

**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 1<sup>st</sup> August, 2016**  
**Academic Council meeting, held on 5 - 10 - 2016**

## **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 1<sup>st</sup> August 2016, 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 2016-17.

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**.

## **OBJECTIVES OF THE SYLLABUS**

The revised syllabus is designed to provide a flexible structure within which students can choose the topic of their interest in addition to a specific knowledge. The syllabus takes into account the requirements for higher education to improve the quality of education and student competency level on par with national and international institutions. The syllabus is structured in such a way so as to ensure that students become aware of the practical applications of scientific knowledge to build careers in the scientific field.

**The syllabus aims to enable students to:**

- Prepare the students for employment and for further studies by acquiring the knowledge and understanding of chemical principles.
- Appreciate, understand and use the scientific method in the solving of problems. Develop the ability to disseminate chemical information effectively.
- Acquire good laboratory skills and practice safety measures when using equipment and chemicals as well as the safe disposal of chemical waste.
- Apply chemical knowledge to everyday life situations and develop inquisitiveness in order to continue the search for new ways in which the resources of our environment can be used in a sustainable way.

## 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
<b>Total</b>	<b>36</b>	<b>18</b>	<b>6*</b>	<b>15</b>	<b>12</b>	<b>4</b>	<b>91</b>

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)

## DISTRIBUTION OF COURSE & CREDITS

### 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	Spectroscopy Methods of Analysis Environmental Chemistry <b>(Any two)</b>	3	30 + 70	3	3	3x2=6
CH S 405		3	30 + 70	3		
CH S 406		3	30 + 70	3		
CH P 407	Inorganic Chemistry Practicals-I	--	30 + 70	4	4	2
CH P 408	Organic Chemistry Practical-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 <b>or</b> CH S 455	Spectroscopy and Analytical Techniques <b>or</b> Chemistry of Bio-molecules	3  3	30 + 70  30 + 70	3  3	3	3x1=3
CH E 456 <b>or</b> CH E 457	Chemistry of Life <b>or</b> Environmental Chemistry	3  3	30 + 70  30 + 70	3  3	3	3x1=3
CH P 458	Inorganic Chemistry Practicals-II	--	30 + 70	4	4	2
CH P 459	Organic Chemistry Practical- II	--	30 + 70	4	4	2
CH P 460	Physical Chemistry Practical- 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 <b>or</b> CH S 505	Chemistry of Synthetic Drugs <b>or</b> Bioorganic Chemistry	3  3	30 + 70  30 + 70	3  3	3	3x1=3
CH E 506 <b>or</b> CH E 507	Medicines in Daily Life <b>or</b> Chemistry of Materials	3	30 + 70	3  3	3	3x1=3
CH P 508	Inorganic Chemistry Practicals-III	--	30 + 70	6	6	3

CH P 509	Organic Chemistry Practicals-III	--	30 + 70	6	6	3
CH P 510	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	Molecular Rearrangements & Heterocyclic Chemistry	3	30 + 70	3	3	3
CH H 553	Polymers & Photochemistry	3	30 + 70	3	3	3
CH S 554	Nuclear, Surface & Nano	3	30 + 70	3		
CH S 555	Chemistry Organometallic	3	30 + 70	3	3	3x2=6
CH S 556	Chemistry Electrochemistry and Reaction Dynamics  (Any two)	3	30 + 70	3		
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 hard core 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 all **nine** sub-divisions from **Question No.1** in **Part A** & any **four** questions from **Part B**.

### **PART - A**

**Answer all**

2x09= 18

1. a.

b. UNIT Ic.



d.

e. UNIT II f.

g.

h. UNIT III i.

**PART - B**

**Answer any 4 questions.**

13x4 = 52

2. a.

b. UNIT I c.

}

3. a

b. UNIT I c.

}

4. a.

b. UNIT II c.

}

5. a.

b. UNIT II c.

}

6. a.

b. UNIT III c.

7. a.

b. UNIT III c.

}

## **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.

## CH H 401: INORGANIC CHEMISTRY

### 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

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

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

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

### UNIT-III

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

## CH H 402: ORGANIC CHEMISTRY

### UNIT-I

15Hrs

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

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

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

### UNIT-II

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

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

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

**UNIT-III: Stereochemistry****15 Hrs**

**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, Pseudoasymmetric 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, Curtin-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus.

11 hrs

**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.

4 hrs

**References:**

1. Organic Chemistry: P.Y. Bruice, Pearson Education Pvt. Ltd., New Delhi, 2002.
2. Stereochemistry, Conformation and Mechanism: P.S. Kalsi, Wiley Eastern, New Delhi, 1993.
3. Stereochemistry of Carbon Compounds: E.L. Eliel, Tata McGraw Hill, New Delhi, 1994.
4. Advanced Organic Chemistry-Reactions, mechanisms & structure: J. March, Wiley, NY, 2000.
5. Organic Chemistry Vol. -1, 2 & 3: Mukherji, Singh and Kapoor, Wiley Eastern, 1994.
6. A guide book of mechanisms in Organic Chemistry: P. Sykes, Orient- Longman, 1985.
7. Organic Chemistry: R.T. Morrison and R.N. Boyd, Prentice Hall, New Delhi, 1994.
8. Organic Chemistry.: S.H. Pine et al., 4<sup>th</sup> Edn, McGraw-Hill, London, 1987.
9. Advanced Organic Chemistry: R.A. Carey and R.J. Sundberg, Plenum, New York, 1990.
10. Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11. A Text book of Organic Chemistry: Tewari, Vishnoi and Mehrotra, Vikas, New Delhi, 1998.
12. A Text book of Organic Chemistry: R.K. Bansal, 3<sup>rd</sup> Edn., New Age, New Delhi, 1997.
13. Organic Chemistry: F.A. Carey, 3<sup>rd</sup> Edn, Tata McGraw Hill, New Delhi, 1996.
14. Organic Chemistry: H. Pine Hendrickson, Cram and Hammond, Mc Graw Hill, 1987.
15. Organic Chemistry: I.L. Finar, ELBS Longmann, Vol. I, 1984.
16. Advanced Organic Chemistry: Dr. Jagdamba Singh, Pragati Prakashan, 2014.

## CH H 403: PHYSICAL CHEMISTRY

### UNIT-I: Chemical Thermodynamics

15 Hrs

Concept of Entropy, Physical significance, entropy change in an ideal gas. Variation of entropy with Temperature, Pressure and Volume. Entropy change in reversible and irreversible processes. Free energy, Helmholtz's and Gibbs free energies, Gibbs – Helmholtz equation and its applications. Maxwell's relations and significance. Thermodynamic equations of state. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.

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

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

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

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

### UNIT- II: Chemical Kinetics

15 Hrs

**Composite reactions:** An overview of basic kinetic concepts and analysis of kinetic results - rates of simple and composite chemical reactions (reversible, parallel and consecutive first order reactions), Chain reactions (hydrogen-halogen reactions with comparison). Transition state theory and its applications. Auto catalytic reactions (Hydrogen-Oxygen reaction). Reactivity - selectivity principles (Hammond's postulate & Curtin-Hammet principle).

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

**Fast reactions-**Introduction, Study of fast reactions by-flow, relaxation, molecular beam, and spectroscopic and analytical methods



### UNIT-III: Quantum Chemistry

15 Hrs

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  $r, \theta, \phi$  equations and their solutions), Angular momenta (commutations, relations, operators).

### References

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

## CH S 404: SPECTROSCOPY

### UNIT-I

12 Hrs

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

**Vibration Spectroscopy:** Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO<sub>2</sub>& H<sub>2</sub>O). Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches.

### 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  $\lambda_{\max}$  of organic compounds. Woodward-Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Empirical rules to calculate  $\lambda_{\max}$ . Application of UV spectroscopy in the structural study of organic molecules.

### UNIT-III: NMR Spectroscopy

12 Hrs

**$^1\text{H}$  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  $^1\text{H}$  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.

**$^{13}\text{C}$  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, 5<sup>th</sup> Edn., Tata McGraw Hill, 2014.
2. Organic Spectroscopy: W. Kemp, 3<sup>rd</sup> Edn., Pargrave Publishers, New York, 1991.
3. Introduction to Spectroscopy: Donald L. Pavia, Gary M. Lampman, G. Cerge S. Kriz, 5<sup>th</sup> Edn., Cengage Learning, 2014.
4. Spectrometric Identification of Organic Compounds: Robert M. Silverstein, Francis X. Webster & David J. Kiemle, 8<sup>th</sup> Edn., Wiley, 2014.
5. Modern spectroscopy: J. Michael Hollas, 4<sup>th</sup> Edn., John Wiley and sons Ltd., 2004.
6. Spectroscopy of Organic Compounds: P. S. Kalsi, 3<sup>rd</sup> Edn., New Age, New Delhi, 2000.

## CH S 405: METHODS OF ANALYSIS

### UNIT-I

12 Hrs

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

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

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

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

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

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

### UNIT-II: Diffraction Techniques

12 Hrs

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

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

### **UNIT-III: Thermoanalytical Techniques**

**12Hrs**

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, 3<sup>rd</sup> Edn. Saunders College Pub., 1985;
4. Instrumental Methods of Chemical Analysis: B.K. Sharma, 19<sup>th</sup> Edn., Goel, 2000.
5. Instrumental methods of chemical analysis: H. Kaur,9<sup>th</sup> Edn., Pragathi, 2013
6. Instrumental methods of chemical analysis: Gurudeep R. Chatwal and Sham K Anand, 5<sup>th</sup> 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, 7<sup>th</sup> Edn., 1988.

## CH S 406: ENVIRONMENTAL CHEMISTRY

### UNIT- I

12 Hrs

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

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

### UNIT-II

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

### UNIT-III

12 Hrs

**Toxic chemicals in the environment:** impact of toxic on enzymes, heavy metal pollution. Detergents- pollution aspects, eutrophication. Pesticides and insecticides- pollution of surface water, biochemical effects.

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

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

**References:**

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

## **CH P 407: INORGANIC CHEMISTRY PRACTICALS – I**

Qualitative Analysis of mixtures of Inorganic Salts containing 4 metal ions and 2 anions (2 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

### **References**

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



## CH P 408: ORGANIC CHEMISTRY PRACTICALS - I

### Single and two stage organic preparations

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

### References

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

## CH P 409: PHYSICAL CHEMISTRY PRACTICALS – I

Any 12 experiments are to be carried out

1. Potentiometric titration of halides in mixtures ( $\text{Cl}^-$ ,  $\text{Br}^-$  and  $\text{I}^-$ ) with silver nitrate
2. Potentiometric determination of redox potentials.
3. Potentiometric determination of dissociation constants of weak acids
4. Potentiometric and conductometric acid –base titrations in partial & non-aqueous media.
5. Conductometric titrations of displacement and precipitation reactions
6. Determination of equivalent conductances and dissociation constants of weak acids.
7. Determination of solubility of lead iodide at different T & hence molar heat of solution
8. Determination of pH of buffer solutions with a pH meter & evaluation of  $\text{pK}_a$  of acids
9. Analysis of a binary mixture and determination of molar refraction of a solid and the composition of chloroform and acetone in its azeotropic mixture by refractometry
10. Analysis of a binary mixture of two miscible liquids by viscometry and the relation between viscosity of a solution and the electrical conductivity
11. Study of variation of viscosity of a liquid with temperature
12. Determination of parachor value for  $\text{CH}_2$  group by S.T method, the composition of a solution by S.T measurement and the CMC of a soap solution by S.T measurement.
13. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode
14. Determination of degree of hydrolysis of  $\text{CH}_3\text{COONa}$  and  $\text{NH}_4\text{Cl}$ .
15. Determination of hydrolysis constant of aniline hydrochloride.
16. Verification of Nernst equation for  $\text{Ag}^+$ ,  $\text{Cu}^{2+}$  and  $\text{Zn}^{2+}$  species.
17. Determination of transport number of ions by emf method ( $\text{Ag}^+$ ,  $\text{Cd}^{2+}$ ,  $\text{NO}_3^{2-}$ ,  $\text{SO}_4^{2-}$  etc.)

## References

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

## II SEMESTER

### CH H 451: ADVANCED INORGANIC CHEMISTRY

#### UNIT- I: Symmetry and Group Theory

15Hrs

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

**Chemistry of higher boranes:** Classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of  $B_5H_9$ ,  $B_{10}H_{14}$  and  $BH_2^-$ . Carboranes and metallocarboranes.

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

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

#### UNIT-III

15 Hrs

Trends in oxidations states, stereochemistry and ionic sizes of metals; comparison of 3d, 4d and 5d series by taking Ti and Ni subgroups as examples. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and

magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

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

### References:

1. Symmetry and Spectroscopy of Molecules: K. Veera Reddy, 2<sup>nd</sup> Edn., New Age Intl Publishers, 2009
2. Group Theory in Chemistry: M.S. Gopinathan, V. Ramakrishnan, 2<sup>nd</sup> Edn., Vishal Publishing, 2007
3. Symmetry and Group theory in Chemistry: R Ameta, 1<sup>st</sup> Edn., New Age, 2013.
4. Inorganic Chemistry: J. E. Huheey, E. A. Keiter, R. L. Keiter & O. K. Medhi, 4<sup>th</sup> Edn., Pearson Education, 2013.
5. Inorganic Chemistry: Shriver, Atkins and Langford, 5<sup>th</sup> Edn., OUP, 2010.
6. Concise Inorganic Chemistry: J. D. Lee, 5<sup>th</sup> Edn., Blackwell Science, 2014.
7. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3<sup>rd</sup> Edn., Wiley, 2007.
8. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2<sup>nd</sup> Edn., Pearson Prentice Hall, 2005
9. Inorganic Chemistry – A Unified Approach: W. W. Porterfield, Elsevier, 2<sup>nd</sup> Edn., 2005.
10. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, 6<sup>th</sup> Edn., Wiley, 2014.
11. Advanced Inorganic Chemistry: Satya Prakash, G. D. Tuli, S. K. Basu, R. D. Madan, Vol. II, 4<sup>th</sup> Edn., S. Chand, 2014.
12. Chemistry of the Elements: N. N. Greenwood and A. Earnshaw, 2<sup>nd</sup> Edition, Pergamon Press, 1997.
13. Principles of Inorganic Chemistry: B. R. Puri, L. R. Sharma, K. C. Kalia, 31<sup>st</sup> Edn., Vishal Publishing, 2013.

## CH H 452: ADVANCED ORGANIC CHEMISTRY

### 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 Vilsmeier-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. Reformatsky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions.

### 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: Chemistry of Heterocyclic Compounds**

**15Hrs**

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

#### **References:**

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

## CH H 453: ADVANCED PHYSICAL CHEMISTRY

### Unit I: Statistical and Irreversible thermodynamics

15Hrs

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

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

### UNIT-II: Electrochemistry

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

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

### UNIT-III: Quantum Chemistry-II

15 Hrs

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, 5<sup>th</sup> Edn., McGraw Hill, Int. St. 2008.
2. Atkin's Physical Chemistry: Peter Atkins, Julio De Paula, 9<sup>th</sup> Edn., OUP, 2011.
3. Thermodynamics for Chemists: S. Glasstone, 8<sup>th</sup> Edn., East-west, 2007.
4. Thermodynamics: Rajaram, Kuriocose, 4<sup>th</sup> Edn., East-West, 2006.
5. Principles of Physical Chemistry: Puri, Sharma, Pathania, 46<sup>th</sup> Edn., Vishal Publishing, 2013.
6. Advanced Physical Chemistry: Gurudeep Raj, 35<sup>th</sup> 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, 2<sup>nd</sup> Edn., Plenum, New York, 1998.
10. Instrumental Methods of Chemical Analysis, Kudesia Sawhney, Pragati Prakasha (Meerut).
11. Introductory Quantum Chemistry: A. K. Chandra, 4<sup>th</sup> Edn., Tata McGraw Hill, 2009.
12. Quantum Chemistry: Ira N. Levine, 7<sup>th</sup> Edn., Prentice Hall, 2013.
13. Quantum Chemistry: R. K. Prasad, 4<sup>th</sup> Edn., New Age International Publications, 2012.
14. Quantum Chemistry: Donald Allan McQuarrie, 5<sup>th</sup> Edn., University Science Books, 2013.

## CH S 454: SPECTROSCOPY AND ANALYTICAL TECHNIQUES

### 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  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds,  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds( nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

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

### UNIT – II

12 Hrs

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

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

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

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

### UNIT-III: Mass Spectrometry

12 Hrs

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

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

#### References:

1. H.Wiliard, L.L.Merrit and J.J.Dean, Instrumental methods of analysis,(7<sup>th</sup> 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-3<sup>rd</sup> Ed.-W.Kemp (Pgrave Publishers, New York), 1991.
5. Introduction to spectroscopy(3<sup>rd</sup> 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 (4<sup>th</sup> Ed.) – J. Michael Hollas, John Wiley and sons Ltd. Chichester, West sussex, 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

### UNIT I

12 Hrs

**Cell Structure and Functions:** Structure of prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of animal and plant cells. Overview of metabolic processes – catabolism and anabolism. ATP- the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems.

**Lipids:** Fatty acids, essential fatty acids, structure and function of triacylglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

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

### Unit II: Amino acids, Nucleic acids and Enzymes

12Hrs

**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. General methods of synthesis of amino acids 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,  $\alpha$ - Carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of  $\alpha$ -amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of carboxylic acids, esters and alcohols- Transesterification. Enzymatic synthesis of  $\alpha$ -amino acids and peptides.

### Unit III: Carbohydrates

12 Hrs

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

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

**References:**

1. Principles of Biochemistry – A L Lehninger, Worth Publishers.
2. Nelson & Cox., Lehninger's Principles of Biochemistry.
3. Harper, Harper's Illustrated Biochemistry
4. Hermann Dugas, Bioorganic Chemistry.
5. J. L. Jain, Fundamentals of Biochemistry, S. Vhand & Company Ltd.
6. Amino acids and Peptides- G. C. barret and D T Elmore (Cambridge university press) 1998.
7. The Carbohydrates Vol. IA I B IIA and IIB – W. Pigman and D. Horton (Academic Press) 1970.
8. Bioorganic chemistry - A chemical approach to enzyme action - Herman Dugas and Christopher Penney.
9. Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.

**Open Elective papers**  
**CH E 456: CHEMISTRY OF LIFE**

**UNIT- I: Cosmetics, Perfumery, Fats, Oils, Soaps and Detergents** **12Hrs**

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

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

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

**UNIT- II: Food and its nutritional aspects** **12Hrs**

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

**UNIT -III: Dyes and Agrochemicals** **12 Hrs**

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

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

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

**References:**

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

## CH E 457: ENVIRONMENTAL CHEMISTRY

### UNIT- I

12 Hrs

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

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

### UNIT-II

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

### UNIT-III

12 Hrs

**Toxic chemicals in the environment:** impact of toxic on enzymes, heavy metal pollution. Detergents- pollution aspects, eutrophication. Pesticides and insecticides- pollution of surface water, biochemical effects.



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

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

**References:**

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

## CH P 458: INORGANIC CHEMISTRY PRACTICALS – II

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  $\text{Ce}^{4+}$ .
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. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
7. Hardness of water
8. Analysis of Halide Mixture - Iodide by  $\text{KIO}_3$  and total halide by gravimetrically.
9. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
10. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
11. Statistical Analysis of Data.

### Reference:

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

## **CH P 459: ORGANIC CHEMISTRY PRACTICALS - II**

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

### **References:**

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

## **CH P 460: PHYSICAL CHEMISTRY PRACTICALS - II**

**At least 12 experiments are to be carried out**

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances using water and benzene as solvents.
2. Detn.of degree of dissociation & Vant Hoff factor of an electrolyte by cryoscopic method.
3. Heat of solution of substances by solubility method.
4. Phase diagram of two component systems by thermal analysis.
5. Kinetics of acid catalysed hydrolysis of methyl acetate and determination of (a) order and rate constant, (b) Relative strength of two acids and c ) Energy of activation.
6. First and second order kinetics of reaction between potassium persulphate and KI.
7. Kinetics of ( a) inversion of cane sugar, (b)sodium formate–iodine reaction .
8. Determination of heat of neutralisation, integral and differential heat of solution calorimetrically. Thermometric titration of an acid with a base.

9. Detn.of association constants carboxylic acids in organic solvents by distribution method.
10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.
12. To study the adsorption of iodine on charcoal from alcoholic solution.
13. To study the effects of gelatin solution on the precipitation values.
14. To compare the cleaning powers of two samples of detergents.

**References:**

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

**THIRD SEMESTER**  
**CH H 501: COORDINATION CHEMISTRY**

**UNIT-I**

**15 Hrs**

Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, Jahn-Teller effect.

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

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

**UNIT-II**

**15 Hrs**

**Spectral and Magnetic properties of complexes:** Term symbols for  $d^n$  ions, spectroscopic ground states, selection rules, nature of spectral bands- band shapes, band intensities, band widths, spin-orbit coupling, vibrational structures.

Orgel diagrams, Tanabe-Sugano diagrams, interpretation of spectra of octahedral, distorted octahedral, tetrahedral and square planar complexes. Charge transfer bands – origin, types, and characteristics. Photochemistry of metal complexes- photosubstitution and photoredox reactions, ligand photoredox reactions, photoreactions and solar energy conversion.

Type of magnetic behaviour, orbital contribution, spin orbit coupling, measurement of magnetic susceptibility–Gouy and Faraday methods, diamagnetic corrections, ferro- and antiferromagnetic coupling, spin cross-over systems.

**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, 4<sup>th</sup> Edn., Pearson Education, 2013.
2. Inorganic Chemistry: Shriver, Atkins and Langford, 5<sup>th</sup> Edn., OUP, 2010.
3. Concise Inorganic Chemistry: J. D. Lee, 5<sup>th</sup> Edn., Blackwell Science, 2014.
4. Concepts & Models of Inorganic Chemistry: B. E. Douglas, D. McDaniel & A. Alexander, 3<sup>rd</sup> Edn., Wiley, 2007.
5. Inorganic Chemistry: Catherine E. Housecroft and Alan G Sharpe, 2<sup>nd</sup> 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.
9. Elements of Magnetochemistry: R. L. Dutta and A. Syamal, Affiliated east-West, 1993.
10. Concise Coordination Chemistry: R. Gopalan and V. Ramalingam, Vikas Publishing, 2014.

## CH H 502: REACTION MECHANISMS & SYNTHETIC METHODS

### UNIT-I: Organic Name reactions

15 Hrs

Reactions, Mechanisms and synthetic uses of the following: Stolbe condensation, Darzen condensation, Gattermann-Koch reaction, Cannizzaro reaction, Chichibabin reaction, Benzoin condensation, Claisen-Schmidt condensation, Claisen reaction, Simon-Smith reaction, Stork Enamine reactions, Sharpless asymmetric epoxidation, Hofmann-Löffler-Freytag reaction, Suzuki coupling, Woodward and Prevost Hydroxylation, Bucherer reaction, Ullmann reaction. Wittig reaction-Mitsunobu reaction.

### UNIT-II: Pericyclic Reactions:

15 Hrs

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl systems. Classifications of Pericyclic reactions. Woodward-Hoffmann correlation diagram and FMO approach.

**Electrocyclic Reactions:** Introduction, Con- rotatory and dis-rotatory Process,  $4n$  and  $4n+2$  systems. Reactions of cations and anions, formation and cyclisation of Dipolar molecules.

**Cycloaddition reaction:** Suprafacial and Antrafacial addition,  $4n$  and  $4n+2$  systems, 1,3-dipolar cyclo additions.

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

### UNIT-III: Oxidation and Reduction Reaction

15Hrs

**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.

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

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

Metal hydride reduction: Reduction with  $\text{LiAlH}_4$  &  $\text{NaBH}_4$ , Stereo chemistry of reduction & other functional groups, Functional group transformation during reduction, Reduction with diborane and related reactions.

Dissolving Metal Reductions: Mechanisms of reduction of conjugated system and carbonyl compounds, Bimolecular reductions of esters, Birch reduction, 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. Favalaro, 2<sup>nd</sup> Edn., John Wiley and sons, Inc., Hoboken, New Jersey, 2005.
2. Named Organic Reactions: Thomas Laue and Andreas Plagens, 2<sup>nd</sup> Edn., John Wiley and sons Ltd. Chichester, West susex, England.
3. Named Reactions: Jie Jack Li, 3<sup>rd</sup> 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: 6<sup>th</sup> 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, 4<sup>th</sup> 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, 3<sup>rd</sup> Ed, New age International publishers, 2013.
9. Modern Organic Reactions: H. O. House, W. A. Benjamin, 1972
10. Organic Synthesis: R. E. Ireland, Prentice Hall India, 1969.
11. Modern Methods of Organic Synthesis: N. Carruthers and Iain Coldham, Cambridge Uni., 2004.
12. Modern Reduction Methods: P. G. Anderson and I. J. Munslow, Wiley-VCH, 2008.

## CH H 503: SOLID STATE CHEMISTRY

### 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  $\text{UO}_2$ ,  $\text{FeO}$  and  $\text{TiO}$ .

**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.

### 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-  $\beta$ -alumina,  $\text{AgI}$ , 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, 2<sup>nd</sup> Edn., New Age International, 2010.
2. Principles of the solid state: H.V.Keer, 1<sup>st</sup> Edn., Wiley Eastern , 1993.
3. Solid state chemistry and its applications: Anthony R. West, Wiley, 1984.
4. L.Smart and E. Moore, Solid State Chemistry –An Introduction (Chapman &Hall)1992.
5. L. Azaroff, An Introduction to Solids ( Mc Graw Hill).
6. M. M. Woolfson, An Introduction to X-ray Crystallography, Vikas, New Delhi (1980).
7. C. Kittel, Introduction to Solid State Physics, Wiley Eastern Ltd., New Delhi (1987)
8. V. Raghavan, Material science and Engineering (3<sup>rd</sup> Ed), (Prentice Hall India)1993.
9. Thermotropic Liquid Crystals, Ed. G.W. Gray, Wiley.
10. S.Chandrasekhar, Liquid Crystals, Cambridge University Press (2<sup>nd</sup> ed), 1994.

## CH S 504: CHEMISTRY OF SYNTHETIC DRUGS

### UNIT-I

12 Hrs

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

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

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

### UNIT-II

12 Hrs

**Antibiotics:** Mechanism of action of following antibiotics, Penicilin- Stereochemistry, Synthesis of Penicillin G, chemical degradation and bacterial resistance. Cephalosporians- Nomenclature, Degradation and B-lactumase resistance. Tetracyclins-SAR studies, Streptomycin- SAR studies, Chloramphenicol- SAR studies

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

**Antiarrhythmic agents-** Introduction, Mechanism of action, Synthesis of Verapamil

**Antihypertensive agents-** Introduction, Mechanism of action, Synthesis of Clonidine and

Hydralazine derivatives. **Hypoglycemic agents-** Introduction, Mechanism of action, Synthesis of Tolbutamide and Tolazamide. **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, Chloradiazepoxide, Diazepam, and Phenobarbital. **Anticonvulsant:** Synthesis of Phenytoin sodium, Trimethadione and Carbamazepine. **CNS stimulants:** Introduction and classification. Synthesis and mechanism of action of Caffeine, Nikethamide, Phetermine, Methylphenidate. **Antihistaminic agents:** Mechanism of action, Synthesis of Diphenhydramine HCl, 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 (Wiley-Eastern , New Delhi)1993.
2. Medicinal and Pharmaceutical Chemistry–H. Singh & V. K. Kapoor (Vallabh Prakashan, New Delhi)1996. Burger's Medicinal Chemistry Series – 7 volumes.
3. Medicinal-Chemistry of Anticancer-Drugs- Carmen Avendano & J.C Menedez (Elsevier B.V-2008)
4. General Analgetics- Daniel Lednicer (John Wiley & Sons Inc 1982)
5. The organic chemistry of drug synthesis Vol III- Daniel Lednicer (John Wiley & Sons Inc 1984)
6. Medicinal Chemistry, a molecular & biochemical approach 3rd ed- Thomas Nogrady & Donald F Weaver (Oxford University press- 2005)

## CH S 505: BIOORGANIC CHEMISTRY

### UNIT-I

12 Hrs

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

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

### UNIT-II

12 Hrs

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

### UNIT-III

12 Hrs

**Vitamins:** Introduction, Classification and Nomenclature-Source and Deficiency diseases- Biological, functions of Vitamins- Study of the following Vitamins: Vitamin A<sub>1</sub> & A<sub>2</sub>, Vitamin B<sub>6</sub> and B<sub>12</sub>, Vitamin C, Vitamin K<sub>1</sub> and K<sub>2</sub>, Pantothenic acid, folic acid.

Lipids: Introduction, classification of lipids, synthesis of fatty acids. Compound lipids- Phospholipids, Glycosphingo lipids and derived lipids.

**References :-**

1. Nelson & Cox., Lehninger's Principles of Biochemistry.
2. Harper, Harper's Illustrated Biochemistry
3. Hermann Dugas, Bioorganic Chemistry.
4. J. L. Jain, Fundamentals of Biochemistry Vol. I & II, S. Vhand & Company Ltd.
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.

## **CH E 506: MEDICINES IN DAILY LIFE**

### **UNIT-I**

**12 Hrs**

Introduction to drugs, chemotherapy, pharmacokinetics and pharmacodynamics, metabolites and antimetabolites. Prodrugs and analogs, agonists and antagonists. Concept of drug receptor, generic drugs. Introduction to common drugs used and their mode of action, classes of drugs, their role in curing the diseases, Introduction to trace elements in biological system, Biological classification of trace elements, essential trace elements. The trace elements in human enzyme system-copper, iron zinc, cobalt, manganese. Clinical Significance of Essential Trace Elements, diseases due to metal deficiency.

### **UNIT-II: Synthetic drugs**

**12 Hrs**

Introduction to medicines used in daily life-Antipyretics-Aspirin, analgesics-paracetamol and anti-inflammatory -Ibuprofen. Antibiotics -Amoxicillin, Cefexime and Streptomycin. Antidiabetics-Insulin and oral hypoglycemic agents. Antihistamines -Methapyrilene, Chlorpheniramine Antineoplastic agents –Mercaptopurine, Fluouracil, Cis-platin and uracil mustards. Anti-virals-Acyclovir, Amantadine. Cardiovascular drugs- Amyl nitrite, sobitite, Guanidine, Methyldopa. Local anti-infective drugs-Sulfonamides, Ciprofloxacin, linezolid, Isoniazid, Chloroquin and primaquin. Natural Psychoactive drugs- the chemotherapy of the mind- Phenobarbital, phenytoin, barbiturates, thiopental sodium and caffeine.

### **UNIT-III: Ayurvedic medicines**

**12 Hrs**

Introduction, classification, identification of biological activity of plants, plant products, bhasmas-formulations-method of formulations and analysis of active ingredient. Medicinal plants-survey of medicinal plants, identification of their occurrence, collection, method of storage, different techniques of extraction of the constituents. Photochemical screening methods, semi purifications for active constituents. Isolation and identification of active molecules from medicinal plants. Chromatographic methods adopted for purification of active ingredients.



**References:**

1. Medicinal Chemistry-Ashutosh Kar (Wiley-Eastern , New Delhi)1993.
2. Medicinal and Pharmaceutical Chemistry–H. Singh & V. K. Kapoor (Vallabh Prakashan, New Delhi)1996. Burger’s Medicinal Chemistry Series – 7 volumes.
3. The organic chemistry of drug synthesis Vol III- Daniel Lednicer (John Wiley & Sons Inc 1984)
4. Advanced Practical Medicinal Chemistry- Ashutosh Kar (New Age International Pvt. Ltd- 2004)
5. Textbook of Organic Medicinal & Pharmaceutical Chemistry-7thEd-Wilson, Giswold & Doerge(Lippincott Company)1977.
6. Principles of Medicinal Chemistry–Vol.-1-Kadam, Mahadik and Bothara.
7. Organic Chemistry-Vol. I and II-I. L. Finar (Longman-ELBS, London)1980.
8. Chemistry of Natural products-Vol. I and II-O.P.Agarwal (Goel Gorakhpur), 1985.

## CH E 507: CHEMISTRY OF MATERIALS

### UNIT-I

12 Hrs

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

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

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

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

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

### UNIT-II

12 Hrs

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

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

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

### **UNIT-III: Polymers**

**12 Hrs**

Introduction, some basic definitions, classification of polymers. Types of polymerization, methods of polymerization, glass transition temperature, structure-property relationship, resins and plastics, moulding of plastics into articles, some commercial polymers-polyethylene, teflon, polyurethanes. Elastomers, synthetic rubbers, adhesives.

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

#### **References:**

1. B.K. Sharma: Introduction to Industrial Chemistry, Goel Publishing, Meerut -1998
2. R. V. Gadag and A. Nityananda Shetty: Engineering Chemistry, IK International Publishing House Pvt. Ltd., Bangalore - 2006.
3. R. Gopalan, D. Venkappayya and Sulochana Nagarajan: Text Book of Engineering chemistry, Vikas Publishing House Pvt. Ltd., New Delhi – 2006.
4. P. Atkins and J. de Paula: Atkin's Physical Chemistry –8<sup>th</sup> Ed., Oxford University Press, 2008.
5. J. R. Fried: Polymer Science and Technology, Prentice Hall.
6. Advanced Physical chemistry, Gurudeep R Chatwal, Goel Publishing, Meerut
7. A Text Book of Engineering Chemistry, S.S. Dara, S. Chand and Company Ltd.
8. Engineering Chemistry, M. M. Uppal, Khanna Publishers

## CH P 508: INORGANIC CHEMISTRY PRACTICALS – III

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

1. Analysis of brass – Cu gravimetrically using  $\alpha$ -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  $\text{KBrO}_3$
5. Quantitative analysis of the constituents & mixtures containing the following radicals
  - (i) Cu(II) + Fe(II) - Cu gravimetrically as  $\text{CuSCN}$  and Fe using Ce(IV).
  - (ii) Fe(II) + Ni(II) – Fe gravimetrically as  $\text{Fe}_2\text{O}_3$  and Ni using EDTA.
  - (iii) Fe(III) + Ca(II) - Fe gravimetrically as  $\text{Fe}_2\text{O}_3$  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  $\text{Mg}^{2+}/\text{Zn}^{2+}$ ,  $\text{Zn}^{2+}/\text{Cd}^{2+}$  &  $\text{Cl}^-/\text{Br}^-$ .

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

## CH P 509: ORGANIC CHEMISTRY PRACTICALS - III

### 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,  $\epsilon$ -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 510: PHYSICAL CHEMISTRY PRACTICALS – III

### A. Electrochemistry:

#### a. Conductometry

1. Determination of hydrolysis constants (aniline hydrochloride etc.).
2. Titration of a mixture of acetic acid, monochloro and trichloroacetic acids with NaOH.
3. Determination of concentrations/amounts of sulphuric acid, acetic acid and copper sulphate by conductometric titration with sodium hydroxide.
4. Determination of oxalic acid by conductometric titration with sodium hydroxide.
5. Measurements of the conductance of a weak acid, HOAc and of the strong electrolytes NaOAc, HCl and NaCl and to calculate the ionisation constant of the acid.
6. Determination of pH and pKa of a given weak acid at various dilutions.
7. Conductometric titration of the mixture of HCl and NH<sub>4</sub>Cl.
8. Determination of activity coefficient of Zinc ions in 0.002M ZnSO<sub>4</sub>.
9. Any other experiments of interest

#### b. Potentiometry

1. Determination of pK values of maleic acid/malonic and phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
2. Determination of acidic and basic dissociation constants and isoelectric point of an amino acid.
3. Determination of the potential of an electrochemical cell and mean ionic activity coefficient.
4. pH titration of (a) HCl versus NaOH, (b) CuSO<sub>4</sub> versus NaOH and (c) HOAc versus NaOH and (d) lead nitrate versus potassium chromate..
5. Determination of pKa values of functional groups in amino acids using a pH meter. Study of potential-pH diagrams.
6. Determination of activity coefficient of an electrolyte at different molalities.
7. Verification of Tafel equation of hydrogen evolution reaction.
8. Determination of pKa values of mono, di and tri-acid base.

## **B. Polymer Chemistry**

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.

## **References:**

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
2. Experiments in Physical Chemistry–James and Prichard.
3. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera(Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (Krishna's Edu. Publishers) 2011.
6. Experiments in Physical Chemistry–J.C.Ghosh ( Bharathi Bhavan)1974.
7. Practical Physical Chemistry – B. Vishwanathan & P.S. Raghavan (Viva Books) 2009



## IV SEMESTER

### CH H 551: BIOINORGANIC CHEMISTRY

#### 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 in cleavage of water.

Metalloproteins as enzymes – carboxy peptidase, carbonic anhydrase, alcohol dehydrogenase, catalases, peroxidases, cytochrome P 450, superoxide dismutase, vitamin B<sub>12</sub> 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<sup>nd</sup> Edn.) Wiley, 1988.
2. Bioinorganic Chemistry: I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, (1<sup>st</sup> 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

### UNIT-I: Synthetic Design

15 Hrs

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

**Retrosynthetic analysis:** Analysis of alcohols, carbonyl compounds cyclic and acyclic alkanes, 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: Molecular Rearrangements

15 Hrs

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 : Heterocyclic Chemistry

15 Hrs

Nomenclature of Heterocycles, Replacement and systematic nomenclature, Hantzsch-Widman

system for monocyclic, fused and bridged heterocycles. Structure, reactivity, synthesis and reaction of the following: Four membered heterocycles-Oxitanes, Azetidines and Thietanes; Five membered heterocycles- Imidazoles , Imidazolines and their benz 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. 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. Ellerl, Frank G. Favalaro, 2<sup>nd</sup> Edn., John Wiley and sons, Inc., Hoboken, New Jersey, 2005.
3. Named Organic Reactions: Thomas Laue and Andreas Plagens, 2<sup>nd</sup> 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, 3<sup>rd</sup> 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, 6<sup>th</sup> Edn., John Wiley and sons Inc. Hoboken, New Jersey, 2007.
7. Advanced Organic Chemistry: Part A &B, F.J. Carrey & R. J. Sundberg, 4<sup>th</sup> 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. Ellerl, Frank G. Favalaro, Jr, 2<sup>nd</sup> Edn., John Wiley and sons, Inc., Hoboken, New Jersey, 2005.
10. Organic Synthesis: R.E. Ireland, Prentice Hall India Pvt Ltd, New Delhi, 1975.
11. Organic Synthesis a Disconnection Approach- Stuart warren, John wiley and sons, 2007.

## **CH H 553: POLYMERS AND PHOTOCHEMISTRY**

### **UNIT-I**

**15 Hrs**

Introduction to Polymers & Techniques of Polymerisation: 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 characterisation: 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, Isomerisation and other rearrangement reactions with specific examples.

**References:**

1. Text book of Polymer Science : F.W. Billmeyer ( Wiley), 3<sup>rd</sup> 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, 3<sup>rd</sup> Edn., New Age International Bangalore, 2014.

## CH S 554: NUCLEAR, SURFACE AND NANO CHEMISTRY

### UNIT-I: Nuclear Chemistry

15 Hrs

Nuclear structure and stability: Nuclear properties - nuclear forces, mass defect and binding energy. Nuclear stability-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  $\alpha$ ,  $\beta$  and  $\gamma$  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: Surface Chemistry and Catalysis

15 Hrs

**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: Nano Chemistry**

**15 Hrs**

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. Arnikaar , 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. Cademartiri, 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

### UNIT-I

12 Hrs

Transition metal-carbon pi complexes: Preparative methods, nature of bonding, structural features of olefinic, acetylenic, allylic, butadiene, cyclobutadiene,  $\eta^5$ -cyclopentadienyl,  $\eta^6$ -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

### 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, microbial 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.

### UNIT-II

12 Hrs

**Photoelectrochemistry**: Introduction, Semiconductor electrodes, photogalvanic cells, photoelectrochemical cells, types and stability of semiconductor electrodes.

**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).

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

### UNIT-III

12 Hrs

**Complex reactions**-Mechanisms of some inorganic and organic reactions, formation and decomposition of phosgene, decomposition of  $N_2O_5$ , ozone, acetaldehyde and ethane.

**Potential energy surfaces** – Features & construction of them. Theoretical calculation of  $E_a$ . 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, protein binding and drugs, 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, 2<sup>nd</sup> 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. Ions in solution-Basic principles of chemical interactions: J. Burgeess (Chichester), 1999.
7. Chemical Kinetics: K. J. Laidler, Pearson Education, 1987.
8. The Physical Basis of Organic Chemistry: H. Maskill, Oxford University Press.
9. Physical Organic Chemistry: N.S.Isaacs, ELBS/Longman, 1988 .
10. Catalysis: J.C. Kuriacose, Macmillan India Ltd., 1991.

## CH P 557: INORGANIC CHEMISTRY PRACTICALS - IV

1. Colorimetric determination of Ti(IV) and Zr(IV)
2. Simultaneous colorimetric determination of two metal ions – Mn and Cr.
3. Flame photometric determination of Na, K, Li and Ca individually and in mixtures.
4. Electrogravimetric determination of (a) Cu-Ni alloy and (b) Pb in Type Metal.
5. Solvent extraction of Ni(II) and UO<sub>2</sub>(II).
6. Preparation of any three of the following complexes, checking the purity of the prepared samples by chemical 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<sub>3</sub>Cr(OX)<sub>3</sub>.3H<sub>2</sub>O vi) Cu(tu)<sub>3</sub>Cl vii)Zn(tu)<sub>3</sub>OSO<sub>3</sub>
7. 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-sulphosalicylic acid complex.
8. Determination of stability constants
  - a) Turner Anderson method : Fe-Tiron system,
  - b) Bejrrums's method : Cu – sulphosalicylic 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, 5<sup>th</sup> Edn., Longman, 1999.

## CH P 558: PHYSICAL CHEMISTRY PRACTICALS- IV

### A. Kinetics and Catalysis

1. 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.
2. Acid catalysed hydrolysis of methyl acetate.
3. Saponification of ethyl acetate by conductivity method.
4. Decomposition of benzenediazonium chloride.
5. Reaction between potassium persulphate and potassium iodide (including the study of salt effect and catalysis by  $\text{Ag}^+$ ,  $\text{Fe}^{2+}$  and  $\text{Cu}^{2+}$  ions).
6. Decomposition of diacetone alcohol by NaOH & Hydrolysis of t-Butylchloride.
7. (i) Reaction between iodine and acetone and (ii) iodination of aniline.
8. Reaction between hydrogen peroxide and HI.
9. Decomposition of  $\text{H}_2\text{O}_2$  (including the study of catalytic effect).
10. Reaction between Chromic acid and oxalic acid. 11. Iodine clock reactions.
11. Reduction of aqueous solution of ferric chloride by stannous chloride.

### B. Radiochemistry Experiments

1. Study of (a) Characteristic plateau, (b) Geometry effects and Statistics of G.M counter
2. Determination of (a) Dead time by double source method. (b)  $E_{\text{max}}$  of  $\beta$  - source  
(c) Back scattering of  $\beta$  and (d)  $\beta$  energy emitted by C- 14.
3. Verification of the inverse square law.
4. Determination of half life of radionuclides
5. Study of self adsorption of rays and determine the adsorption curve.
6. Preparation of Fricke and Ceric sulphate dosimeters & calculation of G-value&dose rate
7. Study of isotope dilution analysis.

### **C. Thermodynamics Experiments**

1. Determination of activities of an electrolyte and non – electrolyte by cryoscopy.
2. Study of association of benzoic acid in benzene.
3. Determination of partial molar volumes of (a) Salts – water and (b) alcohol – water (methanol & ethanol) systems by density method.
4. Study of complex formation between mercury and potassium halides by cryoscopy.
5. Determination of specific heat of liquids and solutions by calorimetry.
6. Determination of stepwise neutralisation of acids.
7. Study of phase diagram of a ternary aqueous system of potassium chloride and water.
8. Study of phase diagram of a ternary system of benzene – acetic acid – water or DMSO-water  
– benzene or ethanol – benzene – water etc.
9. Determination of heat of solution of  $\text{KNO}_3$  in water, integral heat of dilution of  $\text{H}_2\text{SO}_4$  and heat of ionization of acetic acid and ammonium hydroxide calorimetrically.
10. Cryoscopic and ebullioscopic analysis of the given mixture of urea and glucose.
11. Determination of vant Hoff's factor for benzoic and acetic acid mixtures in benzene.
12. Determination cryoscopically the pH value of 0.5 M malonic acid in water.
13. Study of adsorption of picric acid on charcoal using a calorimeter.

### **D. Spectrophotometry**

1. Determination of pKa values of indicators. 2. Determination of Hammett's acidity function.
2. Spectroscopic investigation of partition coefficient of iodine between  $\text{H}_2\text{O}$  and  $\text{CHCl}_3$ .
3. 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.

**References:**

1. Findlay's Practical Physical Chemistry: B. P. Levitt, Longman, London.
2. Experiments in Physical Chemistry: James and Prichard.
3. Experimental Physical Chemistry: Daniels et al.
4. Experimental Physical Chemistry: Das & Behera, Tata McGraw Hill, New Delhi, 1983.
5. Advanced Practical Physical Chemistry: J.D. Yadav, Krishna's Edu. Publishers, 2011.
6. Experiments in Physical Chemistry: J.C. Ghosh, Bharathi Bhavan, 1974.
7. Practical Physical Chemistry: B. Vishwanathan & P.S. Raghavan , Viva Books, 2009

**CH P 559: PROJECT WORK AND DESSERTATION**