

SOPHIA COLLEGE (AUTONOMOUS)  
AFFILIATED TO UNIVERSITY OF MUMBAI



SYLLABUS FOR M.Sc. PART I ANALYTICAL CHEMISTRY  
SEMESTER I AND II

TO BE IMPLEMENTED FROM THE ACADEMIC YEAR 2021-22

FACULTY: SCIENCE  
 COURSE: M.Sc.  
 SEMESTER I

Course Code	Title of the paper	Unit	Topic	Credits
SMSCHE101	PHYSICAL CHEMISTRY	I	Thermodynamics - I	4
		II	Quantum Chemistry – I	
		III	Chemical Dynamics – I	
		IV	Electrochemistry	
SMSCHE102	INORGANIC CHEMISTRY	I	Chemical Bonding	4
		II	Molecular Symmetry and Group Theory	
		III	Materials Chemistry and Nanomaterials	
		IV	Characterization of Coordination Compounds	
SMSCHE103	ORGANIC CHEMISTRY	I	Physical Organic Chemistry	4
		II	Nucleophilic Substitution Reactions and Aromaticity	
		III	Stereochemistry	
		IV	Oxidation and Reduction	
SMSCHE104	ANALYTICAL CHEMISTRY	I	Language and Quality in Analytical Chemistry	4
		II	Calculations based on Chemical Principles	
		III	Optical methods	
		IV	Thermal methods	
SMSCHEP101	PRACTICALS	I	Physical Chemistry	8 (2 credits for each practical)
SMSCHEP102		II	Inorganic Chemistry	
SMSCHEP103		III	Organic Chemistry	
SMSCHEP104		IV	Analytical chemistry	

FACULTY: SCIENCE  
 COURSE: M.Sc.  
 SEMESTER II

Course Code	Title of the paper	Unit	Topic	Credits
SMSCHE201	PHYSICAL CHEMISTRY	I	Thermodynamics – II	4
		II	Quantum Chemistry – II	
		III	Chemical Dynamics – II	
		IV	Solid State Chemistry and Phase Equilibria	
SMSCHE202	INORGANIC CHEMISTRY	I	Inorganic Reaction Mechanism	4
		II	Organometallic Chemistry of Transition metals	
		III	Environmental Chemistry	
		IV	Bioinorganic Chemistry	
SMSCHE203	ORGANIC CHEMISTRY	I	Alkylation and reaction of carbon nucleophiles	4
		II	Reactions and Rearrangements	
		9III	Molecular Orbital Theory	
		IV	Spectroscopy	
SMSCHE204	ANALYTICAL CHEMISTRY	I	Chromatography	4
		II	Spectrometry and Radio-Analytical methods	
		III	Surface Analytical techniques	
		IV	Electroanalytical methods	
SMSCHEP201	PRACTICALS	I	Physical Chemistry	8 (2 credits for each practical)
SMSCHEP202		II	Inorganic Chemistry	
SMSCHEP203		III	Organic Chemistry	
SMSCHEP204		IV	Analytical chemistry	

**PHYSICAL CHEMISTRY**  
**SEMESTER-I**  
**COURSE CODE: SMSCHE101**

**Learning Objectives:**

- To understand and elucidate the third law of thermodynamics and properties like absolute entropies, heat capacity, entropies of vaporization of liquids etc.
- To understand and elucidate the properties of wave function, quantum operators and application of quantum mechanics to different systems
- To understand the mechanism of some composite reactions, kinetics of polymerization reactions and theories for reaction in gas phase
- To study Debye Huckel Onsager equation, deviations from it and to understand different types of fuel cells
- To introduce terms, concepts and derivations involved in bio-electrochemistry

**Learning Outcome : The learner will be able to**

- discuss and elucidate the Third law of thermodynamics, Trouton's rule
- solve problems using the properties and relationships of thermodynamic fluids
- explain and use Quantum operators in solving numericals
- understand and explain Semenov – Hinshelwood and Thompson mechanism, RRK & RRKM theories
- elucidate Debye Huckel Onsager equation, Debye Falkenhagen effect, wein effect
- explain Bio electrochemistry concepts and derive Goldmann equation

UNIT I	THERMODYNAMICS – I	15L
Sub-units	Topics	No. of Lectures
1.1	State function and exact differentials, Joule Thomson experiment, Joule Thomson coefficient, inversion temperature, Joule Thomson coefficient in terms of Van der Waals constants.	
1.2	Third law of Thermodynamics, Entropy change for a phase transition, absolute entropies, determination of absolute entropies in terms of heat capacity, standard molar entropies and their dependence on molecular mass and molecular structure, residual entropy.	
1.3	Entropies of vaporization of liquids – Trouton's rule , Validity, deviation and application, Hildebrand's rule  [Ref 2 and 1,10,11,12 17]	
UNIT II	QUANTUM CHEMISTRY	15L
Sub-units	Topics	No. of Lectures
2.1	Classical Mechanics, failure of classical mechanics: Need for Quantum Mechanics.	
2.2	Particle waves and Schrödinger wave equation, wave functions, properties of wave functions, Normalization of wave functions, orthogonality of wave functions.	

2.3	Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, Eigen functions, Eigen values and Eigen value equation, Schrödinger wave equation as the Eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger's Time independent wave equation from Schrodinger's time dependent wave equation.	
2.4	Application of quantum mechanics to the following systems: a) Free particle, wave function and energy of a free particle. b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels. c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula.  [Ref 7, 8 and 9]	
<b>UNIT III</b>	<b>CHEMICAL DYNAMICS – I</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
3.1	<b>Composite Reactions:</b> Steady state Approximation, rate determining steps, Microscopic Reversibility and Detailed Balanced Chain reactions-chain initiation processes. Some inorganic mechanisms: formation and decomposition of phosgene, decomposition of ozone, Reaction between Hydrogen and Bromine and some general examples Organic Decompositions: Decomposition of ethane, decomposition of acetaldehyde Gas phase combustion: Reaction between hydrogen and oxygen, Semenov – Hinshelwood and Thompson mechanism, Explosion limits and factors affecting explosion limits.	
3.2	<b>Polymerization reactions:</b> Kinetics of stepwise polymerization, Calculation of degree of polymerization for stepwise reaction. Kinetics of free radical chain polymerization, Kinetic chain length and estimation of average no. of monomer units in the polymer produced by chain polymerization.	
3.3	<b>Reaction in Gas Phase:</b> Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.  [Ref. 2 and 15, 17, 18]	
<b>UNIT IV</b>	<b>ELECTROCHEMISTRY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
4.1	Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and its extension to higher concentration (derivations are expected)	
4.2	Electrolytic conductance and ionic interaction, relaxation effect. Debye-Hückel- Onsager equation (derivation expected). Validity of this equation for aqueous and non- aqueous solution, deviations from Onsager equation, Debye -Falkenhagen effect (dispersion of conductance at high frequencies), Wien effect.	

4.3	Batteries: Types of fuel cells- Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]- Principle, construction and working, application in transportation.	
4.4	<p>Bio-electrochemistry: Introduction, cells and membranes, membrane potentials, theory of membrane potentials, interfacial electron transfer in biological systems, adsorption of proteins onto metals from solution, electron transfer from modified metals to dissolved protein in solution, enzymes as electrodes, electrochemical enzyme- catalysed oxidation of styrene. Goldmann equation. (derivations are expected)</p> <p>[Ref: 14 and 16, 17, 18]</p> <p><b>(Note: Numerical and theoretical problems from each unit are expected.)</b></p>	

### REFERENCES

1. Peter Atkins and Julio de Paula, Atkin’s Physical Chemistry, 7<sup>th</sup> Edition, Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Ed., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3<sup>rd</sup> Edition, John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, Physical Chemistry, 5<sup>th</sup> Edition, Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, Physical Chemistry, 3<sup>rd</sup> Edition, Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, Textbook of Physical Chemistry, 2ndEdition., McMillan and Co. Ltd., London, 1962
7. B.K. Sen, Quantum Chemistry including Spectroscopy, Kalyani Publishers, 2003.
8. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw – Hill, 1994.
9. R.K. Prasad, QuantumChemistry, 2<sup>nd</sup> Edition, New Age International Publishers, 2000.
10. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press, New Delhi, 1964.
11. W.G. Davis, Introduction to Chemical Thermodynamics – A Non – Calculus Approach, Saunders, Philadelphia, 19772.
12. Peter A. Rock, Chemical Thermodynamics, University Science Books, Oxford University Press, 1983.
13. Ira N. Levine, Quantum Chemistry, 5<sup>th</sup> Edition, Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
14. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edition, Pearson Education Limited 2013.
15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1<sup>st</sup> Edition, 1992.
16. Bockris, John O’M., Reddy, Amulya K.N., Gamboa-Aldeco, Maria E., Modern Electrochemistry, 2A, Plenum Publishers, 1998.
17. Physical Chemistry by Gurtu and Gurtu
18. A Textbook of Physical Chemistry by K L Kapoor Vol 5, 2ndEdition

### PRACTICALS

**Course Code: SMSCEP101**

#### **Learning Objectives:**

- To train the students in handling various instruments, glassware, chemicals etc. used in various analyses
- To instruct the learner in practical knowledge on planning and performing experiments.
- To elucidate knowledge about the non-instrumental techniques

**Learning Outcomes : The learner will be able to**

- carefully handle and use various instruments used in the lab for performing experiments
- follow instructions thoroughly
- perform experiments with accuracy and perfection

**Non – Instrumental:**

1. Determine the heat of solution ( $\Delta H$ ) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperatures.
2. Investigate the reaction between acetone and iodine.
3. Study the variation in the solubility of  $\text{Ca(OH)}_2$  in presence of NaOH and hence to determine the solubility product of  $\text{Ca(OH)}_2$  at room temperature.
4. Determine the partial molal volume of Ethanol - water mixture at a given composition.

**Instrumental:**

1. Determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
2. Determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
3. Verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.
4. Determine the stability constant of the complex formed between  $\text{Fe}^{3+}$  ion and 5-sulphosalicylic acid at pH 2 and pH 3 by spectrophotometric method

**REFERENCES**

1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3<sup>rd</sup> Edition, Longman Group Ltd., 1974.
3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

**INORGANIC CHEMISTRY**  
**SEMESTER-I**  
**COURSE CODE: SMSCHE102**

**Learning objective**

- To understand wave functions for different hybridizations and bonding in diatomic and polyatomic species
- To understand construction of character tables for different point groups and applications of group theory
- To understand the methods of preparation and properties of co-ordination compounds and nano particles

**Learning outcomes**

The learner will be able to

- derive wave functions for different hybridization and plot MOT diagrams for diatomic and polyatomic species
- construct character tables for different point groups and apply of group theory to inorganic molecules
- write the methods of preparation and explain the properties of co-ordination compounds and nano particles

UNIT I	CHEMICAL BONDING	15L
Sub-units	Topics	No. of Lectures
1.1	<b>Valence Bond Theory</b> Recapitulation of hybridization, Derivation of wave functions for $sp$ , $sp^2$ , $sp^3$ orbital hybridization types considering only sigma bonding, and Critical analysis of VBT.	4L
1.2	<b>Bent's rule:</b> Structure and reactivity of compounds/ complexes	3L
1.3	<b>Molecular Orbital Theory:</b> Molecular Orbital Theory (considering $\sigma$ bonding) for - diatomic species of the first transition series - polyatomic species: electron deficient ( $B_2H_6$ ) and electron rich ( $I_3$ ) molecular species.	5L
1.4	<b>Weak forces of attraction:</b> i) Hydrogen bonding – concept, types, properties, methods of detection and importance. ii) Van der Waal's forces, ion-dipole, dipole-dipole and London forces.	3L
UNIT II	MOLECULAR SYMMETRY AND GROUP THEORY	15L
Sub-units	Topics	No. of Lectures
2.1	Symmetry criterion of optical activity, symmetry restrictions on dipole moment, elements of symmetry, A systematic procedure for symmetry classification of molecules.	3L
2.2	Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups.	3L
2.3	Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem and its application in	5L



	construction of character tables for point groups $C_{2v}$ , $C_{3v}$ and $D_{2h}$ , structure of character tables.	
<b>2.4</b>	Applications of Group Theory (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MOT, sigma bonding in $AB_n$ (Ammonia, $CH_4$ ) molecule. (b) Determination of symmetry species for translations and rotations. (c) Mulliken's notations for irreducible representations. (d) Reduction of reducible representations using reduction formula. (e) Group subgroup relationships. (f) Descent and ascent in symmetry correlation diagrams showing relationship between different groups.	<b>4L</b>
<b>UNIT III</b>	<b>MATERIALS CHEMISTRY AND NANOMATERIALS</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>3.1</b>	<b>Solid State Chemistry</b>	<b>10L</b>
<b>3.1.1</b> <b>3.1.2</b> <b>3.1.3</b>	Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones. Structures of Compounds of the type: $AB$ [nickel arsenide ( $NiAs$ )], $AB_2$ [fluorite ( $CaF_2$ ) and anti-fluorite structures, rutile ( $TiO_2$ ) structure and layer structure [cadmium chloride and iodide ( $CdCl_2$ , $CdI_2$ )]. Methods of preparation for inorganic solids: Ceramic method, precursor method, sol gel method (applications in Biosensors), microwave synthesis (discussion on principles, examples, merits and demerits are expected)	
<b>3.2</b>	<b>Nanomaterials:</b>	<b>5L</b>
<b>3.2.1</b>	Methods of preparation of nanomaterials: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett (L-B) method, Biological methods: Synthesis using microorganisms. SEM, TEM	
<b>UNIT IV</b>	<b>COORDINATION COMPOUNDS: SPECTRAL AND MAGNETIC PROPERTIES</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>4.1</b>	Methods of preparation, thermal studies, Conductivity measurements, electronic, spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods of characterisation.	<b>4L</b>
<b>4.2</b>	Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as $\Delta$ , B, C, Nephelauxetic ratio.	<b>5L</b>
<b>4.3</b>	Magnetic Properties of Coordination Complexes: Origin of magnetism, types of magnetism, Curie law, Curie-Weiss Law, 1st and 2nd Ordered Zeeman effect, quenching of orbital angular momentum by ligand fields, magnetic properties of A, E and T ground terms in complexes, spin free and spin paired equilibria, temperature dependence of magnetism.	<b>6L</b>
<b>REFERENCES</b>		

<p style="text-align: center;"><b>UNIT I</b></p>	<ol style="list-style-type: none"> <li>1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.</li> <li>2. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.</li> <li>3. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson Education Limited, 2nd Edition 2005.</li> <li>4. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure and Reactivity, 4th Ed., Harper Collins, 1993.</li> <li>5. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry, Oxford University Press, 1967.</li> <li>6. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The Benjamin Cummings Publishing Company, 1989.</li> <li>7. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.</li> <li>8. R. Sarkar, General and Inorganic Chemistry, Books &amp; Allied (P) Ltd., 2001.</li> </ol>
<p style="text-align: center;"><b>UNIT II</b></p>	<ol style="list-style-type: none"> <li>1. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley Eastern Ltd., 1989.</li> <li>2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley &amp; Sons, New York, 1996.</li> <li>3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley &amp; Sons, New York, 1998.</li> <li>4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.</li> <li>5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.</li> <li>6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.</li> </ol>
<p style="text-align: center;"><b>UNIT III</b></p>	<ol style="list-style-type: none"> <li>1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-20349635-3, Taylor &amp; Francis Group, LLC.</li> <li>2. Nanomaterials &amp; Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.</li> <li>3. Nanomaterials Chemistry, Recent Developments and New Directions C.N.R. Rao, A. Muller, and A.K. Cheetham, ISBN 978-3-527-31664-9, 2007 WILEY-VCH Verlag GmbH &amp; Co. KGaA, Weinheim.</li> <li>4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.</li> <li>5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH &amp; Co. KGaA, Weinheim, 2004.</li> <li>6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH &amp; Co. KGaA, Weinheim, 2010.</li> </ol>
<p style="text-align: center;"><b>UNIT IV</b></p>	<ol style="list-style-type: none"> <li>1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure and Reactivity, Pearson Education, 2006.</li> <li>2. D. Banerjea ,Coordination Chemistry</li> <li>3. Geary Coordination reviews</li> <li>4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver &amp; Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.</li> <li>5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999,</li> </ol>

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### PRACTICALS

Course Code: SMSCHEP102

#### Learning objectives

- To train students to prepare simple nano particle
- To use classical methods to estimate percentage of metal in alloys/ores
- To use instrumental methods of analysis for estimation of metal ions and inorganic compounds

#### Learning outcomes

The learner will be able to

- Prepare simple nanoparticles and characterize them using absorption methods
- Identify and use simple classical methods and calculate percentage composition of metals in alloys/ores
- Estimate metal ions and inorganic compounds using instrumental methods

(Any seven)

#### I] Analysis of Ores and Alloys/ preparation of compounds

- 1) Analysis of Devarda's alloy
- 2) Analysis of Cu – Ni alloy
- 3) Analysis of Solder alloy
- 4) Analysis of Limestone.
- 5) Analysis of hematite ore.
- 6) Synthesis of Fe<sub>2</sub>O<sub>3</sub> nanoparticles by sol-gel/ coprecipitation/ hydrothermal method (any one)
- 7) Synthesis of ZnO from zinc oxalate - precursor method and determine band gap by absorption spectroscopy

#### II] Instrumentation:

- 1) Estimation of Copper using Iodometric method Potentiometrically.
- 2) Estimation of boric acid conductometrically.

### REFERENCES

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1stEdition., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By:Dr Deepak Pant

### ORGANIC CHEMISTRY

#### SEMESTER-I

COURSE CODE: SMSCHE103

#### Learning Objectives

- Understand the mechanisms of reactions and the effect of various parameters on the rate of the reaction, stereochemistry and selectivity of the product.
- Understand the criteria of aromaticity, thermochemical and magnetic criteria for aromatic compounds of benzenoid and non-benzenoid structures.
- Learn to draw the Frost Musulin Diagrams for various compounds.
- Understand the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers.

- Understand the principles of axial and planar chirality.
- Understand the configurational descriptors to allenes, alkyldiene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
- Understand the concepts of topicity, criteria for enantiotopic and diastereotopic ligands and faces and identify them in a stereoisomer.
- Understand how to assign configurational descriptors for enantiotopic and diastereotopic faces
- Understand the concept of prochirality and predicting them in a molecule

### Learning Outcomes

- Students are expected to predict a mechanism, rate of the reaction, stereochemical outcome of reactions.
- Knowledge of the parameters and evidence used to predict the mechanism of the reaction.
- Understanding the factors affecting acidity and basicity and involvement of acids and bases in determining the mechanism.
- Classify the compounds based on criteria of aromaticity, analyse the thermochemical and magnetic data for aromatic compounds of benzenoid and non-benzenoid structures
- Predicting the aromaticity in cyclic compounds based on Frost Musulin diagram
- Predicting the stereochemical concepts in molecules with constitutionally symmetric and asymmetric stereoisomers.
- Applying the principles of axial and planar chirality.
- Assigning configurational descriptors to allenes, alkyldiene cycloalkanes, spirans, biaryls (including BINOLs and BINAPs), ansa compounds, cyclophanes,
- Predicting topicity, evaluating the criteria for enantiotopic and diastereotopic ligands and faces and identifying them in a stereoisomer and assigning configurational descriptors
- Identifying a prochiral center in a given molecule and assign the configurational descriptors
- Predicting Selectivity and specificity of the various oxidizing and reducing reagents and the mechanisms
- Identifying suitable reagents required for designing synthesis via functional group interconversion.

<b>UNIT I</b>	<b>PHYSICAL ORGANIC CHEMISTRY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>1.1</b>	Thermodynamic and kinetic requirements of a reaction: rate and equilibrium constants, reaction coordinate diagram, transition state (activated complex), nature of activated complex, Hammond postulate, Reactivity vs selectivity, Curtin-Hammett Principle, Microscopic reversibility, Kinetic vs thermodynamic control of organic reactions.	<b>6L</b>
<b>1.2</b>	Determining mechanism of a reaction: Product analysis, kinetic studies, use of isotopes (Kinetic isotope effect – primary and secondary kinetic isotope effect). Detection and trapping of intermediates, crossover experiments and stereochemical evidence.	<b>3L</b>
<b>1.3</b>	Acids and Bases: Factors affecting acidity and basicity: Electronegativity and inductive effect, resonance, bond strength, electrostatic effects, hybridization, aromaticity and solvation. Comparative study of acidity and basicity of organic compounds on the basis of pKa values, Leveling effect and non-aqueous solvents. Acid and base catalysis – general and specific catalysis with examples.	<b>6L</b>
<b>UNIT II</b>	<b>NUCLEOPHILIC SUBSTITUTION REACTIONS AND AROMATICITY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>2.1</b>	<b>Nucleophilic substitution reactions</b>	<b>10L</b>

2.1.1	<b>Aliphatic nucleophilic substitution:</b> $S_N1$ , $S_N2$ , (including effects of solvents on these reactions Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, leaving group and hard-soft interaction.) $S_N^i$ reactions, mixed $S_N1$ and $S_N2$ and SET mechanisms. $S_N$ reactions involving NGP - participation by aryl rings, $\alpha$ and pi-cyclopropane bonds. Ambident nucleophiles. $S_{NCA}$ , $S_N$ at $sp^2$ (vinylic) carbon.	6L
2.1.2	<b>Aromatic nucleophilic substitution:</b> $S_{NAr}$ , $S_N1$ , benzyne mechanisms. Ipso, cine.	2L
2.1.3	<b>Ester hydrolysis:</b> Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.	2L
2.2	<b>Aromaticity:</b>	5L
2.2.1	Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity.	2L
2.2.2	Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's $(4n+2)$ and $4n$ rules.	1L
2.2.3	Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene ( $C_{60}$ ). [Reference Books 1,2 ,13,16]	2L
UNIT III	<b>STEREOCHEMISTRY</b>	15L
Sub-units	<b>Topics</b>	<b>No. of Lectures</b>
3.1	<b>Molecules with tri- and tetra-coordinate centers:</b> Compounds with carbon, silicon, nitrogen, phosphorus and sulphur chiral centers, relative configurational stabilities.	1L
3.2	<b>Molecules with two or more chiral centers:</b> Constitutionally unsymmetrical molecules: erythro-threo and syn-anti systems of nomenclature. Interconversion of Fischer, Sawhorse, Newman and Flying wedge projections. Constitutionally symmetrical molecules with odd and even number of chiral centers: enantiomeric and meso forms, concept of stereogenic, chirotopic, and pseudo asymmetric centres.	4L
3.3	<b>Axial and planar chirality:</b> Principles of axial and planar chirality. Recapitulation of : allenes, alkylidene cycloalkanes, spirans, biaryls. Stereochemical features and configurational descriptors (R, S) for the following classes of compounds: allenes, alkylidene cycloalkanes, spirans, biaryls (buttressing effect) (including BINOLs and BINAPs), ansa compounds, cyclophanes.	3L
3.4	<b>Prochirality:</b> Chiral and prochiral centres; prochiral axis and prochiral plane. Homotopic, heterotopic (enantiotopic and diastereotopic) ligands and faces. Identification using substitution and symmetry criteria. Nomenclature of stereo heterotopic ligands and faces. Symbols for stereo heterotopic ligands in molecules with i) one or more prochiral centres ii) a chiral as well as a prochiral centre, iii) a prochiral axis iv) a prochiral plane v)pro-pseudo asymmetric centre. Symbols for enantiotopic and diastereotopic faces.  [Reference Books: 6-8]	7L

UNIT IV	OXIDATION AND REDUCTION	15L
Sub-units	Topics	No. of Lectures
4.1	<b>Oxidation</b>	8L
4.1.1	<b>Oxidation:</b> General mechanism and selectivity of hydrocarbons, alcohols, carbonyl compounds	
4.1.2	<b>Oxidation of hydrocarbons:</b> <b>Dehydrogenation:</b> Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).	
4.1.3	<b>Oxidation involving C-C bonds cleavage:</b> Glycols using HIO <sub>4</sub> ; cycloalkanones using CrO <sub>3</sub> ; carbon-carbon double bond using ozone, KMnO <sub>4</sub> , NaIO <sub>4</sub> and OsO <sub>4</sub> ; aromatic rings using RuO <sub>4</sub> and NaIO <sub>4</sub> .	
4.1.4	<b>Oxidation involving replacement of hydrogen by oxygen:</b> oxidation of CH <sub>2</sub> to CO by SeO <sub>2</sub> , oxidation of aryl methanes by CrO <sub>2</sub> Cl <sub>2</sub> (Etard oxidation).	
4.1.5	<b>Oxidation of alcohols:</b> Chromium reagents such as K <sub>2</sub> Cr <sub>2</sub> O <sub>7</sub> /H <sub>2</sub> SO <sub>4</sub> (Jones reagent), CrO <sub>3</sub> -pyridine (Collin's reagent), PCC (Corey's reagent) and PDC (Cornforth reagent), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation), Corey-Kim oxidation - advantages over Swern and limitations; and Pfitzner-Moffatt oxidation-DCC and DMSO and Oppenauer oxidation.	
4.1.6	<b>Oxidation of aldehydes and ketones:</b> with H <sub>2</sub> O <sub>2</sub> (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)	
4.2	<b>Reduction</b>	7L
4.2.1	<b>Reduction:</b> General mechanism, selectivity, and important applications of the following reducing reagents:	
4.2.2	<b>Catalytic reduction:</b> Clemmensen reduction, Adams Catalyst, Raney Nickel	
4.2.3	<b>Reduction by hydride:</b> Transfer reagents Boron reagents (NaBH <sub>4</sub> , NaCNBH <sub>3</sub> , diborane, 9-BBN, Na(OAc) <sub>3</sub> BH, aluminium reagents (LiAlH <sub>4</sub> , DIBAL-H, Red Al, L and K-selectrides).	
4.2.4	<b>Dissolving metal reductions:</b> using Zn, Li, Na, and Mg under neutral and acidic conditions, Li/Na-liquid NH <sub>3</sub> mediated reduction (Birch reduction) of aromatic compounds and acetylenes.	
4.2.5	<b>Other Methods of reduction:</b> Wolff Kishner reduction and Huang-Minlon modification. NH <sub>2</sub> NH <sub>2</sub> (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzsch Dihydropyridine).	
<b>REFERENCES</b>		

1. Physical Organic Chemistry, Neil Isaacs
2. Modern Physical Organic Chemistry, Eric V. Anslyn and Dennis A. Dougherty
3. Comprehensive Organic chemistry, Barton and Ollis, Vol 1
4. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.
6. Stereochemistry: Conformation and mechanism, P.S. Kalsi, New Age International, New Delhi.
7. Stereochemistry of carbon compounds, E.L Eliel, S.H Wilen and L.N Manden, Wiley.
8. Stereochemistry of Organic Compounds- Principles and Applications, D. Nasipuri. New International Publishers Ltd.
9. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
10. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
11. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
12. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
13. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
14. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
15. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
16. Mechanism in Organic Chemistry, Peter sykes, 6th edition onwards.
17. Modern Methods of Organic Synthesis, W. Carruthers and Iain Coldham, Cambridge University Press.
18. Organic Synthesis, Jagdamba Singh, L.D.S. Yadav, PragatiPrakashan.

**PRACTICALS**  
**Course Code: SMSCHEP103**

**Learning Objectives:**

**Learner will learn**

- To synthesize organic compounds.
- To purify the given compound by suitable method
- Techniques of TLC to study the progress of a reaction

**Learning Outcomes:**

**Learner will be able to**

- Prepare organic compounds at micro scale
- To assess the purity of the prepared compound
- Monitor the progress of the reaction using TLC

**I. One step preparations (1.0 g scale)**

1. Bromobenzene to p-nitrobromobenzene
2. Anthracene to anthraquinone
3. Benzoin to benzil
4. Anthracene to Anthracene maleic anhydride adduct
5. 2-Naphthol to BINOL
6. p-Benzoquinone to 1,2,4-triacetoxybenzene
7. Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
8. o-Phenylenediamine to 2-methylbenzimidazole
9. o-Phenylenediamine to 2,3-diphenylquinoxaline
10. Urea and benzil to 5,5-diphenylhydantoin

**II. Laboratory preparation of shaving gel**

**III. Plotting TLC for organic synthesis**

**ANALYTICAL CHEMISTRY**  
**SEMESTER-I**  
**COURSE CODE: SMSCHE104**

**Learning Objectives:**

- To introduce important terms involved in analytical chemistry
- To create awareness about quality, accreditation and GLP
- To learn and use appropriate concentration units and predict yield of a reaction.
- To learn about FTIR and UV-Vis spectroscopy as an analytical tool.
- To learn about DSC, DTA and thermometric titration methods as a method for the characterisation of various substances.

**Learning Outcome: The learner will be able to**

- understand the use and importance of various terms used in analytical chemistry.
- be able to comprehend various quality standards and safety rules followed in the laboratories.
- interconvert various concentration units and assess conditions to improve reaction yield.
- explain the working and applications of IR, FTIR and UV-Vis spectroscopy in various fields
- able to solve numerical problems on simultaneous spectroscopy.
- interpret thermograms of various compounds for identification and quantification.

UNIT I	LANGUAGE AND QUALITY OF/IN ANALYTICAL CHEMISTRY	15L
Sub-units	Topics	No. of Lectures
1.1	<b>Language of Analytical Chemistry:</b>	8L
1.1.1	Analytical perspective, Common analytical problems, terms involved in analytical chemistry (analysis, determination, measurement, techniques, methods, procedures and protocol)	
1.1.2	An overview of analytical methods, types of instrumental methods, instruments for analysis, data domains, electrical and non-electrical domains, detectors, transducers and sensors, selection of an analytical method, accuracy, precision, selectivity, sensitivity, detection limit and dynamic range.	
1.1.3	Errors, determinate and indeterminate errors. Types of determinate errors, tackling of errors	
1.1.4	Quantitative methods of analysis: calibration curve, standard addition and internal standard method.	
1.2	<b>Quality in Analytical Chemistry:</b>	7 L



<b>1.2.1</b>	<b>Quality Management System (QMS):</b> Evolution and significance of Quality Management, types of quality standards for laboratories, total quality management (TQM), philosophy implementation of TQM (reference of Kaizen, Six Sigma approach & 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.	
<b>1.2.2</b>	<b>Safety in Laboratories:</b> Basic concepts of Safety in Laboratories, Personal Protection Equipment (PPE), OSHA, Toxic Hazard (TH) classifications, Hazardous Chemical Processes (including process calorimetry / thermal build up concepts).	
<b>1.2.3</b>	<b>Accreditations:</b> Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, Agmark)	
<b>1.2.4</b>	<b>Good Laboratory Practices (GLP):</b> Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score	
<b>UNIT II</b>	<b>CALCULATIONS BASED ON CHEMICAL PRINCIPLES</b> (The topics are to be covered in the form of numerical problems only.)	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>2.1</b>	Concentration of a solution based on volume and mass units.	
<b>2.2</b>	Calculations of ppm, ppb and dilution of the solutions, concept of mmol.	
<b>2.3</b>	Stoichiometry of chemical reactions, concept of kg mol, limiting reactant, theoretical and practical yield.	
<b>2.4</b>	Solubility and solubility equilibria, effect of presence of common ion.	
<b>2.5</b>	Calculations of pH of acids, bases, acidic and basic buffers.	
<b>2.6</b>	Concept of formation constants, stability and instability constants, stepwise formation constants.	<b>15L</b>
<b>2.7</b>	Oxidation number, rules for assigning oxidation number, redox reaction in term of oxidation number, oxidizing and reducing agents, equivalent weight of oxidizing and reducing agents, stoichiometry of redox titration (Normality of a solution of a oxidizing / reducing agent and its relationship with molarity).	
<b>UNIT III</b>	<b>OPTICAL METHODS</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>3.1</b>	<b>Recapitulation and FT Technique:</b>	<b>3L</b>
<b>3.1.1</b>	Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.	
<b>3.1.2</b>	Laser as a source of radiation, Fibre optics	
<b>3.1.3</b>	Introduction of Fourier Transform	
<b>3.2</b>	<b>Molecular Ultraviolet and Visible Spectroscopy: (Numericals are expected)</b>	<b>6 L</b>

<b>3.2.1</b>	Beer- Lambert's Law, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents. Applications of Ultraviolet and Visible spectroscopy: 1. On charge transfer absorption 2. Simultaneous spectroscopy 3. Derivative Spectroscopy	
<b>3.2.2</b>	Dual spectrometry – Introduction, Principle, Instrumentation and Applications	
<b>3.3</b>	<b>Infrared Absorption Spectroscopy:</b>	<b>6 L</b>
<b>3.3.1</b>	Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument	
<b>3.3.2</b>	FTIR and its advantages	
<b>3.3.3</b>	Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on “Finger print” region, Quantitative analysis, Advantages and Limitations of IR	
<b>3.3.4</b>	Introduction and basic principles of diffuse reflectance spectroscopy.	
<b>UNIT IV</b>	<b>THERMAL METHODS</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>4.1</b>	<b>Thermal methods:</b>	<b>9L</b>
<b>4.1.1</b>	<b>Introduction:</b> Recapitulation of types of thermal methods, comparison between TGA and DTA.	
<b>4.1.2</b>	<b>Differential Scanning Calorimetry:</b> Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure).	
<b>4.1.3</b>	<b>Applications:</b> Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Analysis of Polyethylene for its crystallinity.	
<b>4.2</b>	<b>Thermometric titrations:</b> Introduction, instrumentation, applications in the titration of (i) HCl Vs NaOH (ii) Boric acid Vs NaOH (iii) A mixture of Ca <sup>2+</sup> and Mg <sup>2+</sup> Vs EDTA (iv) Zn <sup>2+</sup> with disodium tartarate.	<b>6L</b>
<b>REFERENCES</b>		

<p style="text-align: center;"><b>UNIT I</b></p>	<ol style="list-style-type: none"> <li>1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education</li> <li>2. Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition</li> <li>3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9<sup>th</sup> Edition, 2004, Ch: 5.</li> <li>4. Undergraduate Instrumental Analysis, 6<sup>th</sup> Edition, J W Robinson, Marcel Dekker, Ch:1.</li> <li>5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 &amp; 4) (Free download).</li> <li>6. Quality in the Analytical Laboratory, Elizabeth Prichard, Wiley India, Ch: 5, Ch: 6 &amp; Ch: 7</li> <li>7. Quality Control and Total Quality Management - P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management - Bester field - Pearson Education, Ch:5.</li> <li>8. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. 1. 1998.</li> </ol>
<p style="text-align: center;"><b>UNIT II</b></p>	<ol style="list-style-type: none"> <li>1. 3000 solved problems in chemistry, Schaum's Solved problem series, David E. Goldbers, McGraw Hill international Editions, Chapter 11,15,16,21,22</li> </ol>
<p style="text-align: center;"><b>UNIT III</b></p>	<ol style="list-style-type: none"> <li>1. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5<sup>th</sup> Edition, Harcourt Asia Publisher. Chapter 6, 7.</li> <li>2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis, 6<sup>th</sup> Edition, CBS Publisher. Chapter 2.</li> <li>3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.</li> <li>4. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5<sup>th</sup> Edition, McGraw Hill Publisher, Chapter 3.</li> <li>5. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.</li> </ol>
<p style="text-align: center;"><b>UNIT IV</b></p>	<ol style="list-style-type: none"> <li>1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27</li> <li>2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications</li> <li>3. Instrumental methods of analysis, 7<sup>th</sup> Edition, Willard, Merrit, Dean: Chapter 25</li> <li>4. Instrumental Analysis, 5<sup>th</sup> Edition, Skoog, Holler and Nieman: Chapter 31</li> <li>5. Quantitative Chemical Analysis, 6<sup>th</sup> Edition, Vogel: Chapter 12</li> <li>6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd &amp; Kenneth H. Tonge</li> </ol>
<p><b>PRACTICALS</b>  <b>Course Code: SMSCEP104</b></p> <p><b>Learning Objectives:</b></p> <ul style="list-style-type: none"> <li>● To learn analysis of individual and mixture of components by classical and instrumental methods learnt in theory.</li> <li>● To learn the role of different solvents in sample pre-treatment to enhance accuracy of the result..</li> <li>● To get highly reproducible and accurate results irrespective of the origin of the sample.</li> </ul> <p><b>Learning Outcome: The learner will be able to</b></p> <ul style="list-style-type: none"> <li>● use concepts learnt in theory for solving practical problems.</li> <li>● understand and apply the knowledge acquired in theory to different types of samples for its characterisation and estimation.</li> <li>● be able to work comfortably at different concentrations with the highest degree of accuracy and reproducibility.</li> </ul>	

1	To determine percentage composition of saline injection. Estimation of sodium chloride by Volhard's method and glucose by polarimetry.
2	To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3	To determine the amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
4	To determine the breakthrough capacity of a cation exchange resin.
5	To determine the amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II).
6	To estimate Vitamin B <sub>12</sub> /fluorescein by fluorimetry.
7	Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically

### REFERENCES

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel's, 3<sup>rd</sup> Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals", Part II, 4<sup>th</sup> Ed., A Wiley Interscience Publication, New York,1978.

### PHYSICAL CHEMISTRY SEMESTER-II COURSE CODE: SMSCHE201

#### Learning Objectives:

- To understand the concept of fugacity, Gibbs energy of mixing, relation of partial molal quantity with thermodynamic properties
- To understand thermodynamics of surfaces and free energy changes of biochemical reactions
- To emanate schrodinger equation in spherical coordinates, quantization of rotational energy and spherical harmonics, total wave functions, probability density functions and interdependence of quantum numbers
- To learn kinetics of enzyme catalyzed reactions, different types of inhibitions of enzymes and kinetics of reactions in solid state.
- To understand different types and thermodynamics of formation of defects
- To summarize phase equilibria for two component and three component systems

#### Learning Outcomes : Learner will be able to

- deduce fugacity of real gases using graphical methods.
- elucidate Laplace, Kelvin equation and derive Gibbs adsorption isotherm and BET isotherm
- understand and explain two particle problems and separation of variables, expressions for the total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen.
- elaborate the general mechanisms of acid-base catalysis, enzyme catalysis and effect of pH & temperature on them.
- extrapolate mathematical equation to find concentration of defects and solve numerical problems based on it.

- understand and explain two component systems and three component systems.

<b>UNIT I</b>	<b>CHEMICAL THERMODYNAMICS – II</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>1.1</b>	Fugacity of real gases - Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing.	
<b>1.2</b>	Real solutions- Partial molal quantities, partial molal volume, Gibbs Duhem equation, Relation of partial molal quantity to thermodynamic properties, chemical potential in non-ideal solutions, Gibbs Duhem Margules equation.	
<b>1.3</b>	Thermodynamics of surfaces- Pressure difference across curved surfaces (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).	
<b>1.4</b>	Bioenergetics: standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.	
<b>UNIT II</b>	<b>QUANTUM CHEMISTRY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>2.1</b>	Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wave function, quantum number, the theta equation, wave function, quantization of rotational energy, spherical harmonics.	
<b>2.2</b>	Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the R the $\theta^*$ and the $\phi$ equations, solution of the reequation, introduction of the four quantum numbers and their interdependence on the basis of the solutions of the three equations, total wave function, expression for the energy, probability density function, distances and energies in atomic units, radial and angular plots., points of maximum probability, expressions for the total wave function for 1s,2s, 2p and 3d orbitals of hydrogen.	
<b>2.3</b>	Application of the Schrödinger equation to two electron system, limitations of the equation, need for the approximate solutions, methods of obtaining the approximate solution of the Schrödinger wave equation.	
<b>2.4</b>	Hückel Molecular Orbitals theory for ethylene, 1,3-butadiene and benzene. (Derivation expected)	
<b>UNIT III</b>	<b>CHEMICAL KINETICS AND MOLECULAR REACTION DYNAMICS</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>3.1</b>	General Catalytic Mechanisms – Equilibrium treatment, steady state treatment, Activation energies for catalyzed reactions Acid base Catalysis – general, theory and mechanism	
<b>3.2</b>	Kinetics of reactions catalyzed by enzymes – Michaelis - Menten analysis, Lineweaver-Burk and Eadie Analyses, influence of pH and temperature	

3.3	Inhibition of Enzyme action: Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.	
3.4	Kinetics of reactions in the Solid State:-Factors affecting reactions in solids Rate laws for reactions in solid: The parabolic rate law, The first order rate Law, the contracting sphere rate law, Contracting area rate law, some examples of kinetic studies. (Ref: 7 and 2)	
<b>UNIT IV</b>	<b>SOLID STATE CHEMISTRY AND PHASE EQUILIBRIA</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
<b>4.1</b>	<b>Solid State Chemistry</b>	
<b>4.1.1</b>	Types of Defects and Stoichiometry, Zero dimensional (point) Defects, One dimensional (line) Defects, Two dimensional (Planar) Defects Thermodynamics of formation of defects (Mathematical derivation to find concentration of defects and numerical problems based on it) (Ref: 17, 18 and 19)	
<b>4.2</b>	<b>Phase Equilibria:</b>	
<b>4.2.1</b>	A] Two component system: I. Solid –Gas System : Hydrate formation, Amino compound formation II. Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point (with suitable examples)	
<b>4.2.2</b>	B] Three component system: I. Formation of two pair of partially miscible II. Formation of three pair of partially miscible liquid. III. Solid liquid Equilibria - Ternary solutions with common ions – (NaCl – KCl-H <sub>2</sub> O and NaCl- Na <sub>4</sub> SO <sub>4</sub> - H <sub>2</sub> O) (Ref: 4, 6, 11, 12 ,13,16, 24 )	
<b>REFERENCES</b>		

1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7th Edition, Oxford University Press, 2002.
2. K.J. Laidler and J.H. Meiser, Physical Chemistry, 2nd Edition., CBS Publishers and Distributors, New Delhi, 1999.
3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3rd Edition, John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, Physical Chemistry, 5<sup>th</sup> Edition, Tata McGraw-Hill New Delhi, 2002.
5. S. Glasstone, Text Book of Physical Chemistry, 2nd Edition., McMillan and Co. Ltd., London, 1962.
6. Principles of Chemical Kinetics, 2nd Ed., James E. House, ELSEVIER, 2007.
7. B.K. Sen, Quantum Chemistry including Spectroscopy, Kalyani Publishers, 2003.
8. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press, New Delhi, 1964.
9. W.G. Davis, Introduction to Chemical Thermodynamics – A Non – Calculus Approach, Saunders, Philadelphia, 19772.
10. Peter A. Rock, Chemical Thermodynamics, University Science Books, Oxford University Press, 1983.
11. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edition, Pearson Education Limited 2013.
12. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart & Elaine A. Moore, Taylor & Francis, 2010.
13. The Physics and 'Chemistry of Solids, Stephen Elliott, Willey India, 2010
14. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
15. Principles of physical Chemistry , Marrown and Prutton 5th edition
16. Essentials of Physical Chemistry ArunBahl, B. S Bahl, G. D.Tulli , S Chand and Co. Ltd , 2012 Edition.
17. Introduction of Solids L.V Azaroff , Tata McGraw Hill .
18. A Textbook of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011

## PRACTICALS

Course Code: SMSCHP201

### Learning Objectives:

- To train the students in handling various instruments.
- To get practical knowledge on planning and performing experiments.
- To gain knowledge about the non-instrumental techniques
- To solve equations mathematically to plot graphs and interpret them.

### Learning Outcomes : Learner will be able to

- be equipped with technical skills to work with various instruments.
- correlate the theoretical knowledge with the practical experiments.
- Mathematically solve equations and Interpret graphical plots.

**Non – instrumental:**

1. Study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of  $\text{CaSO}_4$  at room temperature.
2. Study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate
3. Determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.
4. Polar plots of atomic orbitals such as  $1s$ ,  $p_z$  and  $3d_{z^2}$  orbitals by using angular plot of hydrogen atom wave functions.

**Instrumental:**

1. Study the effect of substituent on the dissociation constant of acetic acid conductometrically.
2. Determine the formula of silver ammonia complex by potentiometric method.
3. Determine hydrolysis constant for aniline hydrochloride using conductivity measurements
4. Determine the Michaelis – Menten's constant value ( $K_m$ ) of the enzyme Beta Amylase spectrophotometrically.

**REFERENCES**

1. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books Private Limited, 2005.
2. Practical Physical Chemistry, A.M. James and F.E. Prichard, 3<sup>rd</sup> Edition Longman Group Ltd., 1974.
3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.



**INORGANIC CHEMISTRY**  
**SEMESTER-II**  
**COURSE CODE: SMSCHE202**

**Learning objectives**

- To understand different types of reactions and their mechanisms for inorganic complexes of varying geometry
- To impart knowledge of sources, effects, control measures of radioactive pollutants and heavy metals
- To understand the role of metals in biological systems

**Learning outcomes**

The learner will be able to

- identify different types of reactions and their mechanisms for inorganic complexes of varying geometry
- suggest methods for environmental protection and explain effects of radiation and heavy metal
- explain the role of metals in biological systems

UNIT I	INORGANIC REACTION MECHANISM	15L
Sub-units	Topics	No. of Lectures
1.1	Rate of reactions, factors affecting the rate of reactions, techniques for determination of rate of reaction (Direct chemical analysis, spectrophotometric method, electrochemical and flow methods).	3L
1.2	Ligand substitution reactions of: (Mechanism and factors affecting these substitution reactions.) a) Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method) b) Square planar complexes, trans-effect, its theories and applications. c) tetrahedral complexes	5L
1.3	Redox reactions: electron and atom transfer, inner and outer sphere mechanisms, complimentary and non-complimentary reactions.	4L
1.4	Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)	3L
UNIT II	ORGANOMETALLIC CHEMISTRY OF TRANSITION METALS	15L
Sub-units	Topics	No. of Lectures
2.1	Eighteen and sixteen electron rule comparison and electron counting with examples.	3L
2.2	Preparation and properties of the following compounds (a) Alkyl and aryl derivatives of Pd and Pt complexes (b) Carbenes and carbynes of Cr, Mo and W (c) Alkene derivatives of Pd and Pt (d) Alkyne derivatives of Pd and Pt (e) Allyl derivatives of nickel (f) Sandwich compounds of Cr and Half Sandwich compounds of Cr, Mo. Structure and bonding on the basis of VBT and MOT in the following organometallic compounds:	10L

2.3	Zeise's salt, bis(triphenylphosphine)diphenylacetylene platinum(0) [Pt(PPh <sub>3</sub> ) <sub>2</sub> (HC≡CPh) <sub>2</sub> ] diallyl nickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl ( $\eta^2$ -butadiene) iron(0)	5L
<b>UNIT III</b>	<b>ENVIRONMENTAL CHEMISTRY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
3.1	Introduction and discussion of toxicity of Heavy Metals: Toxicity of metallic species: Mercury, lead, cadmium, arsenic, copper and chromium, with respect to their sources, distribution, speciation, biochemical effects and toxicology, control and treatment.	5L
3.2	Case Studies: For example (a) Itai-itai disease for Cadmium toxicity, (b) Arsenic Poisoning in the Indo-Bangladesh region. (Other relevant examples recent may be included)	5L
3.2	Interaction of radiation in context with the environment: Sources and biological implication of radioactive materials. Effect of low level radiation on cells- Its applications in diagnosis and treatment, Effect of radiation on cell proliferation and cancer.	5L
<b>UNIT IV</b>	<b>BIOINORGANIC CHEMISTRY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
4.1	Biological oxygen carriers- heme and non heme: hemoglobin, hemerythrene and hemocyanin- structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and myoglobin: Cooperativity of oxygen binding in hemoglobin and Hill equation, pH dependence of oxygen affinity in hemoglobin and myoglobin and its implications.	7L
4.2	Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site	3L
4.3	Nitrogen fixation-nitrogenase, hydrogenases	3L
4.4	Metal ion transport and storage: Ionophores and metallothionins	2L
<b>REFERENCES</b>		
<b>UNIT I</b>	<ol style="list-style-type: none"> <li>1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Ed., Oxford University Press, 2010.</li> <li>2. W. H. Malik, G. D. Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8<sup>th</sup> Ed., S. Chand &amp; Company Ltd.</li> <li>3. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.</li> <li>4. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002</li> <li>5. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., Wiley, 1967.</li> <li>6. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.</li> <li>7. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3<sup>rd</sup> Ed., Oxford University Press 2008.</li> </ol>	

<p><b>UNIT II</b></p>	<ol style="list-style-type: none"> <li>1. D. Banerjea, Coordination chemistry. Tata McGraw Hill, New Delhi, 1993.</li> <li>2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2nded, New Age International Pvt Ltd, 2000.</li> <li>3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.</li> <li>4. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2<sup>nd</sup> edition, John Wiley and Sons. 1983.</li> <li>5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.</li> </ol>
<p><b>UNIT III</b></p>	<ol style="list-style-type: none"> <li>1. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.</li> <li>2. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,</li> <li>3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.</li> <li>4. Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.</li> <li>5. Fundamentals of Environmental and Toxicological Chemistry 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor &amp; Francis Group, 2013.</li> <li>6. Living in the Environment 17th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-538-49414-X, Brooks/Cole, Cengage Learning, 2011</li> </ol>
<p><b>UNIT IV</b></p>	<ol style="list-style-type: none"> <li>1. R. W. Hay, Bioinorganic Chemistry, Ellis Harwood, England, 1984.</li> <li>2. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.</li> <li>3. J. A. Cowan, Inorganic Biochemistry-An introduction, VCH Publication, 1993.</li> <li>4. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Publications, Mill Valley, Caligronic, 1994.</li> <li>5. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri&amp; Sons, Calcutta, 1988.</li> <li>6. J.Chem. Educ. (Special issue), Nov, 1985.</li> <li>7. E.Frienden, J.Chem. Educ., 1985, 62.</li> <li>8. Robert R.Crechton, Biological Inorganic Chemistry – An Introduction, Elsevier</li> </ol>
<p><b>PRACTICALS</b>  <b>Course Code: SMSCHEP202</b></p>	

**Learning objectives**

- To train students to prepare and analyze inorganic complexes of various geometries
- To use various optical methods for analysis of inorganic compounds

**Learning outcomes**

The learner will be able to

- prepare and analyze inorganic complexes
- perform analysis of various compounds using suitable optical method

(Any seven)

**I] Inorganic Preparations (Synthesis and Characterization)**

- 1) Bis-(tetraethylammonium) tetrachloroCuprate (II)  $(Et_4 N)_2[CuCl_4]$
- 2) Bis-(tetraethylammonium)tetrachloroNickelate(II)  $(Et_4 N)_2[NiCl_4]$
- 3) Tetramminemonocarbonato Cobalt (III) Nitrate  $[Co(NH_3)_4CO_3]NO_3$
- 4) Hydronium dichlorobis( dimethylglyoximato) Cobaltate(III)  $H[Co(dmgh)_2Cl_2]$
- 5) Bis (ethylenediammine) Copper (II) Sulphate  $[Cu(en)_2]SO_4$

**II] Instrumentation**

- 1) Determination of equilibrium constant by Slope intercept method for  $Fe^{+3}/SCN$  system
- 2) Determination of  $K^+$  in fertilizer sample by standard addition method (flame photometer)
- 3) Simultaneous determination of Ni and Co by spectrophotometry
- 4) Kinetics of formation of Cr(III)-EDTA complex by spectrophotometry

**REFERENCES**

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1<sup>st</sup> Edition., 2010., U.N.Dhur & Sons Pvt Ltd
2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly
3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By:Dr Deepak Pant

**ORGANIC CHEMISTRY**  
**SEMESTER-II**  
**COURSE CODE: SMSCHE203**

**Learning Objective**

- Understanding the formation of enolate.
- Understanding the regioselectivity of alkylation of enolates, Enamines, imines and their nitrogen analogs.
- Understand the mechanisms of reactions and the effect of various parameters on the rate of the reaction, stereochemistry and selectivity of the product.
- Understanding chemical reactions with the help of FMO.
- Understanding HUMO - LUMO gap in UV absorption spectra and interpreting the reactivity of the given compounds.
- Understand the basic concepts of Molecular spectroscopy.

**Learning Outcome:**

- Predict the formation of enolates.
- Predict the mechanism, rate of the reaction, stereochemical outcome of reactions.
- Write the Industrial application of reactions
- Able to draw the FMO's of alkenes, Formaldehyde, allyl anion and cation.
- Apply the concept of FMO's to substitution and addition reactions.
- Able to predict whether the reaction is chemically/ photochemically feasible
- Analyse the effect certain factors on spectrum of the compound
- Interpretation of spectral data and elucidation of structure

UNIT I	ALKYLATION AND REACTION OF CARBON NUCLEOPHILES	15L
Sub-units	Topics	No. of Lectures
<b>1.1</b>	<b>Alkylation of Nucleophilic Carbon Intermediates:</b>	<b>7L</b>
<b>1.1.1</b>	Generation of carbanion, kinetic and thermodynamic enolate formation, Regioselectivity in enolate formation, alkylation of enolates.	
<b>1.1.2</b>	Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.	
<b>1.1.3</b>	Alkylation of aldehydes, ketones, esters, amides and nitriles.	
<b>1.1.4</b>	Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.	
<b>1.1.5</b>	Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).	
<b>1.2</b>	<b>Reaction of carbon nucleophiles with carbonyl groups</b>	<b>8L</b>
<b>1.2.1</b>	Mechanism of Acid and base catalyzed Aldol condensation, Mixed Aldol condensation with aromatic aldehydes, regiochemistry in mixed reactions of aliphatic aldehydes and ketones, intramolecular Aldol reaction and Robinson annulation. Claisen reaction, Perkin Reformatsky Darzens, Knoevenagel reaction.	
<b>1.2.2</b>	Addition reactions with amines and iminium ions; Mannich reaction.	
<b>1.2.3</b>	Acylation of carbanions.	
	[Reference Books: 1-11]	
UNIT II	REACTIONS AND REARRANGEMENTS	15L
Sub-units	Topics	No. of Lectures

	Mechanisms, stereochemistry (if applicable) and applications of the following:	
2.1	<b>Reactions:</b> Baylis-Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction. Wittig	
2.2	<b>Concerted rearrangements:</b> Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.	
2.3	<b>Cationic rearrangements:</b> Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.	
2.4	<b>Anionic rearrangements:</b> Brook, Neber, Von Richter, Wittig, Gabriel-Colman, Payne. [Reference Books: 19-22]	
<b>UNIT III</b>	<b>MOLECULAR ORBITAL THEORY</b>	
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
3.1	<b>Introduction to Molecular Orbital Theory for Organic Chemistry:</b>	<b>8L</b>
3.1.1	<b>Molecular orbitals:</b> Formation of $\sigma$ - and $\pi$ -MOs by using LCAO method. Formation of $\pi$ MOs of ethylene, butadiene, 1, 3, 5-hexatriene,. Concept of nodal planes and energies of $\pi$ -MOs	
3.1.2	<b>Introduction to FMOs:</b> HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra. HOMO and LUMO in MO of allyl cation, anion and radical and regioselectivity in the chemical reactions of allylcation with allyl anion.	
3.1.3	<b>MOs of formaldehyde:</b> The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO ( $\pi$ and $\pi^*$ orbitals) of formaldehyde. Perturbation Theory of Reactivity. Addition of hydride to formaldehyde.	
3.1.4	<b>The Salem-Klopman equation.</b> (no derivation and no remembrance of the equation) Explanation of the three terms in the equation. Hard and Soft Electrophiles and Nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis of MOs.	
3.1.5	<b>Application of FMO</b> concepts in (a) $S_N^2$ reaction, (b) ethylene dimerization to cyclobutane (c) Diels-Alder cycloaddition.	
3.2	<b>Photochemistry:</b>	<b>7L</b>
3.2.1	General Principles	
3.2.2	Orbital Symmetry Considerations for Photochemical Reactions of Alkenes and Dienes, Photochemical Electrocyclic Reactions	
3.2.3	Photochemical cross coupling of alkenes. Photo dimerisation of alkenes.	
3.2.4	Photochemistry of arenes 1,2 ; 1,3 and 1,4 addition photocycloaddition of aromatic rings.	
3.2.5	Photochemically induced radical reactions.	
3.2.6	Chemiluminiscence	
<b>UNIT IV</b>	<b>SPECTROSCOPY</b>	<b>15L</b>
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
4.1	<b>Ultraviolet spectroscopy:</b> Recapitulation - UV spectra of dienes, conjugated polyenes (cyclic and acyclic), carbonyl and unsaturated carbonyl compounds, substituted aromatic compounds. Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, and solvent polarity. Calculation of absorption maxima for above classes of compounds by Woodward-Fieser rules (using Woodward-Fieser tables for values for substituents).	<b>3L</b>

4.2	<p><b>Infrared spectroscopy:</b> Fundamental, overtone and combination bands, vibrational coupling, factors affecting vibrational frequency (atomic weight, conjugation, ring size, solvent and hydrogen bonding). Characteristic vibrational frequencies for alkanes, alkenes, alkynes, aromatics, alcohols, ethers, phenols, amines, nitriles and nitro compounds. Detailed study of vibrational frequencies of carbonyl compounds, aldehydes, ketones, esters, amides, acids, acid halides, anhydrides, lactones, lactams and conjugated carbonyl compounds.</p>	4L
4.3	<p><b>Proton magnetic resonance spectroscopy:</b> Principle, Chemical shift, Factors affecting chemical shift (Electronegativity, H-bonding, Anisotropy effects). Chemical and magnetic equivalence, Chemical shift values and correlation for protons bonded to carbon and other nuclei as in alcohols, phenols, enols, carboxylic acids, amines, amides. Spin-spin coupling, Coupling constant (J), Factors affecting J, geminal, vicinal and long range coupling (allylic and aromatic). First order spectra, Karplus equation. <b><sup>13</sup>C NMR spectroscopy:</b> Theory and comparison with proton NMR, proton coupled and decoupled spectra, off-resonance decoupling. Factors influencing carbon shifts, correlation of chemical shifts of aliphatic, olefin, alkyne, aromatic and carbonyl carbons.</p>	4L
4.4	<p><b>Mass spectrometry:</b> Molecular ion peak, base peak, isotopic abundance, Nitrogen rule, Rule of 13. Determination of molecular formula of organic compounds based on isotopic abundance and HRMS. Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction. <b>Structure determination involving individual or combined use of the above spectral techniques.</b> [Reference Books: 13-18]</p>	4L
<b>REFERENCES</b>		
<ol style="list-style-type: none"> <li>1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.</li> <li>2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A, page no. 713-769, and B, Plenum Press.</li> <li>3. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.</li> <li>4. Organic Chemistry, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7<sup>th</sup> Edition)</li> <li>5. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.</li> <li>6. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.</li> <li>7. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.</li> <li>8. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.</li> <li>9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.</li> <li>10. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.</li> <li>11. Mechanism in Organic Chemistry, Peter Sykes, 6<sup>th</sup> Edition.</li> <li>12. Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley</li> <li>13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.</li> <li>14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.</li> <li>15. Organic Spectroscopy, William Kemp, W.H. Freeman &amp; Company.</li> <li>16. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.</li> <li>17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.</li> </ol>		

18. Spectroscopy of Organic Compounds, P.S. Kalsi, New Age International Ltd.
19. Organic Reaction Mechanisms, V.K. Ahluwalia, R.K. Parasher, Alpha Science .International, 2011.
20. Reactions, Rearrangements and Reagents by S. N. Sanyal
21. Name Reactions, Jie Jack Li, Springer
22. Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, M.G. Ellerdt, and F.G. Favaloro, John Wiley & Sons.

**PRACTICALS**  
**Course Code: SMSCHP203**

**Learning objective:**

**Learner will**

- Understand the method and concept of separation and learn to separate a binary mixture quantitatively by chemical method.
- Learn to perform qualitative analysis, prepare a derivative and identify one of the components
- Learn the method of purification of the components.
- Learn to interpret the spectrum.

**Learning outcomes:**

Learner will be able

- To identify the nature of a binary mixture and separate the mixture quantitatively.
- To perform organic qualitative analysis
- To purify compounds by distilling/recrystallization techniques.
- To elucidate the structure of a compound based on spectra

**I. Separation of Binary mixture using micro-scale technique**

1. Separation of binary mixture using physical and chemical methods.
2. Characterization of one of the components with the help of chemical analysis and confirmation of the structure with the help of derivative preparation and its physical constant.
3. Purification and determination of mass and physical constant of the second component. The following types are expected:
  - a) Water soluble/water insoluble solid and water insoluble solid,
  - b) Non-volatile liquid-Non-volatile liquid (chemical separation)
  - c) Water-insoluble solid-Non-volatile liquid.

**II. Identification of a compound based on spectral interpretation of data of IR <sup>1</sup>H and <sup>13</sup> C NMR and mass spectrum**

**Minimum of 3 mixtures of each type and ten mixtures in total are expected.**

**REFERENCES**

1. Systematic Qualitative organic analysis, H. Middleton (Orient Longman)
2. A Handbook of Organic Analysis, H.T. Clark (Orient Longman)
3. Systematic Identification of organic compounds, R.L. Shriner (John Wiley, New York)
4. Practical Organic Chemistry by Mann and Saunders.
5. Advance Practical Organic Chemistry, N.K. Vishnoi, Vikas Publication



**ANALYTICAL CHEMISTRY  
SEMESTER-II  
COURSE CODE: SMSCHE204**

**Learning Objectives:**

- To learn the principle and working of various chromatographic methods for separation and identification of mixture of unknown compounds by using suitable detectors.
- To understand application of different X-ray spectroscopic methods as a tool for surface studies.
- To learn the principle and working of MS with different analysers as a tool for structural elucidation of organic compounds.
- To learn about advanced electroanalytical methods to analyse mixtures.

**Learning Outcomes: The learner will be able to**

- explain various chromatographic, ICP-AES and X-ray spectroscopic methods with emphasis on principle and working of the instrument.
- draw a simple block/schematic diagram of the instruments learnt and explain the importance of each component.
- carry out structural elucidation of simple organic compounds from the MS data.
- comprehend applications of isotope dilution method and solve numerical problems for a given data.
- explain various types of electroanalytical methods and compare advantages and limitations of one over the other.

UNIT I	CHROMATOGRAPHY	15L
Sub-units	Topics	No. of Lectures
1.1	Concept of plate and rate theories in chromatography: efficiency, resolution, selectivity and separation capability. Van Deemter equation and broadening of chromatographic peaks. Optimization of chromatographic conditions.	4L
1.2	<b>Gas Chromatography:</b> Instrumentation of GC with special reference to sample injection systems – split/splitless, column types, solid/ liquid stationary phases, column switching techniques, temperature programming, Thermionic and mass spectrometric detector, Applications.	3L
1.3	<b>HPTLC:</b> Introduction to HPTLC, techniques in HPTLC. Determination by detectors: single beam densitometer, double beam densitometer, fluorimetric detector. Comparison between TLC and HPTLC. Advantages, limitations and applications of HPTLC	5L
1.4	<b>Size exclusion chromatography:</b> Basic principle and applications in the field of polymers	3L
UNIT II	SPECTROMETRY AND RADIO-ANALYTICAL METHODS	15L
Sub-units	Topics	No. of Lectures
2.1	<b>X-ray spectroscopy:</b> Principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy.	4L

2.2	<b>Mass spectrometry:</b> Recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field desorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications.	6L
2.3	<b>Radio analytical Methods:</b> Recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications.	5L
<b>UNIT III</b>	<b>SURFACE ANALYTICAL TECHNIQUES</b>	15L
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
3.1	<b>Surface Analytical Techniques:</b> Introduction, Principle, Instrumentation and Applications of:	9L
3.1.1	Scanning Electron Microscopy (SEM)	
3.1.2	Scanning Tunnelling Microscopy (STM)	
3.1.3	Transmission Electron Microscopy (TEM)	
3.1.4	Electron Spectroscopy (ESCA and Auger)	
3.2	<b>Atomic Spectroscopy:</b>	6L
3.2.1	Advantages and Limitations of AAS	
3.2.2	Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.	
<b>UNIT IV</b>	<b>ELECTROANALYTICAL METHODS</b>	15L
<b>Sub-units</b>	<b>Topics</b>	<b>No. of Lectures</b>
4.1	<b>Ion selective potentiometry and Polarography:</b>	10L
4.1.1	<b>Ion selective potentiometry:</b> Ion selective electrodes and their applications (solid state, precipitate, liquid –liquid, enzyme and gas sensing electrodes), ion selective field effect transistors, biocatalytic membrane electrodes and enzyme based biosensors.	
4.1.2	<b>Polarography:</b> Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves.	
4.2	<b>Electrogravimetry:</b> Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications.	3L
4.3	<b>Coulometry:</b> Introduction, principle, instrumentation, coulometry at controlled potential and controlled current.	2L
<b>REFERENCES</b>		
<b>UNIT I</b>	1. Instrumental Analysis, Skoog, Holler & Crouch 2. HPTLC Analysis: Dilip Charegaonkar	

<b>UNIT II</b>	<ol style="list-style-type: none"> <li>Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)</li> <li>Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy</li> <li>Principles of Instrumental Analysis - Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 12</li> </ol>
<b>UNIT III</b>	<ol style="list-style-type: none"> <li>Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)</li> <li>Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.</li> <li>Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, NewYork, 1993.</li> <li>Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer</li> <li>Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York</li> <li>Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.</li> </ol>
<b>UNIT IV</b>	<ol style="list-style-type: none"> <li>Principles of Instrumental Analysis – Skoog, Holler, Nieman, 5<sup>th</sup> Edition, Harcourt College Publishers, 1998. Chapters - 23, 24, 25.</li> <li>Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).</li> <li>Vogel’s Textbook of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).</li> <li>Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).</li> <li>Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.</li> </ol>
<p><b>PRACTICALS</b>  <b>Course Code: SMSCHEP204</b></p> <p><b>Learning Objectives:</b></p> <ul style="list-style-type: none"> <li>To learn analysis of the mixture of two or more species using a classical or instrumental method.</li> <li>To learn handling of different instruments.</li> <li>To use a given method to comment on the quality of the compound.</li> </ul> <p><b>Learning Outcomes: The learner will be able to</b></p> <ul style="list-style-type: none"> <li>analyse a given mixture with the highest degree of accuracy by using classical or instrumental method of analysis.</li> <li>check the quality of any given compound.</li> <li>handle various instruments confidently.</li> <li>perform analysis at various concentrations.</li> </ul>	

1	To determine the amount of Ti (III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
2	To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine/ajino motto) by titration with perchloric acid in a non- aqueous medium using a glass calomel system potentiometrically.
3	To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10-phenanthroline spectrophotometrically.
4	To determine the percentage composition of HCl and H <sub>2</sub> SO <sub>4</sub> on weight basis in a mixture of two by conductometric titration with NaOH and BaCl <sub>2</sub> .
5	Demonstration separation of test dyes/ Separation and identification of a marker compound in a herbal formulation using HPTLC.
6	Simultaneous determination of Cd <sup>2+</sup> and Zn <sup>2+</sup> in an industrial effluent sample using calibration curve method polarographically.
7	To determine the amount of calcium in milk powder by flame photometry.
<b>REFERENCES</b>	
<ol style="list-style-type: none"> <li>1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3<sup>rd</sup> Ed. ELBS (1964)</li> <li>2. Standard Instrumental Methods of Chemical Analysis, F. J. Welcher</li> </ol>	

**Internal Assessment:** 1. One test of 10 marks on self-study topic(50%- 100% for self study topic/ Other topics from the unit)

2. One test of 10 marks on any other unit.

3. Seminar on a given topic\*/ 2- Infographs on given topics /2-concept maps/ Peer teaching (in-house students)/short term course related to the subject\*-20 marks

4. Active participation in department activities/ participation in inter and intra-collegiate activities/outreach activity/internship-10

**Semester End Exam:** Subjective (offline)

Five questions of 12 marks each

Each question A/A, B/B and C-----4 M each (sub-questions)