor, McMillan, (1978).
6. Organic Chemistry, P. Y. Bruice, Pearson Education, (2002).
7. Organic Reaction Mechanism, R. K. Bansal, Wiley Eastern, (1993).
8. A guide book of mechanisms in Organic Chemistry, P. Sykes, Orient- Longman, (1985).
9. Advanced Organic Chemistry, Vol-1, I. L. Finar, Longmann, (1984).
10. Advanced General Organic Chemistry, S. K. Ghosh, Book and Allied, (1998).
11. Synthetic Organic Chemistry, G. R. Chatwal, Himalaya, (1994).
12. Organic Reaction Mechanisms, V. K. Ahluwalia & R. K. Parashar, Narosa, (2006).
13. Advanced Organic Chemistry, 3rd edn., F. A. Carey and R. J. Sundberg, Part A & B, Plenum Press, (1990).
14. Organic Chemistry, J. Clayden, N. Greeves and S. Warren Oxford University Press, (2001).
15. Name reactions and reagents in organic synthesis, B. P. Mundy, M. G. Ellerd, F. G. Favaloro, 2nd edn., John Wiley and sons, (2005).
16. Named organic reactions, 2nd edn., T. Laue and A. Plagens, John Wiley and sons, (2005).
17. Named Reactions, J. J. Li, 3rd edn, Springer Verlag, (2006).

CH 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).

CH 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).

CH 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).

CH 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).

CH 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).

CH 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, method of separation and systematic semimicro qualitative analysis by the Identification of the functional group(s) present in each of them and preparation of one solid derivative for the conformation of each of the functional group(s).

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).

CH 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 CH 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

CH H 511: COORDINATION CHEMISTRY

Course Outcome

- The students will learn the application of Crystal Field Theory, Molecular Orbital Theory and J-T effect in the study of complexes.
- Understand the application of spectrophotometric and polarographic methods in the determination of stability of metal complexes.
- Demonstrate the interpretation of spectra and magnetic properties of complexes.
- Understanding reaction mechanism in transition metal complexes.

UNIT-I **[12 Hours]**

Coordination numbers 2-10 and their geometry, Crystal Field Theory- Salient features, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, Jahn-Teller distortions, measurement of 10 Dq and factors affecting it. Evidences for ligand field splitting. Molecular Orbital Theory-MOT of coordination compounds and MO diagrams for octahedral, tetrahedral and square planar complexes without and with pi-bonding. Preparation of coordination compounds-Simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions. Stability of Metal Complexes-Step-wise and overall formation constants, factors affecting stability of metal complexes, determination of stability constants of metal complexes by spectrophotometric and polarographic methods.

UNIT-II **[12 Hours]**

Spectral properties of complexes: Term symbols for d^n ions, spectroscopic ground states, selection rules, nature of spectral bands- band shapes, band intensities, band widths, spin-orbit coupling, vibrational structures. Orgel diagrams, Tanabe-Sugano diagrams, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes, Determination of o from spectra. Charge transfer bands-origin, types, and characteristics. Photochemistry of metal complexes-photosubstitution and photoredox reactions, ligand photoredox reactions, photoreactions and solar energy conversion.

UNIT-III **[12 Hours]**

Type of magnetic behaviour, orbital contribution, spin orbit coupling, spin cross-over systems. Measurement of magnetic susceptibility-Gouy and Faraday methods, diamagnetic corrections, ferro- and antiferro-magnetic coupling, super paramagnetism. High and low spin equilibria. Magnetic properties of lanthanides and actinides. Infrared spectra of metal complexes, Group frequency concept. Changes in ligand vibrations on coordination- metal ligand vibrations. Spectral applications of coordination compounds-IR spectra of metal carbonyls-ESR spectra-Application to copper complexes, Mossbauer spectra-Application to iron complexes. NMR spectra-Application to diamagnetic complexes.

UNIT-IV **[12 Hours]**

Reaction Mechanisms in Transition Metal Complexes: Energy profile of a reaction, inert and labile complexes, kinetics of octahedral substitution and mechanistic aspects. Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism and evidences in its favour. Anation reactions, reactions without M-L bond cleavage. Substitution reactions in square planar complexes, trans effect, mechanisms of substitution. Substitution reactions in tetrahedral complexes. Isomerization and racemization reactions of coordination compounds. Electron transfer reactions-inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

References
1. Concise Coordination Chemistry: R. Gopalan and V. Ramalingam, Vikas Publishing, 2014.
2. Inorganic Chemistry, 4th edn., C. E. Housecroft and A. G. Sharpe, Pearson Education (2012).
3. Inorganic Chemistry, 5th edn., G. L. Miessler, P. J. Fischer and D. A. Tarr, Pearson (2014).
4. Inorganic Chemistry, 6th edn., D. F. Shriver, M. Weller, T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
5. Physical Inorganic Chemistry: A Coordination Chemistry Approach, S. F. A. Kettle, Spektrum, Oxford (1996).
6. Inorganic Chemistry, 3rd edn., James E. Huheey, Harper and Row Publishers (1983).
7. Basic Inorganic Chemistry, 3rd edn., F. A. Cotton, G. Wilkinson and P. L. Gaus, John Wiley and Sons (2002).
8. Infrared and Raman Spectra of Coordination Compounds-Part-B, 6th edn., K. Nakamoto, John Wiley and Sons (2009).
9. Electronic absorption Spectroscopy and Related Techniques, D. N. Satyanarayana, OUP (2001).
10. Inorganic Reaction Mechanisms, F. Basolo and R. G. Pearson, Wiley Eastern (1979).
11. Inorganic chemistry-A Unified Approach, W. W. Porterfield, Elsevier (2005).
12. Elements of Magnetochemistry, R. L. Dutta and A. Syamal, Affiliated East-West (1993).
13. Inorganic Chemistry, 4th edn., J. E. Huheey, R. L. Keiter and A. L. Keiter, Addison Wesley (2000).
14. Inorganic Chemistry, 4th edn., J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, Pearson Education (2013).

CH H 512: REAGENTS IN ORGANIC SYNTHESIS AND 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, concepts of pericyclic reactions, diverse types of electrocyclic, cycloaddition and sigmatropic reactions with multiple examples.
- 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.

UNIT-I: **[12 Hours]**

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

UNIT-II: **[12 Hours]**

Organic Photochemistry: Bonding and antibonding orbital, Chemistry of excited states of organic molecules, Jablonski diagram and quantum yield, Photodissociation, Photoreduction, Photochemical isomerisation, Norrish Type-I and Type-II reactions, Yang cyclization, Barton reaction and Paterno-Buchi reaction, photo oxidation.

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 & dis-rotatory Process, 4n & 4n+2 systems.

Cycloaddition reaction: Suprafacial and Antarafacial addition, 2+2 and 4+2 systems. 1,3-Dipolar cycloaddition reactions.

Sigmatropic reactions: Suprafacial and Antarafacial shift of H, [1,3] & [1,5] - sigmatropic shifts.

UNIT-III: 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-IV: Reagents in Organic Synthesis-II **[12 Hours]**

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

References

1. Organic Photochemistry. O. L. Chapman, Vol I & II. Marcel Dekker, (1967).
2. Advanced Organic Chemistry-Part A & B, F. A Carey and R. J. Sundberg, (Plenum), (2007).
3. Synthetic Organic Chemistry, G. R. Chatwal, Himalaya, (1994).
4. Organic Reaction Mechanisms, V. K. Ahluwalia & R. K. Parashar, Narosa, (2006).
5. Organic Chemistry, Vol I-II, I. L. Finar, Longmann ELBS, London, (1973).
6. Advanced Organic Chemistry - Reaction Mechanisms, R. Bruckner, Academic, (2005).
7. Organic Reactions and their Mechanisms - P. S. Kalsi, New Age, New Delhi, (1996).
8. An Introduction to the Chemistry of Heterocyclic Compounds, Acheson, Wiley–Eastern, (1987).
9. Heterocyclic Chemistry, J. Joule & G. Smith, Van-Nostrand, (1978).
10. Heterocyclic Chemistry, 3rd edition, R. K. Bansal, New Age International, (2005).
11. Organic Chemistry, P. Y. Bruice, Pearson Education, (2002).
12. Comprehensive Heterocyclic Chemistry Vol-I-VI, Katritzky & Rees, Pergamon, (1984).
13. Advanced Organic Chemistry, J. March, 6th edn, John Wiley and Sons, (2007).
14. Organic Chemistry, J. Clayden, N. Greeves and S. Warren, Oxford, (2001).
15. Advanced General Organic Chemistry, S. K. Ghosh, Book & Alleied (P) Ltd, (1998).

CH H 513: SOLID STATE CHEMISTRY

Course Outcome

- It is an interdisciplinary course falling at the boundary of physics and chemistry.
- It is aimed at understanding the properties of solids and their possible applications in materials science as superconductors, semiconductors, liquid crystal materials and as magnetic materials.
- Emphasis has been given to the methods of preparation of solids, understanding the structure-property relationships and their possible applications.
- Preparation, properties and applications of nanomaterials has also been considered.

UNIT-I **[12 hours]**

Crystal Defects and Non-Stoichiometry: Imperfections and defects in crystals. Vacancy, Schottky and Frenkel defects, Dislocations. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Solid State Reactions: General Principles, Wagner's theory. Order - disorder transitions in solids-Bragg- William's theory Mechanism of diffusion, Kirkendall effect.

Preparative Methods: Ceramic, sol-gel, precursor and chemical vapour deposition (CVD) methods. Nucleation & crystal growth techniques; pulling, zoning, flame fusion & skull melting.
Basic methods of preparation of thin films (PVD and CVD techniques).

UNIT-II **[12 hours]**

Electronic Properties and Band Theory: Free electron theory to band theory of solids, electrical conductivity, Hall effect. Metals, Insulators and Semiconductors. Intrinsic and extrinsic semiconductors, hopping semiconductors. Metal - semiconductor and p-n junctions.

Ionic Conductors: Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples; β-alumina, AgI, halide and oxide ion conductors.

UNIT-III **[12 hours]**

Superconductivity: Meissner effects; Types I and II superconductors, Features of super-conductors, isotope effect, high Tc materials. Basics of low temperature superconductivity.

Magnetic properties: Classification of magnetic materials; dia, para, ferro, ferri, antiferro & antiferri magnetic types, Langevin diamagnetism. Selected magnetic materials such as spinels & garnets.

Insulators: Dielectric properties, Piezo and inverse Piezo electric effect, ferroelectricity, ferroelectric transitions in $BaTiO_3$.

UNIT IV **[12 hours]**

Liquid Crystals: Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics chiral nematics, molecular arrangements in smectic A & C phases. Optical properties of liquid crystals.

Nanomaterials: Types (Nanolayers, Carbon nanotubes, Nanowires, Quantum dots) and importance. Synthesis of metal nanomaterials: Physical methods (Laser Ablation, Evaporation, sputtering and solvated metal dispersion), chemical methods (Thermolysis, Sonochemical approach, reduction of metal ions by hydrogen and methanol). Characterization: morphology, geometric structure, electronic structure, optical properties). Applications of nanomaterials.

References

1. Solid State Chemistry, D. K. Chakrabarty, 2nd edn., New Academic Science (2010).
2. Principles of the Solid State, H. V. Keer, Wiley Eastern (1993).
3. Solid State Chemistry and its applications, 2nd edn., A. R. West, Wiley (2014).
4. Solid State Chemistry - An Introduction, 4th edn., L. Smart and E. Moore, Chapman & Hall Press (2012).
5. Introduction to Solids, L. V. Azaroff, India Tata Mc Graw Hill (1977).
6. Material Science and Engineering- A first course, 6th edn., V. Raghavan, Prentice Hall India (2015).
7. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley (1987).
8. Liquid Crystals, 2nd edn., S. Chandrasekhar, Cambridge University Press (1992).
9. Introduction to Nanotechnology, 1st edn., C. P. Poole and F. K. Owens, Wiley-Interscience, (2003).
10. Nano: The Essentials: Understanding Nanoscience and Nanotechnology, 1st edn., T. Pradeep, McGraw Hill Education, New Delhi (2017).
11. Basics of Nano Chemistry, Mamta V. Sachdeva, Anmol Publications Pvt Ltd, New Delhi, (2011).
12. Modern Heterogeneous Oxidation Catalysis: Design, Reactions and Characterization, 1st edn., Ed. Noritaka Mizuno, Wiley (2009).
13. Nanoscale materials in Chemistry, 2nd edn., Ed. K. J. Klabunde and R. M. Richards, Wiley (2009).
14. Introduction to Nanotechnology, C. P. Poole and F. J. Owens, Wiley-Interscience, (2003).

CH S 514: MEDICINAL AND NATURAL PRODUCTS CHEMISTRY

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 get a good understanding of isolation, classification, methods of structure elucidation and synthesis of various types of alkaloids, terpenoids and steroids with suitable examples.

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 **c**lassification, synthesis & mode of action of methoxy fluorane, 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]**

Alkaloids: Classification and general methods of structure elucidation. Structure and synthesis of Papaverine, Adrenaline and Reserpine.

Terpenoids: Introduction and classification, isoprene rule and general methods of structure determination. Structure and synthesis of Menthol, α-Pinene, Camphor and Zingiberene.

Steroids: Introduction, Blanc's rule, Chemistry of Cholesterol, Oestrone and Progesterone.

References

1. Medicinal Chemistry, Ashutosh Kar New Age, (2005).
2. Medicinal Chemistry, G. R. Chatwal, Himalaya, (2002).
3. Principles of Drug Action, A. Goldstein, L. Aronow & S. M. Kalman, Wiley Int. Ed., 1973
4. Natural Products Chemistry, Vol-I & II, G. R. Chatwal, Himalaya, (1990).
5. Organic Chemistry, Vol I & II, I. L. Finar, Longmann ELBS, (1973).
6. Chemistry of Natural Products, Vol-I & II, O. P. Agarwal, Goel, (1985).
7. Chemistry of Natural Products: A Unified Approach, N. R. Krishnaswamy, University Press, (1999).

CH 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.

References

1. Fatty acid and Lipid Chemistry, F. D. Gustone, Wiley (1996).
2. Chemistry of Biomolecules, S. P. Bhtani, CRC Press (2010).
3. Organic Chemistry-Vol. I and II, I. L. Finar, ELBS Longmann (1984).
4. Principles of Biochemistry, 1st edn., K. Albert, L. Lehninger, D. L. Nelson and M. M. Cox, CBZ publishers, New Delhi (1993).
5. Harper's Biochemistry, 22nd edn., Ed. R. Harper, Prentice Hall Press, New York (1990).
6. Natural Products-Chemistry and Biological Significance, J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J. B. Harbome, Longman (1994).
7. Lehninger Principles of Biochemistry, 7th edn., David L. Nelson and Michael M. Cox, W H Freeman and Co. (2017).
8. Biochemistry, 4th edn., C. B. Power and G. R. Chatwal, Himalayan Publishing House (1999).
9. Instant notes on Medicinal Chemistry, 1st edn., G. Patrick. Viva Books (2002).
10. Bioorganic Chemistry-A Chemical Approach to Enzyme Action, Hermann Dugas and C.
11. Penny, Springer-Verlag (1981).
12. Organic Chemistry of Natural Products-Volume I and II, G. Chatwal, Himalaya Publishing House (1988).
13. Chemistry of Organic Natural Products, Volume I and II, O.P. Agarwal, Goel Publishing House (1988).
14. Chemistry of Natural Products, 1st edn., V. K. Ahluwalia, Ane Books (2006).
15. Biochemistry, 2nd edn., U. Satyanaraya, Uppala Author- Publisher Interlinks (2003).
16. Fundamentals of Biochemistry, J. L. Jain, S. Chand and Co., New Delhi (2007).
17. Chemistry of Biomolecules-An Introduction, R. J. Simmonds, Royal Society of Chemistry (1992).
18. Lehninger Principles of Biochemistry, 7th edn., David L. Nelson and Michael M. Cox, W. H. Freeman and Co. (2017).
19. Bioorganic and Bioinorganic and Supramilecular Chemistry, 2nd edn., P. S. Kalsi, New Age International (2010).
20. Biochemistry, 4th edn., C.B. Power and G.R. Chatwal, Himalayan Publishing House (1999).

21. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford Univ. Press (2001).
22. Understanding Enzymes, 4th edn., Trevor Palmer, Prentice Hall (1995).
23. Enzyme Chemistry-Impact and Applications, Ed. Collin J. Suckling, Chapman and Hall (1990).
24. Enzyme Mechanisms, Ed. M. I. Page and A. Williams, Royal Society of Chemistry (1987).
25. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman and Co., Oxford (1979).
26. Fundamentals of Enzymology, 3rd edn., N. C. Price and L. Slovens, Oxford University Press (2000).

CH E 516: ANALYTICAL AND GREEN CHEMISTRY

Course Outcome

- Enable the students to understand the basic principles and theory of UV/Electronic, Infra-Red, Nuclear Magnetic Resonance and Mass Spectroscopy.
- Study the utility of these techniques in structure elucidation of simple organic molecules.
- Know about water cycle, water sources, water quality, and significant measurements of water parameters and treatment of water for drinking and industrial purposes.
- Learn about principles and use of green chemistry in laboratory synthesis.
- Understand the green chemistry principles, basic principles and utility of sonochemistry and Microwave induced organic synthesis.

UNIT-I **[12 Hours]**

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

IR Spectroscopy: Basic principles, Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. 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-spincoupling, coupling constant. Shielding and deshielding. High resolution ^{1}HNMR. 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. 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. Treatment of liquid radioactive wastes.

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, Phase transfer catalyst catalysed reactions (Quaternary ammonium salts & Crown ethers), enzymatic transformations & reactions in ionic liquids.

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

Microwave induced organic synthesis: Introduction, reaction vessel and reaction medium, concept, specific effect, 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, orthoester Claisen rearrangement.

References

1. Organic Spectroscopy, 3rd edn., W. Kemp, Pagrave Publishers (1991).
2. Spectrometric Identification of Organic Compounds,8th edn., R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, Wiley (2014).
3. Applications of Absorption Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall (1965).
4. Spectroscopy of Organic Compounds, 3rd edn., P. S. Kalsi, NewAge, (2000).
5. Spectroscopic Methods in Organic Chemistry, D. Williams and I. Fleming, McGraw-Hill (1995).
6. Environmental Chemistry, A. K. De, Wiley Eastern Ltd. (1990).
7. Environmental Chemistry, S. K. Banerji, PrenticeHall India (1993).
8. Chemistry of Water Treatment, S. D. Faust and O.M. Aly, Butterworths (1983).
9. Chemistry for Environmental Engineering, 3rd edn., C. N. Sawyer and P. L. McCarty, McGrawHill (1978).
10. Environmental Chemistry, I. Williams, John Wiley (2001).
11. Environmental Pollution Analysis, S. M. Khopkar, Wiley Eastern (1993).
12. Organic Synthesis, Special Techniques, V. K. Ahluwalia and R. Aggarwal, Narosa (2001).
13. Green Chemistry, Environment friendly alternatives, R. Sanghi and M. M. Srivatsava, Narosa (2003).
14. Green Chemistry-Environment benign reactions, V. K. Ahluwalia, Ane Books India (2006).

CH P 517: INORGANIC CHEMISTRY PRACTICALS – III

Course Outcome

- The students will have hands on experience in the analysis of Brass, Stainless Steel.
- Understand the analysis of Type metal and quantitative analysis of the constituents of mixtures containing the radicals such as Fe + Ni, Fe + Ca, Cr + Fe.
- Train the students in separation and determination of Mg^{2+}/Zn^{2+}, Zn^{2+}/Cd^{2+} by Ion-Exchange Chromatography in Part A and in Part B
- Able to determine COD, DO, nitrate, nitrite and alkalinity, fluoride in various water samples.
- The students will acquire practical experience in determination of Na, K, Li and Ca by Flame photometry and Solvent extraction of Ni(II) and UO_2(II).
- Learn the preparation and analysis of complexes and measurement of magnetic susceptibility.
- Demonstrate skills related to determination of composition of complexes by Job's method, Mole ratio method and Slope ratio method.
- Understand the determination of stability constants of complexes.

A. Any four of the following experiments are to be carried out:

1. Analysis of brass-Cu gravimetrically using α-Benzoinoxime and Zn complexometrically.
2. Analysis of Stainless Steel-Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) and Cr(III) volumetrically by persulphate oxidation.
3. Quantitative analysis of the constituents and mixtures containing the following radicals:

a) Fe(II) + Ni(II) - Fe gravimetrically as Fe_2O_3 and Ni using EDTA.
b) Fe(III) + Ca(II) - Fe gravimetrically as Fe_2O_3 and Ca using EDTA.
c) Cr(III) + Fe(III) - Using EDTA by Kinetic masking method.

4. Analysis of chalcopyrites, magnetite and ilmenite.
5. Ion-exchange chromatography: Separation and determination of Mg^{2+}/Zn^{2+}, Zn^{2+}/Cd^{2+} and Cl^-/ Br^-.

B. Any four of the following experiments are to be carried out:

1. Determination of i) COD ii) dissolved oxygen (DO) iii) alkalinity of a water sample.
2. Determination of nitrate & nitrite in water samples and sea water.
3. Analysis of heavy metals in waste water, sea water (Pb, Hg etc. by spectrophotometry)
4. Nephelometric determination of sulphate/phosphate.
5. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode.

C. Any four of the following experiments are to be carried out:

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Determination of composition of complexes:
   Job's method: Fe-phenanthroline complex
   Mole ratio method: Zr-Alizarin red S complex,
   Slope ratio method: Cu ethylenediamine complex
3. Determination of stability constants of Fe-Tiron system by Turner Anderson method.
4. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
5. Electrogravimetric determination of Cu-Ni alloy in Type Metal.
6. Solvent extraction of Ni(II) and UO_2(II).
7. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemicals analysis, structural study of the prepared complexes using conductance and magnetic susceptibility measurements, recording the electronic and infrared spectra:
   i) Chloropentamminecobalt(III) chloride
   ii) Hexamminecobalt(III)chloride.

References

1. Standard Method for the Examination of water and Waste Water, Ed. A. E. Greenberg, L. S. Clesceri and A. D. Eaton, American Public Health Association (1989).
2. Quantitative Chemical Analysis, I. M. Kolthof and E. P. Sandell, McMillan (1980).
3. Environmental Chemistry, I. Williams, Wiley (2001).
4. Spectrochemical Trace Analysis for Metals and Metalloids: Comprehensive Analytical Chemistry-Vol. 30, R. Lobinski and Z. Marczenko, Elsevier (1996).
5. Vogel's Text Book of Quantitative Chemical Analysis, 5th edn.,G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, Longman (1999).

CH P 518: ORGANIC CHEMISTRY PRACTICALS – III

Course Outcome

- Enable the students to understand and learn the principles of quantitative determinations of different types of organic molecules.
- Learn and identify the concepts of a standard solutions, primary and secondary standards
- Demonstrate the methods of organic preparations using multistep synthetic protocol.
- Learn the isolation and purification of intermediate and final products.
- 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.
- Apply the spectroscopic techniques to interpret the structure by analysing the spectral data.

Quantitative Determinations (Any five determinations are to be carried out)

1. Quantitative determination of equivalent weight of acids by titrimetric/silver salt method
2. Quantitative determination of aromatic amines/phenols by bromide-bromate & acetylation methods.
3. Quantitative determination of amino acids by formal titration method
4. Quantitative determination of sugars by Bertrand's/Fehling's solution method.
5. Quantitative determinationsof acid & ester and acid & amide in the given mixtures.
6. Quantitative determinations of ketones by haloform reaction and oxime method.
7. Quantitative determinations of aldehydes & ketones by using 2,4-dinitrophenyl hydrazine method.
8. Quantitative determinations of hydroxyl, amino, nitro and amide groups.

Multi Step Organic Synthesis (Any five preparations are to be carried out)

1. Preparation of *o*-aminobenzoic acid from phthalic anhydride.
2. Preparation benzilic acid from benzoin.
3. Preparation of benzanilide from benzophenone*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. Preparation of anthraquinone from phthalicanhydride.
9. Preparation of 4-bromoaniline from acetanilide.
10. Preparation of 4-nitroaniline from acetanilide.
11. Preparation of acetanilide from acetophenone*via* Beckmann rearrangement.

Separation Techniques (Any two separations are to be carried out)

Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation and steam distillation.

Identification/separation of components from the mixture of organic compounds by Paper, TLC and column chromatography.

Spectroscopic Techniques (Any five spectral problems are to be solved)

Interpretation of structure of organic molecules by the joint application of UV-Vis., IR, NMR and Mass spectra.

Demonstration of recording of UV-Visible, IR, NMR and LC Mass spectra of organic compounds.

References

1. Practical Organic Chemistry, Ajay Kumar Manna, Books & Allied (2018).
2. Advanced Practical Organic Chemistry-Vol. II, Jag Mohan, Himalaya Publishing House (1992).
3. Elementary Practical Organic Chemistry-Vol. III, Quantitative Organic Analysis, A. I. Vogel, Pearson (2011).
4. Vogel's Text Book of Quantitative Chemical Analysis, 4^{th} & 6^{th} edn., J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, Pearson Education Asia (2009).
5. Laboratory Manual in Organic Chemistry, 3^{rd} edn., R. K. Bansal, New Age (1996).
6. Experimental Organic Chemistry–Vol. I & II, P. R. Singh, D. S. Gupta and, K. S. Bajpai, Tata McGraw-Hill (1981).
7. Laboratory Manual in Organic Chemistry, B. B. Dey and M. V. Sitaraman, Allied (1992).
8. Vogel's Text Book of Practical Organic Chemistry, 5^{th} edn., B. S. Furniss, P. W. Smith, A. R. Tatchell and A. R. Tatchell, Longman-ELBS (2005).
9. A Text Book of Practical Organic Chemistry including Qualitative Organic Analysis, A.I. Vogel, Longman (1970).
10. Practical Organic Chemistry, F. G. Mann & B. C. Saunders, Orient Longmann (2004).
11. Advanced Practical Organic Chemistry, J. Leonard, B. Lygo and G. Proctor, CRC Press (2013).
12. Techniques and Experiments for Organic Chemistry, 6^{th} edn., Addison Ault, University Science Book (1998).
13. Comprehensive Practical Organic Chemistry-Preparation and Qualitative Analysis, V. K. Ahluwalia and Renu Aggarwal, Sangam Books Ltd. (2001).
14. An Advanced Course in Practical Chemistry, 3^{rd} edn., A. K. Nad, B. Mahapatra and A. Ghoshal, New Central Book Agency (2011).
15. Experimental Organic Chemistry, Vol. I & II, P. R. Singh, Tata McGraw-Hill, (1981).
16. Laboratory Experiments in Organic Chemistry, R. Adams, J. R. Johnson and C. F. Wicox, McMillan (1979).
17. Experimental Organic Chemistry, H. D. Durst and G. E. Goke, McGraw-Hill (1980).
18. W. Kemp, Organic Spectroscopy, Pagrave Publishers (1991).
19. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley & Sons (1981).
20. Applications of Absorption Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall, (1965).
21. Spectroscopy of Organic Compounds, P. S. Kalsi, New Age (2000).
22. Spectroscopic Methods in Organic Chemistry, D. Williams and I. Fleming, TMH (2020).
23. Organic structures from spectra, 5^{th} edn., L. D. Field, S. Sternhell and J. R. Kalman, John Wiley & Sons (2013).

IV SEMESTER

CH H 561: ORGANOMETALLIC CHEMISTRY

Course Outcome

- The students will learn historical development of organometallic compounds and classification.
- Understand the chemistry of transition metal-carbon multiple bonded compounds andtransition metal-carbon pi complexes.
- Application of catalysis by organometallic compounds, homogeneous catalysis by organometallics and hydrocarbonylation of olefins.
- Acquire knowledge on Ziegler-Natta catalyst, Fischer-Tropsch and Water Gas Shift reactions.

UNIT-I **[12 Hours]**

Historical development-Classification and nomenclature, bond energies and stability. 16- and 18-electron rules. Transition metal alkyls and aryls-types, routes of synthesis, stability and decomposition pathways, Nucleophilic and electrophilic cleavage of metal-carbon sigma bonded compounds. Alkane activation.

Transition metal-carbon multiple-bonded compounds-Carbenes, carbynes, synthesis, nature of bond, agostic interactions, structural characteristics and reactivity. Transition metal hydrides-Synthetic routes, properties, structure and reactivity, synthetic applications.

UNIT-II **[12 hours]**

Transition metal-carbon, pi-complexes-Preparativemethods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene, η^5- cyclopentadienyl, η^6-benzene and other arenes, cycloheptatriene and cyclooctatetraene complexes. Important reactions relating to nucleophilic and electrophilic attack on ligands. Fluxional isomerism in olefin, allyl, dienyl and cyclopentadienyl complexes. Carbene complexes and metallacycles, arene complexes. Isolobal concept.

UNIT-III **[12 hours]**

Catalysis by organometallic compounds: oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics: Hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts, Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), Wacker process. Carbonylation of alcohols-Monsanto acetic acid process.

Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer–Tropsch reaction, Water Gas Shift reactions.

Unit-IV **[12 Hours]**

Metal complexes as drugs and therapeutic agents: Antibacterial agents, antiviral agents, metal complexes in cancer therapy, metal complexes for the treatment of rheumatoid arthritis–Gold based therapeutic agents, vanadium in diabetes, metal complexes as radio diagnostic agents.

Treatment of toxicity due to inorganics: General aspects of mechanism of metal ion toxicity- i) Mechanism of antidote complex with poison, rendering it inert: arsenic, lead, mercury, iron, copper; ii) Antidote accelerated metabolic conversion of poison to non-toxic product: cyanide and carbon monoxide.

References

1. Principles and Applications of organotransition Metal Chemistry, J. P. Collman, L. S. Hegedus, J. R. Norton and R. G. Finke, University Science Books (1987).
2. Organometallic Chemistry, R. C. Mehrotra and A. Singh, New Age International (1999).
3. Organometallic Chemistry of Transition Metals, R. H. Crabtree, Wiley (1999).
4. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson, Wiley (1991).
5. Organometallic Chemistry, G. S. Sodhi, Ane books (2009).
6. Principles and Applications of Organo-transition Metal Chemistry, J. P. Collman, L. S. Hegedus, J. R. Norton and R. G. Finke, University Science Books (1987).
7. Basic Organometallic Chemistry, B. D. Gupta and A. J. Elias, Universities Press (2013).
8. Medicinal Applications of Coodination Chemistry, C. Jones and J. Thornback, RSC Publishing (2007).
9. Transition Metal Complexes as Drugs and Chemotherapeutic Agents, N. Farrell, Kluwer, Academic Publishers (1989).
10. Bioinorganic Medicinal Chemistry, Ed. E. Alessio, Wiley-VCH Verlag (2011).

CH H 562: ORGANIC SYNTHETIC METHODS

Course Outcome

Enable the students:

- 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.
- Students will understand the systematic nomenclature of various types of heterocyclic compounds with multiple examples.
- Students will get the sound knowledge on the structure, synthesis and reactions of various three, four, five, six and fused heterocyclic compounds.
- 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.

UNIT-I **[12 Hours]**

Reduction Reactions: Catalytic hydrogenation-catalysts and solvents, mechanisms and stereochemistry. Hydrogenolysis and homogeneous catalytic hydrogenation.

Metal hydride reduction: Reduction with $LiAlH_4$ and $NaBH_4$, Stereo chemistry of reduction, Reduction with diborane.

Dissolving Metal Reductions: Mechanisms of reduction of carbonyl compounds, Bimolecular reductions of esters, Birch reduction.

Wolf-Kishner reduction and reduction with diimide.

Oxidation reactions: Mechanism of oxidation with chromium and manganese salts, Osmium tetroxide, peracids, periodic acid and Lead tetra acetate.

Halogenation: Halogenation of carbonyl compounds. Benzyllic and Allylic halogenations.

UNIT-II **[12 Hours]**

Heterocyclic Chemistry: Hantzsch-Widman system of nomenclature for monocyclic, fused and bridged heterocycles. Structure, synthesis and reactions of aziridines, episulfides, azetidines, thietanes, furan, pyrrole, thiophene, oxazoles, imidazoles, thiazoles, pyridine, pyrimidine and fused hetercycles-Indoles, benzofurans and quinolines.

UNIT- III **[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- IV **[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*-methoxy acetophenone, 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.

References

1. Modern Synthetic Reactions H. O. House, 2nd edn, W. A. Benjamin Inc, (1972).
2. Organic Synthesis, R. E. Ireland, Prentice Hall India, (1969).
3. Art in Organic Synthesis, Anand, Bindra & Ranganath, Wiley, (1970).
4. Organic Synthesis a Disconnection Approach, S. Warren and P. Wyatt, 2nd edn, Wiley (2008).
5. Advanced Organic Chemistry, Part A & B, F. A. Carrey & R. J. Sundberg, Plenum Press, (1990).
6. Modern Methods of Organic Synthesis, N. Carruthers, Cambridge University, (1996).
7. Selected Organic Synthesis, I. Fleming, John Wiley & Sons, (1973).
8. An Introduction to the Chemistry of Heterocyclic Compounds, Acheson, Wiley Eastern, (1997).
9. Heterocyclic Chemistry, J. Joule & G. Smith, Van Nostrand ELBS, (1978).
10. Comprehensive Heterocyclic Chemistry, Vol – I to VI, Katritzky & Rees, Pergamon, (1984).
11. Organic Chemistry, Vol I & II, I. L. Finar, Longmann ELBS, (1973).

CH H 563: ADVANCED ELECTROCHEMISTRY

Course Outcome

- It is an advanced level course on electrochemical processes and their applications in chemical industries.
- This course content trains students on alternate methods of synthesis using electrochemical concepts.
- The course enables them to learn the functioning of electrochemical energy systems such as batteries and fuel cells.

UNIT-I **[12 hours]**

Electrocatalysis: Introduction. Electrocatalysis in reactions involving adsorbed species, concept and process of electrogrowth on electrodes. Deposition to crystallization, mechanism of electrogrowth. Special features of electrocatalysis. Hydrogen evolution and reactions. Electronation of oxygen and their mechanisms.

Photo-electrocatalysis: History of photocatalysis, Principles and Developments in photo-electrochemistry. Semiconductor-electrolyte solution interface. Effect of light at semiconductor interface. Capacity of space charge - Mott-Schottky plot. Photo cells-PEC cells and Photogalvanic cells.

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

UNIT-II **[12 hours]**

Electrode Processes: Charge transfer across the interface and its implications. Basic electrodic reactions: Butler - Volmer equation. Current potential laws at charged interface. Quantum aspects of charge transfer reactions. Concepts of over voltage, Theory of hydrogen and oxygen overvoltage. Mechanism of cathodic and anodic reactions, Dependence of current density on overvoltage: Tafel equation.

The Electrified Interface: Electrification of interfaces, experimental techniques used in studying interface (Low energy electron diffraction, X-ray photoelectron spectroscopy). The potential difference across Electrified interface. The accumulation and depletion of substances at an interface. Thermodynamics of an electrified interface. Brief introduction to the structure of electrified interfaces (models).

UNIT-III **[12 hours]**

Electrochemical Energy System: Electricity Storage-Importance, storage density, Fundamentals and classification of batteries, Primary battery (Laclanche-dry cell and Alkaline cell). Secondary battery (acid and alkaline). Reserve batteries. Lithium batteries - (primary and secondary and lithium based conducting polymer battery). Fuel cells – introduction, classification, H_2-O_2 and bio-cells.

Sensors: Biosensors: Introduction electrochemical bio-sensors- characteristics, use as a transducer, types.

Ion-Sensors: Ion-selective electrode: Introduction, Types. Analytical and biological applications of sensors.

Electrosynthesis: Electro-organic synthesis (Kolbes synthesis, oxidation and reduction of hydrocarbons, reduction of nitro-compounds); Electro inorganic synthesis of fluorine and ozone. Synthesis of metal salts via anodic dissolution.

UNIT-IV **[12 hours]**

Metallurgical Processing: Electroplating-fundamentals, mechanism of electrodeposition of metals, application of electroplating. Brief account of Electroless plating, Conversion coatings, Electrophoretic painting.

Metals and materials processing: Theory and applications of Electroforming and Electrochemical etching. Production of metals by electro winning and electrorefining. Applications of electrochemistry in fixing of CO_2, treatment of waste, Metal ion removal and metal recovery. Treatment of liquors containing dissolved chromium.

References

1. Modern Electrochemistry, Vol.1, 2A & 2B, 2nd edn., J. O. M. Bockris and A. K. N. Reddy, Plenum, New York (1998).
2. Chemical and Electrochemical Energy Systems, B. Narayan and R. Viswanathan, Univ. Press, Hyderabad (1998).
3. Fundamentals of Electrochemistry, 2nd edn., L. R. Fulkner and A. J. Bard, Wiley India, (2006).
4. Ions in solution: Basic principles of chemical interactions, J. Burgeess, Chichester: Horwood Publisher (1999).
5. Electrochemistry-Principles, Methods and Applications, A. M. O. Brett and C. M. A. Brett, Oxford Science, (1993).
6. Industrial Electrochemistry, 2nd edn., D. Pletcher & F. C. Walsh, Chapman & Hall (1990).
7. Biosensors: theory and Applications, D. G. Burek, Technomic Publishing Company, (1993).
8. Principles and Applications of Electrochemistry, 4th edn., D. R. Crow, CRC Press, (1994).

CH S 564: BIOINORGANIC CHEMISTRY

Course Outcome

- Students will learn metal and non-metal ions in biological systems and understand theirrole biological systems.
- Gain knowledge on biological nitrogen fixation andphotocatalysis.
- Explain the transport and storage of dioxygen, metal storage and transport.
- Demonstrate the role of metalloproteins as enzymes.
- Describe the therapeutic uses of metals, metal complexes as drugs and treatment of toxicity due to inorganics.

UNIT-I **[12 Hours]**

Metal and non-metal ions in biological systems-essential and trace metals, deficiency of trace metal ions (Fe, Zn, Cu and Mn), ion transport across membranes, active transport of ions across biological membranes.

Iron-Sulfur proteins (rubredoxins and ferredoxins) and cytochromes including cytochrome P450.

Non-redox metalloenzymes: Structure and reactivity of carboxypeptidase-A, alcohol dehydrogenase, leucine aminopeptidase and carbonic anhydrase.

UNIT-II **[12 Hours]**

Transport and storage of dioxygen, haemoglobin, myoglobin, hemerythrin and hemocyanins, heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers.

Metal storage and transport-Ferritin, transferrin and ceruloplasmin. Electron transfer proteins-cytochromes, iron-sulphur proteins. Metalloproteins as enzymes-Structure and reactivity of catalase, peroxidase, superoxide dismutase, copper oxidases.

Vitamin B_{12} and Coenzymes: Structural feature, names of different forms, chemistry of cobalamin, biochemical functions of cobalamins, model compounds. Special characteristics of B_{12} co-enzyme.

UNIT-III **[12 Hours]**

Therapeutic uses of Metals: Metals in medicine-Metals and human biochemistry, general requirements. Disease due to metal deficiency and treatment: Iron, zinc, copper, sodium, potassium, magnesium, calcium and selenium.

Biochemistry of non-metals: Biomineralization, biological role of some trace nonmetals. Biological importance of Nitric oxide.

Biological nitrogen fixation, Molybdenum nitrogenase, Model compounds, *in vitro* fixation of nitrogen through dinitrogen complexes.

Metal complexes in transmission of energy-chlorophylls. Photosystems I and II in cleavage of water, model systems.

References

1. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Berg, Panima Publishing (1997).
2. Inorganic Chemistry of Biological Processes, 2nd edn., M. N. Hughes, Wiley (1988).
3. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Viva Books (1998).
4. Inorganic Chemistry, 4th edn.,J. E. Huheey, R. L. Keiter and A. L. Keiter, Addison Wesley, (2000).
5. Bioinorganic Chemistry, K. Hussain Reddy, New Age International (2003).
6. Bioinorganic Chemistry, R. W. Hay, Ellis Horwood (1984).

7. Bioinorganic Chemistry, A. K. Das, Books & Allied (2007).
8. Biocoordination Chemistry, D. E. Fenton, Oxford University Press (1996).
9. Metal ions of Biological Systems, H. Siegel and T. G. Spiro, Mercel-Dekker (1979).
10. Principles of Biochemistry, A. L. Lehninger, Worth (1982).
11. Essentials of Inorganic Chemistry for Students of Pharmacy, Pharmaceutical Sciences and Medicinal Chemistry, Katja A. Strohfeldt, John Wiley & Sons (2015).
12. Inorganic chemistry, C. E. Housecraft and A. G. Sharpe, Pearson-Prentice Hall (2001).
13. Bioinorganic Chemistry-A Survey, E. Ochiai, Academic Press (2008).
14. Bioinorganic Chemistry-A Short Course, 2nd edn., R. M. Roat-Malone, Wiley Interscience (2007).
15. Medicinal Applications of Coodination Chemistry, C. Jones and J. Thornback, RSC Publishing (2007).
16. Transition Metal Complexes as Drugs and Chemotherapeutic Agents, N. Farrell, Kluwer, Academic Publishers (1989).
17. The Biological Chemistry of the Elements-The Inorganic Chemistry of Life, 2nd edn., J. J. R. Frausto da Silva and R. J. P. Williams, Oxford University Press (2001).
18. Essentials of Inorganic Chemistry, K. A. Strohfeldt, John Wiley and Sons (2015).
19. Bioinorganic Medicinal Chemistry, Ed. E. Alessio, Wiley-VCH Verlag (2011).

CH S 565: POLYMER CHEMISTRY

Course Outcome

- This is an introductory course on highly useful materials, namely the polymers.
- The course content is of interdisciplinary interest.
- It enables students to learn about general information about plastics, rubber and fibre materials.
- The applications of these materials in daily life, engineering and biomedical field have been emphasized.
- The students are made aware of the problems of polymer waste management and the strategies developed to minimize plastic pollution.

UNIT-I **[12 hours]**

Terminology and basic concepts: General structure, naming, preparation, properties and uses of polymers (polyethylene, polypropylene, polystyrene, PVC, polyacrylics, polyesters, polyamides, and regenerated cellulose).

Classification based on various considerations: Source, preparation methods, thermal behaviour, chain structure etc**.**

Types: Homopolymers and copolymers; Linear, branched and network polymers.

Techniques of polymerization: Techniques of preparation of addition and condensation polymers.

Kinetics of polymerization: Kinetics of addition and condensation polymerization. Kinetics of copolymerization.

UNIT-II **[12 hours]**

Stereochemistry of polymers: Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers. Expressions for average molecular weight. Molecular weight distribution and Polydispersity**.**

Determination of molecular weight: Osmometry, viscometry, ultracentrifugation, electrodialysis and GPC methods.

Thermal Characterization: Glass Transition and melting-correlation with structure-Factors affecting T_g and T_m. Techniques of thermal characterization: DSC, DTA, DTG and TGA techniques.

UNIT-III **[12 hours]**

Structural features, properties and uses of commercial polymers: Polyurethanes, polycarbonates, formaldehyde based resins, epoxy resins and aromatic polyamides.

Properties and uses of Specialty polymers: Composites, Conducting polymers and Biomedical polymers.

Polymer degradation and stability: Thermal, oxidative, photo, chemical and radiation affected degradation. Plastic waste management-incineration, recycling and biodegradation.

Polymer processing Techniques: Compounding - role of additives. Casting, calendaring, moulding, foaming, reinforcing and spinning techniques.

References

1. Textbook of Polymers, 3rd edn., F. W. Billmeyer, Wiley (1984).
2. Contemporary Polymer Chemistry, 3rd edn., H. R. Allcock, J. E. Mark and F. W. Lampe Prentice Hall (2003).
3. Polymer Science and Technology, 3rd edn., J. R. Fried, Prentice Hall (2014).
4. Polymer Science, 4th edn., V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, New Age International Pvt. Ltd. (2021).
5. Principles of Polymer Science, 2nd edn., P. Bahadur and N. V. Sastry, Narosa Publishers (2006).

CH P 566: PHYSICAL CHEMISTRY PRACTICALS-III

Course Outcome

- Enables the students to learn different principles of chemical kinetics.
- The course also enables students to understand the use spectrophotometry in determination of physicochemical parameters of molecules.
- It enables students to get hands on training on the use of electrochemical techniques namely, conductometry, potentiometry and polarography.
- This course enhances the skill of students in quantitative analysis.

a. Kinetics and Catalysis (Any six experiments to be carried out)

1. Saponification of ethyl acetate by conductivity method: Determination of thermodynamic parameters.
2. Reaction between potassium persulphate and potassium iodide: Determination of order w.r.t. KI
3. Reaction between potassium persulphate and potassium iodide: Determination of order w.r.t. $K_2S_2O_8$.
4. Reaction between potassium persulphate and potassium iodide: Determination of effect of ionic strength.
5. Reaction between potassium persulphate and potassium iodide: Determination of thermodynamic parameters.
6. Reaction between potassium persulphate and potassium iodide: Effect of dielectric constant.
7. Decomposition of diacetone alcohol by NaOH: Determination of order w.r.t. NaOH.
8. Decomposition of diacetone alcohol by NaOH: Determination of thermodynamic parameters.

b. Instrumentation methods (Any six experiments to be carried out)

(i)Spectrophotometric Experiments

1. Determination of pK_a value of an indicator.
2. Determination of composition and Stability constant of metal complex [Fe(III) - Salicylic acid complex].

(ii)Electrochemistry

a. Conductometry

1. Titration of a mixture of acetic acid, monochloro and trichloacetic acids with NaOH.
2. Determination of concentrations of sulphuric acid, acetic acid and copper sulphate in a mixture by conductometric titration with NaOH.

b. Potentiometry & pH metry

1. Potentiometric titration of (a) Non aqueous system and (b) mixture of strong (HCl) and weak acid (HOAc) with NaOH / NH_4OH and to find the strength of the acids in mixture.
2. Determination of acidic and basic dissociation constants and isoelectric point an amino acid pH metrically.
3. pH/potentio metric titration of mixture of bases (Na_2CO_3 & $NaHCO_3$) with standard HCl.

c. Polarography Experiments

1. Determination of the half-wave potential of Cd (II), Cu (II) & Zn (II) ions individually and in mixtures.

Any other experiments of interest.

References

1. Practical Physical Chemistry, A. 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., Daniels and Farrington, McGraw Hill Book Co., New York, (1970).
4. Experimental Physical Chemistry, R. C. Das and B. Behera, Tata McGraw Hill Education, (1983).
5. Advanced Practical Physical Chemistry, J. B. Yadav, Krishna prakashan Media Publication, (2016).
6. Experiments in Physical Chemistry, J. C. Ghosh, Bharathi Bhavan, New Delhi (1974).
7. Practical Physical Chemistry, B. Viswanathan and P. S Raghavan, Viva Books, New Delhi, (2017).

CH 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.