SRI DHARMASTHALA MANJUNATHESHWARA COLLEGE, UJIRE-574240

(Autonomous)

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

PG DEPARTMENT OF CHEMISTRY

Syllabus of
Masters' Degree in
CHEMISTRY

(CHOICE BASED CREDIT SYSTEM)
2016 - 2017 onwards.

Approved by the BOS meeting held on 27th August 2020
Academic Council meeting, held on 10-11-2020

Preamble

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

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

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

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

The syllabus is structured in a view to equip the students with the potential to contribute to academic and industrial environments. Chemistry being an experimental science, sufficient emphasis is given in the syllabus for training in laboratory skills and instrumentation. The units of the syllabus are well defined. The number of contact hours required for each unit is also given. A list of reference books is provided at the end of the each semester.

ELIGIBILITY FOR ADMISSION

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

Faculty of PG Studies in Chemistry: PGCHE052

Programme Specific Outcomes:

PSO1: Show the ability to plan, design and carry out scientific experiments as well as accurately record and analyze the results of such experiments.

PSO2: Exhibit skills in problem solving, critical thinking and analytical reasoning as applied to scientific problems.

PSO3: Demonstrate the ability to apply green chemistry techniques in daily life.

PSO4: Be able to appreciate the central role of chemistry in our society and use this as a basis for ethical behavior in issues facing chemists including an understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.

PSO5: Exhibit competency to take up teaching profession, industrial jobs.

PSO6: Show an interest to start small scale industries with the available resources.

PSO7: Develop an aspiration to clear the UGC/NET/KSET and Civil services examinations.

COURSE/CREDIT PATTERN

Semester	Credits						Total
	Theory (T)			Practical (P)		Project (P)	
	Hard Core (H)	Soft Core (S)	Elective (E)	Hard Core (H)	Soft Core (S)	Hard Core (H)	
First	9	6	--	--	6	--	21
Second	9	3	3	--	6	--	21
Third	9	3	3	9	--	--	24
Fourth	9	6	--	6	--	4	25
Total	36	18	6*	15	12	4	**91**

Total Credits from all the Four Semesters = 91

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

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

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

COURSE PATTERN AND SCHEME OF EXAMINATION

I Semester

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

II Semester

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

III Semester

Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
CH H 501	Coordination Chemistry	3	30 + 70	3	3	3
CH H 502	Reaction Mechanisms and Synthetic Methods	3	30 + 70	3	3	3
CH H 503	Solid State Chemistry	3	30 + 70	3	3	3
CH S 504 **or** CH S 505	Chemistry of Synthetic Drugs **or** Computational and Theoretical Chemistry	3 3	30 + 70 30 + 70	3 3	3	3x1=3
CH E 506 **or** CH E 507 or CH E 508	Biomolecules and Medicines **or** Chemistry of Materials or Food Chemistry	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x1=3
CH P 509	Inorganic Chemistry Practicals-III	--	30 + 70	6	6	3
CH P 510	Organic Chemistry Practicals-III	--	30 + 70	6	6	3
CH P 511	Physical Chemistry Practicals-III	--	30 + 70	6	6	3

IV Semester

Course Code	Course Title	No of Units	Evaluation IA+ Exam	Teaching Hrs/ week	Exam Hrs	Credits
CH H 551	Bioinorganic Chemistry	3	30 + 70	3	3	3
CH H 552	Synthetic Methods, Molecular Rearrangements & Heterocyclic Chemistry	3	30 + 70	3	3	3
CH H 553	Polymers & Photochemistry	3	30 + 70	3	3	3
CH S 554 CH S 555 CH S 556	Nuclear, Surface & Nano Chemistry Organometallic Chemistry Electrochemistry and Reaction Dynamics **(Any two)**	3 3 3	30 + 70 30 + 70 30 + 70	3 3 3	3	3x2=6
CH P 557	Inorganic Chemistry Practicals–IV	6 Hrs	30 + 70	6	6	3
CH P 558	Physical Chemistry Practicals–IV	6 Hrs	30 + 70	6	6	3
CH P 559	Project Work & Dissertation	8 Hrs	30 + 70	8	--	4

BASIS FOR INTERNAL ASSESSMENT

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

THEORY QUESTION PAPERS PATTERN

The Syllabus of each hardcore course shall be grouped into three units of 15 teaching hours and that of soft core and open elective courses shall be of three units of 12 teaching hours. Question Papers in all the four semesters shall consist of Two Parts, Part-A and Part-B. Part-A shall contain Nine (09) objective short answer type questions carrying 2 marks each, drawn equally from all the three units of the syllabus. All the nine subdivisions are to be answered. Part B shall contain Six (06) brief and/or long answer questions carrying 13 marks each drawn from all the three units of the syllabus (2 questions per unit). There should be three sub-divisions per question. Four out of Six questions are to be answered.

M.Sc. Chemistry

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

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

PART - A

Answer any Nine subdivisions

2x9= 18

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

f. UNIT II

g.

h.

i.

j.

k. UNIT III

l.

PART – B

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

UNIT I

2. a.

b.

c. 5+4+4

3. a

b.

c. 5+4+4

UNIT II

4. a.

b.

c. 5+4+4

5. a.

b.

c. 5+4+4

UNIT III

6. a.

b.

c. 5+4+4

7. a.

b.

c. 5+4+4

M.Sc. Chemistry Open Elective Paper

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

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

PART - A

Answer any Nine subdivisions 2x9= 18

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

e.
f. UNIT II
g.
h.

i.
j.
k. UNIT III
l.

PART – B

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

UNIT I

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

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

UNIT II

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

5. a.

b.

c. 5+4+4

UNIT III

6. a.

b.

c. 5+4+4

7. a.

b.

c. 5+4+4

PRACTICAL EXAMINATION PATTERN

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

I SEMESTER

CH H 401: INORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT-I **15 Hrs**

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

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

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

UNIT-II **15 Hrs**

Compounds of Main Group elements

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

Graphite and intercalation compounds, carbides, silicates, zeolites.

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

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

UNIT-III **15 Hrs**

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

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

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

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

References:

1. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, 4th Edn., Pearson Education, 2013.
2. Inorganic Chemistry: Shriver, Atkins and Langford, 5th Edn., OUP, 2010.
3. Concise Inorganic Chemistry: J. D. Lee, 5th Edn., Blackwell Science, 2014.
4. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3rd Edn., Wiley, 2007.
5. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2nd Edn., Pearson Prentice Hall, 2005.
6. Inorganic Chemistry – A Unified Approach: W. W. Porterfield, Elsevier, 2nd Edn., 2005.

7. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6th Edn., Wiley, 2014.
8. Quantitative Analysis: R. A. Day and A. L. Underwood, 6th Edn., Prentice Hall, 2012.
9. Analytical Chemistry: Dhruba Charan Dash, 1st Edn., PHI Learning Private Limited, 2011.
10. Basic Concepts of Analytical Chemistry: S. M. Khopkar, 3rd Edn., New Age International, 2008.

CH H 402: ORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT–I **15 Hrs**

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

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

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

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

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

UNIT-II **15 Hrs**

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

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

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

UNIT-III **15 Hrs**

Stereochemistry

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

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

References:

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

CH H 403: PHYSICAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

CO3: Role of quantum Chemistry in understanding properties of molecules

UNIT-I **15 Hrs**

Chemical Thermodynamics

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

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

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

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

Thermodynamics of real gases

Concept of activity, choice of standard states, variation of activity and activity coefficient of a gas with pressure and temperature, activity of solids and liquids, concept of fugacity, variation of

fugacity with pressure and temperature, fugacity of solids and liquids, fugacity of a gas in mixture of real gases, determination of fugacity of gas in a mixture

UNIT- II **15 Hrs**

Chemical Kinetics

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

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

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

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

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

UNIT-III **15 Hrs**

Quantum Chemistry

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

References:

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

CH S 404: SPECTROSCOPY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

CO2: Knowledge on Electronic spectra of molecules

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

UNIT-I **12 Hrs**

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

UNIT–II **12 Hrs**

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

hydrogen bonding, phase and solvents on vibrational frequencies, overtones, combination bands and Fermi resonance.

UV/Electronic Spectroscopy: Basic principle, Chromophores, auxochromes, Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

UNIT-III **12 Hrs**

NMR Spectroscopy

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

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

References:

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

CH S 405: METHODS OF ANALYSIS

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Objectives:

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

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

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

UNIT-I **12 Hrs**

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

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

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

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

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

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

UNIT-II **12 Hrs**

Diffraction Techniques

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

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

UNIT-III **12 Hrs**

Thermoanalytical Techniques

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

Radiochemical Methods of Analysis

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

References:

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

CH S 406: ENVIRONMENTAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

CO2: Identification of impurities in waste water and their removal

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

UNIT-I **12 Hrs**

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

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

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

UNIT-II **12 Hrs**

Water, Waste Water Treatment and Analysis: Hydrologic cycle, sources, chemistry of sea water, criteria & standards of water quality- safe drinking water, maximum contamination levels of inorganic & organic chemicals, radiological contaminants, turbidity, microbial contaminants.Water pollution control and management. Drinking water supplies, Trace elements in water. DO, COD, BOD, TOC. Monitoring techniques and methods: Determination of pH,

conductance, fluoride, dissolved oxygen by Winkler's method, nitrate/nitrite by diazo coupling, chloride by Mohrs and Volhard's method, and fluoride by Alizarin Visual method, Water contamination with cyanide, sulfide, sulphate, phosphate and total hardness. Analysis of Arsenic by Atomic absorption spectroscopy (AAS), cadmium and mercury by dithizone method, chromium by diphenyl carbazide method, lead by polarographic method. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis

UNIT-III **12 Hrs**

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

References:

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

CH P 407: INORGANIC CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

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

References

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

CH P 408: ORGANIC CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

Single stage organic preparations

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

References

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

CH P 409: PHYSICAL CHEMISTRY PRACTICALS – I

Teaching Hours: 4 Hrs per week

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

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

References

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

II SEMESTER

CH H 451: ADVANCED INORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT- I **15 Hrs**

Symmetry and Group Theory

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

UNIT-II **15 Hrs**

Metallurgy and redox potentials

Methods of reduction of oxide ores, chemical and electrolytic reductions, Ellingham diagram, Specialized techniques for the extraction of metals –Amalgamation, Hydrometallurgy, Solvent Extraction, Ion exchange chromatography. Reduction potentials, Latimer and Frost diagrams – features and applications.

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

UNIT-III **15 Hrs**

Chemistry of Ti subgroup and inner transition elements

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

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

References:

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

CH H 452: ADVANCED ORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT-I **15 Hrs**

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

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

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

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

UNIT-II **15 Hrs**

Free Radical Reactions: Types, mechanisms of free radical substitution reactions & neighboring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead, reactivity of attacking radical and effect of solvent on reactivity. Auto-oxidation,

coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsdiecker reactions.

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

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

UNIT-III **15 Hrs**

Chemistry of Heterocyclic Compounds

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

References:

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

CH H 453: ADVANCED PHYSICAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

CO3: Need for approximate methods for structure-property relationships

Unit I **15 Hrs**

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

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

UNIT-II **15 Hrs**

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

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

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

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

Unit-III: 15 Hrs

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

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

References:

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

CH S 454: SPECTROSCOPY AND ANALYTICAL TECHNIQUES

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT- I **12 Hrs**

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

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

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

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

UNIT – II **12 Hrs**

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

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

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

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

UNIT-III **12 Hrs**

Mass Spectrometry

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

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

References:

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

CH S 455: CHEMISTRY OF BIOMOLECULES

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

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

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

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

UNIT I **12 Hrs**

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

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

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

Unit II **12 Hrs**

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

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

Unit III **12 Hrs**

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

References:

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

Open Elective papers

CH E 456: COLOUR CHEMISTRY: APPLICATIONS IN DAILY LIFE
Teaching Hours: 3 Hrs per week

Learning Objectives:

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

LO2: To understand the role of pigments in surface coatings

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

Course Outcomes:

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

CO2: Will realize the importance and technological application of pigments

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

UNIT-I 12 Hrs

Synthetic Dyes

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

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

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

UNIT-II12 Hrs

Paints and Pigments

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

UNIT-III 12 Hrs

Colourants in Cosmetics and High Technology

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

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

References:

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

CH E 457: ENVIRONMENTAL CHEMISTRY FOR SUSTAINABLE FUTURE

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

LO2: Identification of toxic and solid pollutants in environment

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

Course Outcomes:

CO1: Able to create an awareness on environmental pollutants.

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

CO3: Knowledge about Chemical toxicology.

UNIT-I **12 Hrs**

Air pollution

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

UNIT-II **12 Hrs**

Water pollution

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

UNIT-III **12 Hrs**

Soil pollution and Chemical toxicology

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

References:

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

CH E 458: CHEMISTRY IN THE COMMUNITY
Teaching Hours: 3 Hrs per week

Learning Objectives:
LO1: To have a brief knowledge on water, food and conservation of chemical resources
LO2: To understand the concept of personal chemistry and atmospheric chemistry
LO3: To learn concepts of pesticide chemistry

Course Outcomes:
CO1: Awareness on quality of water, food and conservation of chemical resources
CO2: Knowledge on Human body's internal chemistry and atmospheric chemistry
CO3: Understanding role of fertilizer, insecticides and pesticides.

UNIT-I **12 Hrs**

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

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

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

UNIT-II **12 Hrs**

Personal Chemistry and choices

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

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

Personal choices and risk assessment:

UNIT-III **12 Hrs**

Pesticide Chemistry

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

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

Fungicides-characteristics, classification, uses and impact on environment

Herbicides-Classification, mechanism of degradation and impact on environment

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

References:

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

CH P 459: INORGANIC CHEMISTRY PRACTICALS – II

Teaching Hours: 4 Hrs per week

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

Reference:

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

CH P 460: ORGANIC CHEMISTRY PRACTICALS – II

Teaching Hours: 4 Hrs per week

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

References:

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

CH P 461: PHYSICAL CHEMISTRY PRACTICALS – II

Teaching Hours: 4 Hrs per week

At least 12 experiments are to be carried out

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.
2. Determination of degree of dissociation, Vant Hoff factor and molecular weight of an electrolyte by cryoscopy method using copper calorimeter/Dewar flask..
3. Heat of solution of a sparingly soluble compound in water by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Phase diagram of three component system (a) 3 liquids with single binodal curve, and b) two liquids and one solid
6. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of (a) order and rate constant and (b) Energy of activation.
7. Determination of a) Energy of activation & b) rate constant for the First and second order kinetics of reaction between potassium persulphate and potassium iodide.
8. Kinetics of sodium formate – iodine reaction.
9. Determination of the latent heat of evaporation of carbon tetrachloride.

10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
12. To study the adsorption of iodine on charcoal from alcoholic solution.
13. To study the effects of gelatin solution on the precipitation values.
14. Comparison of detergent action of detergents and determination of interfacial tension.
15. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene.
16. Study of association of benzoic acid in benzene/toluene.

Any other relevant experiments of interest.

Computer related Practicals

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

References:

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

III SEMESTER

CH H 501: COORDINATION CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To understand coordinate covalent bonds and effects of CFS
2. To render knowledge on spectral and magnetic properties of complexes
3. To explicit the reaction mechanisms in transition metal complexes

Course Outcomes:

CO1: Application of CFT, MOT, J-T effect in the study of complexes

CO2: Interpretation of spectra and magnetic properties of complexes

CO3: Understanding reaction mechanism in transition metal complexes

UNIT-I **15 Hrs**

Modern theories of Metal – ligand bond and thermodynamic effects of crystal field effects.

Crystal field theory of coordination compounds, d-orbital splitting in octahedral, square planar and tetrahedral fields, spectrochemical series, Factors influencing the magnitude of crystal field splitting.

MO theory of coordination compounds - MO energy level diagrams for octahedral and tetrahedral complexes. Structural evidences for ligand field splitting – hydration, ligation and lattice energies, site preference energies. Jahn-Teller effect.

Factors affecting stability of metal complexes, stepwise and overall formation constants, determination of binary formation constants by pH-metry and spectrophotometry.

UNIT-II **15 Hrs**

Spectral properties of complexes: Coupling of single electron angular momenta, energy terms, energy states, coupling schemes, ground terms, spectroscopic ground states, selection rules, relaxation of selection rules, band shapes, band intensities and band widths. Effect of V_{oct} & V_{tet} on the terms, interpretation of electron absorption spectra of coordination compounds- Orgel diagram, Tanabe-Sugano diagrams, Charge transfer bands.

Magnetic properties of complexes: Origin of magnetism, types of magnetic behavior, diamagnetic corrections, measurement of magnetic susceptibility- Guoy and Faraday's methods, ferro- and antiferromagnetic coupling, valence bond and crystal field approach to explain magnetic behavior.

UNIT-III **15 Hrs**

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. Electron transfer reactions- inner sphere and outer sphere reactions, complimentary and non-complimentary reactions.

References:

1. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, 4th Edn., Pearson Education, 2013.
2. Inorganic Chemistry: Shriver, Atkins and Langford, 5th Edn., OUP, 2010.
3. Concise Inorganic Chemistry: J. D. Lee, 5th Edn., Blackwell Science, 2014.
4. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3rd Edn., Wiley, 2007.
5. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2nd Edn., Pearson Prentice Hall, 2005
6. Electronic absorption Spectroscopy and Related Techniques: D. N. Satyanarayana, OUP, 2001.
7. Inorganic Reaction Mechanisms: F. Basolo, R. G. Pearson, Wiley Eastern, 1979.
8. Elements of Magnetochemistry: R. L. Dutta and A. Syamal, Affiliated east-West, 1993.
9. Concise Coordination Chemistry: R. Gopalan and V. Ramalingam, Vikas Publishing, 2014.

CH H 502: REACTION MECHANISMS & SYNTHETIC METHODS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To study the mechanism and synthetic uses of organic name reactions
2. To enable the students to analyze the pericyclic reaction using FMO method and correlation diagram
3. To develop the knowledge on mechanism of oxidation and reduction reaction using various agents

Course Outcomes:

CO1: Reaction mechanism and synthetic uses of organic named reactions

CO2: Knowledge on different pericyclic reactions

CO3: Use of oxidizing and reducing reagents in organic reactions

UNIT-I **15 Hrs**

Organic Name reactions: Reactions, Mechanisms and synthetic uses of the following: Stobbe condensation, Darzen condensation, Bayil-Hillman reaction, Cannizzaro reaction, Chichibabin reaction, Swern oxidation, Oppenauer oxidation, Simon-Smith reaction, Stork Enamine reactions, Prins reaction, Yamada reaction, Suzuki coupling, Woodward and Prevost Hydroxylation, Bucherer reaction, Wittig reaction, Mitsunobu reaction.

UNIT-II **15 Hrs**

Pericyclic Reactions: Classifications of Pericyclic reactions, Theories of pericyclic reaction, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, 1,3,5,7-Octatetraene, allyl systems and 2,4-pentadienyl system. Molecular orbital symmetry. Woodward-Hoffmann correlation diagram and FMO approach.

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

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

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

UNIT-III **15 Hrs**

Oxidation and Reduction Reaction: Oxidation reactions: Introduction and different oxidative processes, Mechanism of oxidation reaction with chromium and manganese salts, peracids and peresters, periodic acid, Lead tetra acetate, Ozone, Osmium tetroxide.

Reduction Reactions: Catalytic hydrogenation: Introduction, catalysts and solvents employed, reduction of functional groups. Hydrogenolysis, and homogeneous catalytic hydrogenation.

Metal hydride reduction: Reduction with LiAlH4 & NaBH4, Stereo chemistry of reduction & other functional groups, Functional group transformation during reduction, Reduction with diborane and related reactions.

Dissolving Metal Reductions: Birch reduction,Clemmenson and Wolf-Kishner reductions. Reduction with diimide and related compounds.

References:

1. Name reactions and Reagents in Organic synthesis: Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, 2nd Edn., John Wiley and sons, New Jersey, 2005.
2. Named Organic Reactions: Thomas Laue and Andreas Plagens, 2nd Edn., John Wiley and sons Ltd. Chichester, West susex, England.
3. Named Reactions: Jie Jack Li, 3rd edn, Springer Verlag Berlin. Heidelberg, Newyork, 2006
4. Reactions, Rearrangements and Reagents: S.N.Sanyal, Bharathi Bhavan publisher, New Delhi, 2007
5. Advanced Organic Chemistry- Reaction, Mechanism and structure: 6th Ed, Michael B. Smith, Jerry March, John Wiley and sons,Inc., Hoboken, New Jersey 2007
6. Advanced Organic Chemistry Part A &B: F. J.Carrey & R.J.Sundberg, 4th Edn., Kluwer, 2001.
7. Organic Chemistry: J. Clayden, N. Greeves, S.Warren and P. Wothers, Oxford University Press.
8. Photochemistry and Pericyclic Reactions: Jagadamba Singh and Jaya Singh, 3rd Ed, New age International publishers, 2013.
9. Modern Methods of Organic Synthesis: N. Carruthers and Iain Coldham, Cambridge Uni., 2004.
10. Modern Reduction Methods: P. G. Anderson and I. J. Munslow, Wiley-VCH, 2008.

CH H 503: SOLID STATE CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To acquaint the students with various types of defects and principles of solid state reaction
2. To understand the electronic properties and applications of solids
3. To learn the properties and applications of ionic conductors, new materials and liquid crystals

Course Outcomes:

CO1: Study of crystal defects and non-stoichiometry, solid state reactions and preparatory methods

CO2: Knowledge on electronic properties, Band theory, and magnetic properties of materials

CO3: Study of liquid crystals, superconductivity and organic conducting polymers.

UNIT–I **15 Hrs**

Crystal Defects and Non-Stoichiometry: Perfect and imperfect crystals, intrinsic and extrinsic defects- point, line and plane defects. Vacancy, Schottky and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects – Structures of UO_2, FeO and TiO.

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.

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UNIT–II **15 Hrs**

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.

Insulators-Dielectric, ferroelectric, pyroelectric & piezoelectric properties & their applications.

Magnetic properties: Classification of magnetic materials – dia, para, ferro, ferri, antiferro &

antiferri magnetic types Langevin diamagnetism. Selected magnetic materials such as spinels & garnets.

UNIT–III **15 Hrs**

Ionic Conductors: Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors; phase transitions and mechanism of conduction in super ionic conductors, examples- β-alumina, AgI, halide and oxide ion conductors. **Superconductivity:** Meisner effects; Types I and II superconductors, Features of super-conductors, isotope effect, high T_c materials. Principle of low temperature superconductivity. **New Materials:** An introduction to Zeolites and Organic conducting materials-polyacetylenes, polyparaphenylenes and polyanilines. **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 and smectic C phases. Optical properties of liquid crystals.

References:

1. Solid state Chemistry: D. K. Chakrabarty, 2nd Edn., New Age International, 2010.
2. Principles of the solid state: H.V.Keer,1st Edn., Wiley Eastern , 1993.
3. Solid state chemistry and its applications: Anthony R. West, 2nd Edn., Wiley, 2014.
4. Solid State Chemistry –An Introduction: L. Smart and E. Moore, 4th Edn., Chapman & Hall, 2012.
5. An Introduction to X-ray Crystallography M. M. Woolfson, Vikas, New Delhi, 1980.
6. Introduction to Solid State Physics, C. Kittel, Wiley Eastern Ltd., 8th Edn., New Delhi, 2005.
7. Material science and Engineering, V. Raghavan, 3rd Ed, (Prentice Hall India), 2011.
8. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
9. Liquid Crystals, S. Chandrasekhar, 2nd ed, Cambridge University Press, 2005.

CH S 504: CHEMISTRY OF SYNTHETIC DRUGS

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

CO1: Imparting knowledge on drug design, structure activity relationship on pharmacokinetics

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

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

Unit I: **12 Hrs**

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

General anaesthetics: Synthesis of Halothane, & Methohexital sodium.

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

UNIT-II **12 Hrs**

Antibiotics: Introduction, classification, mode of action of β-lactum antibiotics. Penicillin-Synthesis of Penicillin V, chemical degradation and bacterial resistance. Cephalosporians-

Nomenclature, Classification, β-lactamase resistance. Structure and mode of action of Tetracyclins, Streptomycin and Chloramphenicol.

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

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

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

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

UNIT-III **12 Hrs**

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

Anticonvulsant: Synthesis of Phenytoin sodium, Trimethadione and Carbamazepine

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

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

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

References:

1. Medicinal Chemistry: Ashutosh Kar, 4th Edn., Wiley-Eastern, New Delhi, 2006.
2. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi,1996.
3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby, Elsevier, 2006.
4. Medicinal-Chemistry of Anticancer-Drugs: Carmen Avendano & J. C Menedez, Elsevier B.V, 2008.
5. The organic chemistry of drug synthesis Vol. III: Daniel Lednicer, John Wiley & Sons Inc., 1984
6. Medicinal Chemistry, a Molecular & Biochemical Approach: Thomas Nogrady & Donald F Weaver, 3rd Edn., Oxford University Press, 2005.
7. Advanced Practical Medicinal Chemistry: Ashutosh Kar, New Age International Pvt. Ltd., 2004.
8. Textbook of Organic Medicinal & Pharmaceutical Chemistry: Wilson, Giswold & Doerge 7th Edn., Lippincott Company, 1977.
9. Pharmacology & Pharmacotherapeutics-Part I and II: Satoskar and Bhandarkar 10th Edn., Bombay Popular Prakashan, 1986.
10. Principles of Medicinal Chemistry: Foye: 3rd Edn., Varghese Publishing House, 2008.
11. Medicinal and Pharmaceutical Chemistry: H. Singh & V. K. Kapoor, Vallabh Prakashan, New Delhi, 1996.
12. Burger's Medicinal Chemistry-Part–I-III: 4th Edn., Wolff, Wiley Eastern, NewYork, 1980.
13. Organic Chemistry-Vol. I and II: I. L. Finar, 6th Edn., Longman-ELBS, London, 2009.
14. Synthesis of Essential Drugs: R. S. Vardanya and V. J. Hruby, Elesvier, 2006.

CH S 505: COMPUTATIONAL AND THEORETICAL CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes:

CO1: Knowledge structural and synthesis of amino acids, proteins and their linkages

CO2: Decoding the synthesis of nucleoside and nucleotides and study of DNA and RNA structure

CO3: Learning classification and nomenclature of Vitamins and their deficiency diseases

UNIT-I **12 Hrs**

Introduction: computational chemistry as a tool and its scope.

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

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

UNIT-II **12 Hrs**

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

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

UNIT-III **12 Hrs**

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

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

References:

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

CH E 506: BIOMOLECULES AND MEDICINES

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

Course Outcomes

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

UNIT-I 12 Hrs

Synthetic drugs

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

UNIT-II 12 Hrs

Metals in Medicine

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

Biological Trace elements: Introduction to trace elements in biological system, Biological classification of trace elements, essential trace elements. The trace elements in human enzyme system-copper, iron zinc, cobalt, manganese. Clinical Significance of Essential Trace Elements, diseases due to metal deficiency.

UNIT-III 12 Hrs

Chemistry of Biomolecules

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

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

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

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

References:

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

CH E 507: CHEMISTRY OF MATERIALS

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

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

LO3: To study about bio-materials

Course Outcomes:

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

CO2: Ability to understand the industrial utility of materials

CO3: Knowledge on biological applications of materials

UNIT-I **12 Hrs**

Cementitious Materials

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

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

Ceramic Materials

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

UNIT-II **12 Hrs**

Composite Materials

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

Bio-materials

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

UNIT-III **12 Hrs**

Superconducting Materials

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

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

References:

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

CH E 508: FOOD CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

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

LO2: To understand the science and few aspects of cooking

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

Course Outcomes:

CO1: Knowledge on food, nutrition and food additives
CO2: Understanding of science behind cooking
CO3: Information on food metabolism & impact of food factors on our body

UNIT-I **12Hrs**

Food, nutrition & food additives

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

UNIT-II **12 Hrs**

The Science of cooking

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

UNIT-III **12 Hrs**

Eat right for good metabolism and health

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

References:

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

CH P 509: INORGANIC CHEMISTRY PRACTICALS – III

Teaching Hours: 6 Hrs per week

A. Any five of the following experiments are to be carriedout:

1. Analysis of brass – Cu gravimetrically using ∝-Benzoinoxime and Zinc complexometrically.
2. Analysis Cu-Ni alloy .
3. Analysis of Stainless Steel – Insoluble residue by gravimetry, Ni gravimetrically using DMG, Fe volumetrically using Ce(IV) & Cr(III) volumetrically by persulphate oxidation.
4. Analysis of Type metal –Sn gravimetrically, Pb electrogravimetrically and Sb titrimetrically using KBrO3
5. Quantitative analysis of the constituents & mixtures containing the following radicals
   (i) Cu(II) + Fe(II) - Cu gravimetrically as CuSCN and Fe using Ce(IV).
   (ii) Fe(II) + Ni(II) – Fe gravimetrically as Fe2O3 and Ni using EDTA.
   (iii) Fe(III) + Ca(II) - Fe gravimetrically as Fe2O3 and Ca using EDTA.
   (iv) Cr(III) + Fe(III) – Using EDTA by Kinetic masking method.
6. Analysis of chalcopyrites, magnetite and ilmenite.
7. Ion-exchange chromatography: Separation and determination of Mg2+/Zn2+, Zn2+/Cd2+ & Cl-/ Br-.

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

8. Determination of COD of a water sample
9. Determination of Phosphorus.
10. Determination of dissolved oxygen (DO) by Winkler's method
11. Determination of nitrate & nitrite in water samples and sea water.
12. Analysis of heavy metals in waste water, sea water (Pb, Hg by spectrophotometry)
13. Determination of available K in soil,
14. Nephelometric determination of sulphate/phosphate.

15. Determination of alkalinity of water samples
16. Determination of fluoride in drinking water by spectrophotometry and ion selective electrode
17. Determination of phosphates in detergents
18. Spectrophotometric determination of sulphur and phosphorus present in soil.

References:

1. A. I. Vogel : A Text book of Quantitative Inorganic Analysis, (ELBS), 1978.
1. APHA, AWWA and WPCF: Standard Method for the Examination of water and Waste Water (Washington DC),1989,
2. I. M. Kolthof and E.P. Sandell: Quantitative Chemical Analysis.McMillan,1980
3. I. Williams, Environmental Chemistry, Wiley, 2001
4. Lobinski and Marczenko, Comprehensive Analytical Chemistry, Vol.30, Elsevier, 1996.

CH P 510: ORGANIC CHEMISTRY PRACTICALS – III

Teaching Hours: 6 Hrs per week

Quantitative Estimation

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

Determination of functional groups like hydroxyl, vic-hydroxyl, enol, amino, amide.

Multi Step Organic Synthesis

Ethyl resorcinol from Resorcinol, 3-Bromo-4-methyl benzaldehyde from p-Toludine, ε-Caprolactam from cyclohexanone, p-Amionobenzoic acid from p-Nitrotoludine, s-Tribromobenzene from aniline, o-hydroxy acetophenone from phenol, Benzanilide from Benzophenone, Benzylic acid from Benzoin, Benzopinacolone from Benzophenone, p-Chlorotoluine from p-Toludine, 2,5-Dihydroxy acetophenone from Hydroquinone, 2,4-Dinitrophenylhydrazine from Chlorobenzene, m-Nitrobenzoic acid from Benzoic acid

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

References:

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

CH P 511: PHYSICAL CHEMISTRY PRACTICALS – III

Teaching Hours: 6 Hrs per week

A. Electrochemistry:

a. Conductometry (At least four experiments to be carried out)

1. Titration of a mixture of acetic acid, monochloro and trichloacetic acids with NaOH.
2. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate by conductometric titration with sodium hydroxide.
3. Measurements of the conductance of a weak acid, (a) HOAC and of the strong electrolytes NaOAc, HCl and NaCl and (b) HCOOH and of the strong electrolytes HCOONa, HCl and NaCl) and to calculate the ionization constant of the acid.
4. Titration of mixture of strong acid and weak acid with weak base (HCl + HAC against NH4OH).
5. Determination of pKa of a given weak acid by pH measurements at various dilutions.
6. Conductometric titration of the mixture of (a) HCl and NH4Cl and (b) HCl and acetic acid.
7. Determination of activity coefficient of Zinc ions in 0.002M ZnSO4.
8. Conductometric determination of Critical Micelle Concentration.
9. Synthesis of a n – type semiconductor (e.g ZnO) and measurement of its electrical conductivity at different temperatures
10. Synthesis of a p – type semiconductor (e.g NiO) and measurement of its electrical conductivity at different temperatures.

b. Potentiometry (At least four experiments are to be carried out)

1. Composition of Zinc Ferrocyanide Complex by potentiometric Titration.
2. Potentiometric titration of (a) Non aqueous system and (b) mixture of strong (HCl) and weak (HAC) acid with NaOH / NH4OH and find the strength of the acids in mixture.
3. Determination of decomposition potential of an aqueous electrolytic solution.
4. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
5. Determination of acidic and basic dissociation constants and isoelectric point an amino

acid pH metrically..

6. pH titration of (a) HCl versus NaOH, (b) HOAC versus NaOH and (c) lead nitrate versus potassium chromate, and Titration of mixture of bases (Na2CO3& NaHCO3) with standard HCl..

7. Determination of pKa values of functional groups in amino acids using a pH meter.

8. Determination of Hammett constants of o-, m-, p- amino/nitro benzoic acid by pH measurements.

9. Verification of Tafel equation of hydrogen evolution reaction.

10. Study of rate of corrosion and inhibition efficiency of an inhibitor on mild steel/Al/Cu by weight loss method i) at different time intervals and ii) at different temperatures (to evaluate thermodynamic parameters)

B. Dry experiments (At least two experiments to be carried out)

1. Interpretation of X-ray diffractogram

2. Analysis of an ESR spectrum of an organic/inorganic radical.

3. Derivation of geometric and spectroscopic and rotation-vibration spectra of linear molecules.

4. Interpretation of electronic spectrum/identifying chromophores and solvent effect studies.

5. Interpretation of TGA curve

C. Computational chemistry experiments (At least two experiments to be carried out)

Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

Single point energy, Geometry optimization and MO energy, Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

REFERENCES:

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

Ab initio, semiempirical and DFT:

1. Firefly / PC GAMESS available from http://classic.chem.msu.su/gran/gamess/
2. WINGAMESS available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

1. Gabedit available from http://gabedit.sourceforge.net/
2. wxMacMolPlt available from http://www.scl.ameslab.gov/MacMolPlt/
3. Avogadro from http://avogadro.openmolecules.net/wiki/Get_Avogadro

IV SEMESTER

CH H 551: BIOINORGANIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To acquire the knowledge on metal ions in transmission of energy and bio-functions of metalloenzymes
2. To understand the role of metals in metabolic activities and medicines
3. To study biochemical aspects of non-metals.

Course Outcomes:

CO1: Able to understand the role of metal ions in biological systems, energy and enzymes

CO2: Importance of oxygen carriers, metal storage and nitrogen fixation in biological systems

CO3: Knowledge on biochemistry of non-metals and Chelation in Medicine

UNIT-I **15 Hrs**

Metal ions in biological systems: Essential and trace metals, ion transport across membranes, active transport of ions, ionophores.

Metal complexes in transmission of energy: Chlorophyll, Photosystem I & II, Mechanism of photosynthesis- light reactions.

Metalloproteins as enzymes: Carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P 450, superoxide dismutase, vitamin B_{12} coenzyme.

UNIT-II **15 Hrs**

Transport and storage of dioxygen: 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. Biological nitrogen fixation, nitrogenase.

Metals in medicine: metal deficiency, metal toxicity

UNIT-III **15 Hrs**

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

Chelation in Medicine: Metal ion detoxification – Chelating drugs having –SH groups, polyamino carboxylic acids as chelating drugs, Desferrioxamines as chelating drugs. Limitations of chelation therapy in metal ion detoxification.

Radio protective chelating drugs and therapeutic activities of some special chelating agents inhibiting the metalloenzymes. Metal – metal detoxification, Antimicrobial activities of metal chelates and chelating ligands, Chrysotherapy. Metals used in diagnosis. Anticancer activity of platinum complexes.

References:

1. Inorganic Chemistry of Biological Processes: M. N. Hughes (2^{nd} Edn.) Wiley,1988.
2. Bioinorganic Chemistry: I. Bertini. H. B. Gray, S. J. Lippard and J. S. Valentine, (1^{st} Edn.) Viva Books, 1988
3. Principles of Bioinorganic Chemistry: Lippard S. J. and Berg J. M., University Science Books, 1994.
4. Biocoordination Chemistry (Chemistry Primer 26): Fenton D. E., Oxford University Press, 1996.
5. Metal ions of Biological Systems: H. Siegel and T. G. Spiro, Mercel – Dekker, 1980 to present.
6. Principles of Biochemistry: Lehninger A. L., New York, Worth, 1982.
7. Bioinorganic Chemistry: Asim K Das, Books & Allied Ltd, 2013.
8. Bioinorganic Chemistry: K. Hussain Reddy, New Age International, 2007.

CH H 552: SYNTHETIC DESIGN, MOLECULAR REARRANGEMENTS AND HETEROCYCLIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To gain the knowledge of retrosynthetic approach in the multistep synthesis
2. To familiarize with different molecular rearrangement reactions
3. To study heterocycles and their biological importance

Course Outcomes:

CO1: Illustration on basic principles and techniques used in disconnection approach

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

CO3: Understanding nomenclature, structure, synthesis and reaction of four and five membered heterocycles.

UNIT-I **15 Hrs**

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

Retrosynthetic analysis: Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, Benzocaine, p-methoxyacetophenone, acetonecyanohydrin, 2-methyl-6-methoxy-indole-3-acetic acid, 6-methyl quinoline and 1-phenyl-4-p-methoxyphenyl-1,3-butadiene.

Illustrative Synthesis: Juvabione, Longifolene, 7-isopropyl-trans-3,7-octadienol, 4,6-dimethoxyphalaldehydic acid, 6-methoxy tryptamine, 2-(3-butenyl)-3-methylcyclohexenone and 4-(3-butenyl)-3-methylcyclohexenone and Zearalenone.

UNIT-II **15 Hrs**

Molecular Rearrangements: Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements. Intermolecular and Intramolecular migration, nature of migration and migratory aptitudes. Mechanism of Wagner-Meerwein, Dienone-Phenol,

Pinacol-Pinacolone, Demaynov, Benzil-Benzilic acid, Fries, Wolff, Favorskii, Neber, Benzidine, Baeyer-Villiger, Beckmann, Lossen, Curtius, Schmidt, Stevens, Shapiro, Baker-Venkatraman and Amadori rearrangement. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement

UNIT-III: 15 Hrs

Heterocyclic Chemistry: Structure, reactivity, synthesis and reaction of the following: Four membered heterocycles-Oxetanes, Azetidines and Thietanes; Five membered heterocycles-Imidazoles, Oxazole, Imidazolines and their benzo analogues. Pyrazoles, Pyrazolines, and benzopyrazoles. Thiazoles and Thiazolidines. Oxadiazole, and Oxadiazolines. Thiadiazoles and Thiadiazolines. 1,2,4-Triazoles and 1,2,3- Triazoles. Oxazoles and Benzoxazoles. Isoxazoles and Osoxazolines. Coumarin. Biological importance of Purines and Pyrimidines.

References:

1. Organic Chemistry: P.Y Bruice , Pearson Education (Singapore) Pvt. Ltd., Delhi, 2003.
2. Name reactions and Reagents in Organic synthesis: Bradford P.Mundy, Michael G. Ellerd, Frank G. Favaloro, 2nd Edn., John Wiley and sons,Inc.,Hoboken, New Jersey, 2005.
3. Named Organic Reactions: Thomas Laue and Andreas Plagens, 2nd Edn., John Wiley and sons Ltd. Chichester, West susex, England, 2005.
4. Named Reactions: Jie Jack Li, Named Organic Reactions: Thomas Laue and Andreas Plagens, 3rd Edn., John Springer Verlag Berlin. Heidelberg, Newyork, 2006.
5. Reactions, Rearrangements and Reagents: S. N. Sanyal, Bharathi Bhavan publisher, New Delhi, 2007.
6. Advanced Organic Chemistry- Reaction, Mechanism and structure: Michael B. Smith, Jerry March, 6th Edn., John Wiley and sons Inc. Hoboken, New Jersey, 2007.
7. Advanced Organic Chemistry: Part A &B, F.J. Carrey & R. J. Sundberg, 4th Edn., (Kluwer) 2001.
8. Organic Chemistry: J.Clayden, N.Greeves, S.Warren and P.Wothers, Oxford University Press, 2001
9. Name Reactions and Reagents in Organic Synthesis: Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Jr, 2nd Edn., John Wiley and sons, Inc., Hoboken, New Jersey, 2005.
10. Organic Synthesis a Disconnection Approach- Stuart warren, John wiley and sons, 2007.

CH H 553: POLYMERS AND PHOTOCHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

LO1: To understand the mechanism and kinetics of polymerization reactions

LO2: To acquire the knowledge of stereochemistry and application of polymers

LO3: To study different types of photochemical reactions and their kinetics

Course Outcomes:

CO1: Understanding techniques and kinetics of polymerization.

CO2: Study of stereochemistry, phase transition, solutions and conducting properties of polymers

CO3: Learning photochemical reactions, their properties, kinetics and their rearrangement reactions.

UNIT-I **15 Hrs**

Introduction to Polymers & Techniques of Polymerization: Bulk, Solution, Suspension & Emulsion methods. Polycondensation techniques.

Polymer Molecular weight: Average molecular weight concept - averages, polydispersity and molecular weight distribution. Fractionation methods. Methods of Molecular weight determinations–osmometry, viscometry, ultracentrifugation. & gel permeation chromatography

Size of Polymer Molecules: Average dimensions of polymer chains- end to end distance and radius of gyration calculations.

Kinetics of Polymerisation: Addition (free radical and ionic) and Condensation kinetics. Kinetics of Copolymerisation-reactivity ratio and copolymer types.

UNIT-II **15 Hrs**

Stereochemistry of polymers- geometric and optical isomers. Stereospecific polymers using coordination catalysts.

Phase transitions in polymers and thermal characterization: Glass transition, crystallinity and melting- correlation with the polymer structure.

Polymers in solution: Criteria of polymer solubility. Thermodynamics of polymer solutions. Conducting polymers, liquid crystal polymers, polyelectrolyte. Polymers for high temperature applications, biodegradable polymers, drug delivery polymers.

UNIT-III **15 Hrs**

Introduction to photochemistry. Quantum yield and its determinations, experimental methods in photochemistry, Actinometry. Physicochemical properties of electronically excited molecules-excited state dipole moments, acidity constants.

Photochemical kinetics of unimolecular and bimolecular processes. Quenching-collisions in the gas phase, solution (Stern-Volmer equation) & by added substances. Photophysical Reactions-Types-Photo-dissociation, Isomerization and other rearrangement reactions with specific examples.

References:

1. Text book of Polymer Science F.W. Billmeyer (Wiley), 3rd Edn., 2007.
2. Contemporary Polymer Chemistry: H.R. Allcock and F.W. Lampe, Pearson/Prentice Hall, 2003
3. Polymer Science: V. R. Gowariker, N. V. Viswanathan & T. Sreedhar, New Age international, 2015
4. Polymer science and Technology: J. R. Fried, Prentice Hall, 1995.
5. Advanced Polymer Chemistry- A problem solving guide: Manas Chanda, Marcel Dekker, 2000.
6. Engineering materials: Properties and Selection: K. G. Budinski, Prentice Hall, 2000.
7. Fundamentals of Photochemistry – K. K. Rohatgi and Mukherje, 3rd Edn., New Age International Bangalore, 2014.

CH S 554: NUCLEAR, SURFACE AND NANO CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To gain the knowledge of the Radioactivity, Radiation Detection and Measurement
2. To understand the mechanism of surface reactions and catalysis
3. To study synthesis and characterization nanomaterials

Course Outcomes:

CO1: Studying of the concepts radioactivity, decay and nuclear power reactors

CO2: Study of surface reactions, mechanisms

CO3: Understanding introduction to nano materials, their synthesis and characterization and their application

UNIT-I **15 Hrs**

Nuclear Chemistry: Nuclear structure and stability: Nuclear properties - nuclear forces, mass defect and binding energy. Nuclearstability-Liquid drop, shell and collective models.

Radioactivity and Nuclear Decay - Decay modes of natural and artificial nuclides- Determination of half life, growth kinetics. Conditions of equilibrium. Theories of $\propto$, $\beta$and γ emissions.

Radiation Detection and Measurement: Experimental techniques in the assay of radioactive isotopes. Radiation Detectors-ionisation chambers, proportional and Geiger-Muller, scintillation and semiconductor radiation detectors (NaI-Tl and Ge(Li), HPGe solid state detectors). Liquid scintillators and multichannel analysers.

Nuclear Reactions, Energy and Nuclear Power reactors - Nuclear fission and fusion. Types of nuclear power reactors, basic features and components of a nuclear power reactor. An introduction to breeder reactors.

UNIT- II **15 Hrs**

Surface Chemistry and Catalysis: Surface reaction kinetics: A review of adsorption isotherms, uni- and bi-molecular reactions. multilayer adsorption-BET equation- application in surface area determination.

Reactions at Surfaces: Structures of solid surfaces & adsorbed layers. Mechanisms of surface reactions- kinetic effects of surface heterogeneity & interactions – surface inhibition and activation energies –reactions between two adsorbed molecules – surface exchange reactions – Transition state theory of surface reactions – unimolecular and bimolecular reactions.

Catalysis: Acid-base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed reactions- Michaelis-Menten equation, Effect of pH, temperature& inhibitors

Acidity functions - Hammett acidity function, Zucker–Hammett hypothesis. Bunnett hypothesis. Industrial catalysts: Catalyst carrier, promoter, inhibitor & catalyst poison.

UNIT-III **15 Hrs**

Nano Chemistry

Nanomaterials: definition, importance, classification, 0D, 1D, 2D structures – size effects, the general methods for the synthesis of nanostructures (sol-gel method, co-precipitation, microemulsion, solvothermal, sonochemical reaction etc), Solution growth techniques of 1D-2D nano structures: Synthesis of metallic, semiconducting and oxide nanoparticles – homo- and hetero-nucleation growth methods – template-based synthesis, different characterization techniques (XRD, TEM, SEM, AFM, XPS, Raman study etc) and their application

References:

1. Nuclear and Radiation Chemistry: Friedlander, Kennedy Macias & Miller , Wiley, 1981
2. Essentials of Nuclear Chemistry: H. J. Arnikar , Wiley Eastern, 1987.
3. An Introduction to Radiation Chemistry: Spinks and Woods, Wiley, New York, 1990.
4. Catalysis: J.C. Kuriacose, Macmillan India Ltd., 1991.
5. Nanochemistry: A Chemical approach to Nano materials-: G.A. Ozin, A. C. Arsenault and L. Cadematiri, Royal Society of Chemistry, London, 2009.
6. The Chemistry of Nano structured Materials: P. D. Yang, World Scientific Publishing, Singapore, 2003.

CH S 555: ORGANOMETALLIC CHEMISTRY

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To study preparation and reactions of transition metal pi complexes
2. To gain the knowledge of organometallic reactions
3. To understand the application of organometallics in organic synthesis

Course Outcomes:

CO1: Learning structural features of transition metal-carbon pi complexes

CO2: Studying catalysis by organometallic compounds

CO3: Using of organometallics in organic synthesis

UNIT-I **12 Hrs**

Transition metal-carbon pi complexes: Preparative methods, 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.

Isolobal concept.

UNIT- II **12 Hrs**

Catalysis by organometallic compounds:16- and 18-electron rules, oxidative addition, insertion, deinsertion and reductive elimination reactions.

Homogeneous catalysis by organometallics- hydrogenation, hydrosilation, hydrocyanation and isomerization of olefins, immobilisation of homogeneous hydrogenation catalysts,

Hydrocarbonylation of olefins (oxo reaction–cobalt and rhodium oxo catalysts), carbonylation of alcohols- Monsanto acetic acid process. Polymerization of olefins and acetylenes: Ziegler-Natta catalyst systems. Fischer – Tropsch reaction , Water Gas Shift reactions.

UNIT-III **12 Hrs**

Organometallics in Organic Synthesis: Main group organometallics- preparation, properties and applications of organometallic compounds of Li, Mg, Hg, Zn, Cd and Sn. Synthetic applications of organo-transition metal compounds: organocuprates. Hydrozirconation, transmetallation reactions by organopalladiums and organonickels, carbonylation by metal carbonylates, decarbonylation, carbene complexes and metallacycles, arene complexes.

References:

1. 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.
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.

CH S 556: ELECTROCHEMISTRY AND REACTION DYNAMICS

Teaching Hours: 3 Hrs per week

Learning Objectives:

1. To acquire the knowledge of electro-organic synthesis and corrosion concepts
2. To familiarize with electrochemical energy systems
3. To study complex reactions and pharmco kinetics

Course Outcomes:

CO1: Able to Differentiate electrorganic synthesis with conventional synthesis and corrosion types and its control. Role of electrocatalysis in hydrogen preparation.

CO2: Imparts knowledge on solar energy conversion to chemical energy and application of batteries, fuel cells

CO3: Understanding of Complex reactions, Potential energy surfaces, Theory of kinetic isotope effects and Pharmaco kinetics

UNIT-I **12 Hrs**

Industrial Electrochemistry: Fundamentals, electro- organic synthesis (Kolbes synthesis, adiponitrile, oxidation & reduction of hydrocarbons, reduction of nitro-compounds). Electro-inorganic synthesis of fluorine, chlorates & ozone

Corrosion: Introduction, Importance and principles, Forms of corrosion (Galvanic, Atmospheric, stress and soil). Techniques of Corrosion rate measurement (instrumental and non-instrumental). EMF series & Galvanic series and their limitations. Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), effect of oxidizer and passivity of corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating).

Electrocatalysis- Introduction and its future. Electrogrowth of metals on electrodes, its importance and consequences. Hydrogen evolution reaction.

Photoelectrochemistry: photogalvenic cells, photoelectrochemical cells, types and stability of semiconductor electrodes

UNIT-II **12 Hrs**

Electrochemical Energy System: Chemical energy sources and their limitations. Introduction to electrochemical energy systems and solar energy system, Electricity storage-Importance, storage density; Primary battery (Laclanche-dry cell and Alkaline cell). Secondary battery (acid and alkaline). Reverse batteries. Fuel cells (H_2-O_2 , methanol, bio-cells).

Biosensors: Introduction, Bio-recognition elements in biosensors, immobilization methods, principles of biorecognition, natural, semi-synthetic and synthetic biorecognition elements. **Electrochemical biosensors**: Amperometric, potentiometric and conductometric biosensors.

UNIT-III **12 Hrs**

Complex reactions–Mechanisms of some inorganic and organic reactions, formation and decomposition of phosgene, decomposition of N_2O_5, ozone and acetaldehyde.

Linear Free Energy Relationship: Okemoto Brown equation and its application. Swain Scott and Edward equation. Winstein - Grunwald relationship.

Dynamics of unimolecular reactions-Lindemann, Hinshelwood, RRK & RRKM theories.

Theory of kinetic isotope effects - Primary, secondary and solvent kinetic isotope effects. Tunneling effect. Isotope effects with heavier atoms.

Pharmaco kinetics: Pharma concentration time curve, drug dissolution rate, pharmacokinetics applied to one-component open model (calculation of elimination rate constant & metabolism constant).

References:

1. Modern Electrochemistry (Vol.1, 2A &2B): Bockris and Reddy, 2nd Edn., Plenum, New York, 1998.
2. Chemical and Electrochemical Energy Systems: Narayan & Viswanathan, Univ. Press, 1998.
3. Industrial Electrochemistry: D. Peltcher and F. C. Walsh, Chapman & Hall-Cambridge, 1990.
4. Fundamentals of Electrochemistry: Fulkner and J.Bard, wiley, 2000
5. Biosensors-Theory and Applications: Donald G.Buerk, Technomic Publishing Co., 1993.
6. Biosensors: Fundamentals and Applications, Bansi Dhar Malhotra and Chandra, Mouli Pandey, Smither Group Co., 2017.
7. Biosensors: Techniques and Instrumentations in Analytical Chemistry, Frieder Scheller and Florian Schubert, Vol. 11, Elsevier Sci. Publishers, 1992.
8. Chemical Sensors and Biosensors, Brian R. Eggins, John Wiley & Sons Ltd, UK, 2004.
9. Chemical Kinetics: K. J. Laidler, Pearson Education, 1987.
10. Medicinal and Pharmacuetical chemisty, Harkishan Singh, V K Kapoor, Mackhingee Publisher,2017.

CH P 557: INORGANIC CHEMISTRY PRACTICALS – IV

Teaching Hours: 6 Hrs per week

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
3. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
4. 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.

iii) Potassium trisoxalatoferrate(III) and iv) Potassium hexathiocyanatochromate(III)

v) $K_3Cr(OX)_3.3H_2O$ vi) $Cu(tu)_3Cl$ vii)$Zn(tu)_3OSO_3$

5. Determination of composition of complexes:
   a) Job's method: Fe-phenanthroline complex
   b) Mole ratio method: Zr-Alizarin red S complex,
   c) Slope ratio method: Cu ethylenediamine complex,
   d)Limiting logarithmic method:Uranyl-sulphosalicyclic acid complex.
6. Determination of stability constants
   a) Turner Anderson method : Fe-Tiron system,
   b) Bejrrums's method : Cu – sulphosalicyclic acid system,
   c) Polarographic method :Cu-glycinate or Pb -oxalate system.

References:

1. Physicochemical Experiments: J. Rose, I. Pitman, 2007
2. Vogel's Text Book of Quantitative Chemical Analysis: G. H. Jeffrey, J. Bassette, J. Mendham and R. C. Denny, 5th Edn., Longman, 1999.

CH P 558: PHYSICAL CHEMISTRY PRACTICALS- IV

Teaching Hours: 6 Hrs per week

A. Kinetics and Catalysis (Any Four Experiments are to be carried out)

Determination of reaction order and activation parameters, study of acidity/salt/solvent/catalytic effects on reaction rates of any FIVE of the reactions listed below.

1. Acid catalyzed hydrolysis of methyl acetate.
2. Saponification of ethyl acetate by conductivity method.
3. Decomposition of benzenediazonium chloride.
4. Reaction between potassium persulphate and potassium iodide (including the study of salt effect and catalysis by Ag^{+}, Fe^{2+} and Cu^{2+} ions).
5. Decomposition of diacetone alcohol by NaOH& Hydrolysis of t-butylchloride.
6. (i) Reaction between iodine and acetone, and (ii) iodination of aniline.
7. Reaction between hydrogen peroxide and HI.
8. Decomposition of H_2O_2 (including the study of catalytic effect).
9. Reaction between Chromic acid and oxalic acid.
10. Reduction of aqueous solution of ferric chloride by stannous chloride.
11. Determination of the mechanism of the oxidation of an organic compound from kinetic data.
12. Determination of catalytic constant of an acid.
13. Determination of effect of surface area of catalyst and temperature on the kinetics of Metal-acid reaction.
14. Determination of dissociation of trichloroacetic acid-Kinetic method.
15. Determination of equilibrium constant for homogeneous equilibria and determining the concentration of a given solution.
16. Determine the molecular formula of copper-ammonia complex by the partition coefficient method.
17. Alkaline hydrolysis of ethyl acetate volumetrically.
18. Effect of reaction surface area of catalyst and temperature, concentration on the kinetics of metal-acid

B. Polymer Chemistry (Any Two experiments are to be carried out)

1. Determination of molecular weight and size parameters of polymers by viscometry.
2. Determination of sequences in polyvinylalcohol by viscometry.
3. Determination of molecular weight of a polymer by turbidimetry.
4. Preparation of Polymethylmethacrylate by suspension polymerization / polystyrene by free radical polymerization / Nylon by interfacial polymerization / Polyacrylamide by solution polymerisation method / polyvinylalcohol from polyvinylacetate / Phenol formaldehyde/ urea formaldehyde resins / thin films of polymers.

C. Thermodynamics Experiments (Any Four experiments to be carried out)

1. Determination of activities of an electrolyte and non-electrolyte by cryoscopy.
2. Determination of partial molar volumes of (a) Salts-water and (b) alcohol-water (methanol & ethanol) systems by density method.
3. Study of complex formation between mercury and potassium halides by cryoscopy.
4. Determination of specific heat of liquids and solutions by calorimetry.
5. Determination of stepwise neutralisation of acids.
6. Determination of heat of solution of KNO3 in water, integral heat of dilution of H2SO4 and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
7. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
8. Determination of vant Hoff's factor for benzoic and acetic acid mixtures in benzene.
9. Velocity of sound in liquid-ultrasonic interferometry

D. Spectroscopic Experiments (Any Two experiments to be carried out)

1. Kinetics of oxidation of alcohol by potassium dichromate – spectrophotometrically.
2.Simultaneous determination of Manganese and chromium in a solution of dichromate and Permanganate mixture.
3. Determination of pKa of an indicator.
4. Spectroscopic investigation of partition coefficient of iodine between H_2O and $CHCl_3$.
5. Study of the effect of ionic strength on the pH of the given acid with the help of Indicators using buffer solution by colorimetric method.

E. Radiochemistry Experiments (At least Two experiments to be carried out)

1. Study of (a) Characteristic plateau, (b) Geometry effects and Statistics of G.M counter
2. Determination of (a) Dead time by single source & double source method. (b) Emax of □-

source (c) Back scattering of □and (d) □energy emitted by C-14.

3. Verification of the inverse square law.

4. Determination of half life of radionuclides.

4. Determination of Linear and mass attenuation coefficient.

5. Preparation of Fricke and Ceric sulphate dosimeters & calculation of G-value & dose rate.

6. Study of isotope dilution analysis;

8. Radiochemical Determination of I-131 in sea water.

7. Determination of β-particle range and, axmum energy (by half thickness method).

8. Percentage purity of copper sulphate by electrogravimetric method.

F. Adsorption

1. Synthesis of a suitable adsorbent (e.g activated carbon) and its characterization by surface area, iodine value, total acidity and pzc

2. Adsorption of monovalent and divalent metal ions and their mixture on a suitable adsorbent. Applicability of Freundlich and Langmuir Adsorption isotherms.

3. Adsorption characteristics of pollutants such as dyes and/or surfactants on a suitable adsorbent.

4. Investigation of adsorption charactrisitics of different dyes (cationic andanionic) on two different types of activated carbons.

References:

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

CH P 559: PROJECT WORK AND DESSERTATION

Teaching Hours: 8 Hrs per week

References:

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

VALUE ADDED COURSES

CERTIFICATE COURSE ON APPLICATIONS OF CHEMISTRY SOFTWARE AND RESEARCH METHODOLOGY

Total Teaching Hours: 40 Hrs

Unit I: 20 Hrs

Computer applications for chemists

Chemsketch 6 Hrs

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

Origin Graphing and Analysis for Chemistry: 4 Hrs

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

Microsoft Excel® 6 Hrs

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

Mercury program for visualizing crystal structures 4 Hrs

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

Unit II 20 Hrs

Research, Industrial pharmacy and Safety

Fundamentals of research: 6 Hrs

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

Industrial pharmacy: 10 Hrs

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

Chemical and hazardous materials safety. 4 Hrs

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

References

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