

# **SEMESTER - I**

	Contents:			
Paper I	:	Physical Chemistry		
SIPSCHE11.1	:	Thermodynamics - I		
SIPSCHE11.2	:	Quantum Chemistry		
SIPSCHE11.3	•	Chemical Dynamics - I		
SIPSCHE11.4	:	Electrochemistry		
Paper II	:	Inorganic Chemistry		
SIPSCHE12.1	:	Chemical Bonding		
SIPSCHE12.2	:	Molecular Symmetry and Group Theory		
SIPSCHE12.3	:	Materials Chemistry and Nanomaterials		
SIPSCHE12.4	:	Characterization of Coordination compounds		
Paper III	:	Organic Chemistry		
SIPSCHE13.1	:	Physical Organic Chemistry		
SIPSCHE13.2	:	Nucleophilic substitution reactions and Aromaticity		
SIPSCHE13.3	:	Stereochemistry		
SIPSCHE13.4		Oxidation and Reduction		
Paper IV		Analytical Chemistry		
SIPSCHE14.1	:	Language of Analytical Chemistry		
SIPSCHE14.2	:	Calculations based on Chemical Principles		
SIPSCHE14.3	Ģ	Optical Methods		
SIPSCHE14.4	•	Thermal Methods		
Practical				
SIPSCHE1P1	:	Physical Chemistry Practical		
SIPSCHE1P2	:	Inorganic Chemistry Practical		
SIPSCHE1P3	:	Organic Chemistry Practical		
SIPSCHE1P4	:	Analytical Chemistry Practical		

# **SEMESTER - II**

Contents:			
Paper I	•	Physical Chemistry	
SIPSCHE21.1	:	Chemical Thermodynamics II	
SIPSCHE21.2	:	Quantum Chemistry II	
SIPSCHE21.3	:	Chemical Kinetics and Molecular Reaction Dynamics	
SIPSCHE21.4	:	Solid State Chemistry and Phase Equilibria	
Paper II	:	Inorganic Chemistry	
SIPSCHE22.1	:	Inorganic Reaction Mechanism	
SIPSCHE22.2	:	Organometallic Chemistry of Transition metals	
SIPSCHE22.3	:	Environmental Chemistry	
SIPSCHE22.4	:	Bioinorganic Chemistry	
Paper III	:	Organic Chemistry	
SIPSCHE23.1	:	Alkylation of Nucleophilic Carbon Intermediates and Reaction of carbon nucleophiles with carbonyl groups	
SIPSCHE23.2	:	Reactions and Rearrangements	
SIPSCHE23.3	:	Introduction to Molecular Orbital Theory for Organic Chemistry and	
		Applications of UV and IR spectroscopy	
SIPSCHE23.4		NMR spectroscopy and Mass spectrometry	
Paper IV		Analytical Chemistry	
SIPSCHE24.1	÷	Chromatography	
SIPSCHE24.2	÷	Instrumental methods of Chemical Analysis	
SIPSCHE24.3	:	Surface Analytical Techniques and Atomic Spectroscopy	
SIPSCHE24.4	:	Electroanalytical Methods	
Practical			
SIPSCHE2P1	:	Physical Chemistry Practical	
SIPSCHE2P2	:	Inorganic Chemistry Practical	
SIPSCHE2P3	:	Organic Chemistry Practical	
SIPSCHE2P4	:	Analytical Chemistry Practical	

# **SEMESTER - I**

### **Course Code: SIPSCHE11**

## **Paper I : Physical Chemistry**

### **CREDITS: 4**

### **LECTURES: 60**

	Physical Chemistry	
	UNIT- I, 1L/week	
	COURSE CODE: SIPSCHE11.1	
LEA	RNING OBJECTIVES:	
1) To	learn the concept of exact differentials in relation to thermodynamics.	
2) Im	portance of third law of thermodynamics.	
3) Ap	plication of standard molar entropies.	
1 The	ermodynamics - I	15L
1.1	State function and exact differentials. Maxwell equations, Maxwell thermodynamic Relations; it's significance and applications to ideal gases, 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.	
	UNIT- II, 1L/week	
	COURSE CODE: SIPSCHE11.2	
LEA	RNING OBJECTIVES:	
1. To	learn the need for quantum mechanics.	
2. Ap	plication of Schrodinger wave equation.	
3. To	study different types of operators and harmonic oscillator.	
2 Qua	antum Chemistry	15L
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, Schrödinger's Time independent wave equation from Schrödinger'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.	
	UNIT III, 1L/week	
	COURSE CODE: SIPSCHE11.3	
LEA	RNING OBJECTIVES:	
1. To study the kinetics of polymerisation reaction and reaction in gas phase.		
3 Ch	emical Dynamics - I	15L
3 Cho 3.1	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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.	15L
3 Ch 3.1 3.2	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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. Polymerization reactions: 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 number of monomer units in the polymer produced by chain polymerization.	15L
3 Ch 3.1 3.2 3.2	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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. Polymerization reactions: 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 number of monomer units in the polymer produced by chain polymerization. Reaction in Gas Phase: Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice- Ramsperger-Kassel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory.	15L
3 Ch 3.1 3.2 3.3	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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. Polymerization reactions: 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 number of monomer units in the polymer produced by chain polymerization. Reaction in Gas Phase: Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice- Ramsperger-Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory. Unit – IV, 1L/week	15L
3 Ch 3.1 3.2 3.3	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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. Polymerization reactions: 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 number of monomer units in the polymer produced by chain polymerization. Reaction in Gas Phase: Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice- Ramsperger-Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory. Unit – IV, 1L/week COURSE CODE: SIPSCHE11.4	15L
3 Ch 3.1 3.2 3.3 LEA	emical Dynamics - I Composite Reactions: Recapitulation: Rate laws, Differential rate equations Consecutive reactions, 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. Polymerization reactions: 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 number of monomer units in the polymer produced by chain polymerization. Reaction in Gas Phase: Unimolecular Reactions: Lindeman-Hinshelwood theory, Rice- Ramsperger-Kasssel (RRK) theory, Rice-Ramsperger-Kassel Marcus (RRKM) theory. Unit – IV, 1L/week COURSE CODE: SIPSCHE11.4 RNING OBJECTIVES:	15L

C	equeous solution.	
<b>2</b> .To	study different kinds of fuel cells and its applications.	
<b>3</b> .To	introduce the learner to concept in Bio-electrochemistry.	
4. Ele	ectrochemistry	15L
4.1	Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's 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: Alkaline fuel cells, Phosphoric acid fuel cells, High temperature fuel cells [Solid –Oxide Fuel Cells (SOFC) and Molten Carbonate Fuel Cells]	
4.4	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)	

### SUGGESTED REFERENCE SIPSCHE11

- 1. Peter Atkins and Julio de Paula, Atkin's Physical Chemistry, 7<sup>th</sup> Edn., Oxford University Press, 2002.
- K.J. Laidler and J.H. Meiser, Physical Chemistry, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
- 3. Robert J. Silby and Robert A. Alberty, Physical Chemistry, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, Physical Chemistry, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, Physical Chemistry, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, Text Book of Physical Chemistry, 2<sup>nd</sup> Edn., 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, Quantum Chemistry, 2<sup>nd</sup> Edn., 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, 5th Edn., Pearson Education (Singapore) Pte. Ltd., Indian Branch, New Delhi, 2000.
- 14. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
- 15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1<sup>st</sup> Edn., 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 Text book of Physical Chemistry by K L Kapoor Vol 5, 2<sup>nd</sup> Edn

### **Paper II: Inorganic Chemistry**

CR	EDITS: 4 LECTURES: 60	
	UNIT- I , 1L/week	
	Course Code: SIPSCHE12.1	
	RNING OBJECTIVES:	
$\begin{array}{c} 1 \\ 1 \\ 2 \\ 2 \\ \end{array}$	study the concept of hybridization and molecular orbital theory.	
(2) Ap	plication to poly atomic species hydrogen bond and its different types.	
1	Chemical Bonding:	15L
1.1	Recapitulation of hybridization, Derivation of wave functions for sp, $sp^2$ , $sp^3$ orbital hybridization types considering only sigma bonding. Discussion of involvement of $d$ orbitals in various types of hybridization. Concept of resonance, resonance energy derivation expected. Formal charge with examples. Critical analysis of VBT.	
1.2	Molecular Orbital Theory for diatomic species of First transition Series. Molecular Orbital Theory for Polyatomic species considering $\sigma$ bonding for SF <sub>6</sub> , CO <sub>2</sub> , B <sub>2</sub> H <sub>6</sub> , I <sub>3</sub> <sup>-</sup> molecular species.	
1.3	Weak forces of attraction: Hydrogen bonding – concept, types, properties, methods of detection and importance. Van der Waal's forces, ion-dipole, dipole-dipole, London forces.	
	UNIT- II, 1L/week	
	Course Code: SIPSCHE12.2	
LEA	RNING OBJECTIVES:	
1. To	study the primary understanding of Group Theory and Molecular Symmetry.	
2 Mo	lecular Symmetry and Group Theory	15L
2.1	Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. Concepts of Groups, Sub- groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non- Abelian point groups.	
2.2	Representation of Groups: Matrix representation of symmetry operations, reducible and	

	irreducible representations. The Great Orthogonality Theorem and its application in construction of character tables for point groups $C_2v$ , $C_3v$ and $D_{2h}$ , structure of character tables.	
2.3	Applications of Group Theory	
	(a)Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in AB <sub>n</sub> (Ammonia, CH <sub>4</sub> ) 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.	
	UNIT III, 1L/week	
	Course Code: SIPSCHE12.3	
LEAF	RNING OBJECTIVES:	
1. To understand the electronic structure of solids and methods for preparation of inorganic solids.		
2. To study nanomaterials and its application in various field.		
3 Mat	erials Chemistry and Nanomaterials	15L
3.1	Solid State Chemistry: 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 <sub>2</sub> [fluorite (CaF <sub>2</sub> ) and anti-fluorite structures, rutile (TiO <sub>2</sub> ) structure and layer structure [Cadmium chloride and iodide (CdCl <sub>2</sub> , CdI <sub>2</sub> )]. 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)	
3.2	Nanomaterials: Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett (L-B) method, Biological methods: Synthesis using microorganisms. Applications in the field of semiconductors and solar cells.	
	Unit – IV, 1L/week	
	Course Code: SIPSCHE12.4	
LEAF	RNING OBJECTIVES:	
1.To	study the spectral properties Coordination compound.	
2. т	o learn spectral calculations	

4 Cha	4 Characterization of Coordination compounds	
4.1	Formation, thermal studies, Conductivity measurements, electronic spectral and magnetic measurements, IR, NMR and ESR spectroscopic methods.	
4.2	Spectral calculations using Orgel and Tanabe-Sugano diagram, calculation of electronic parameters such as $\Delta$ , $\beta$ , C, Nephelauxetic ratio.	
4.3	Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.	

### SUGGESTED REFERENCE SIPSCHE12.2

#### Unit - I

- 1. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
- 2. W. W. Porterfield, Inorganic Chemistry-A Unified Approach, 2nd Ed., Academic Press, 1993.
- 3. B. W. Pfennig, Principles of Inorganic Chemistry, Wiley, 2015.
- 4. C. E. Housecroft and A. G. Sharpe, Inorganic Chemistry, Pearson EducationLimited, 2nd Edition 2005.
- 5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles ofStructure and Reactivity, 4th Ed., Harper Collins, 1993.
- 6. P. J. Durrant and B. Durrant, Introduction to Advanced Inorganic Chemistry,Oxford University Press, 1967.
- 7. R. L. Dekock and H.B.Gray, Chemical Structure and Bonding, The BenjaminCummings Publishing Company, 1989.
- 8. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.
- 9. R. Sarkar, General and Inorganic Chemistry, Books and Allied (P) Ltd., 2001.
- 10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East WestPress Pvt. Ltd., 1985.
- 11. J. N. Murrell, S. F. A. Kettle and J. M. Tedder, The Chemical Bond, Wiley, 1978.
- 12. G. A. Jeffrey, An Introduction to Hydrogen Bonding, Oxford University Press, Inc., 1997.

Unit - II

- 1. F. A. Cotton, Chemical Applications of Group Theory, 2nd Edition, Wiley EasternLtd., 1989.
- 2. H. H. Jaffe and M. Orchin, Symmetry in Chemistry, John Wiley and Sons, New York, 1996.
- 3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley and Sons, NewYork, 1998.
- 4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New AgeInternational Publishers, New Delhi, 2009.
- 5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications inChemistry, PHI Learning, 2012.
- 6. P. K. Bhattacharya, Group Theory and its Chemical Applications, HimalayaPublishing House. 2014.

7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to GroupTheory in Chemistry, Universities Press, 2008.

#### Unit - III

- 1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-203-49635-3, Taylor and Francis Group, LLC.
- 2. Nanomaterials and Nanochemistry, 2007, Catherine Brechignac, Philippe Houdy, Marcel Lahmani, ISBN 978-3-540-72992-1 Springer Berlin Heidelberg New York.
- 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 and Co. KGaA, Weinheim.
- 4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, MarcelDekker Inc. New York.
- 5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCHVerlag GmbH and Co. KGaA, Weinheim, 2004.
- 6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH and Co. KGaA, Weinheim, 2010.

#### Unit - IV

- 1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles ofStructure and Reactivity, Pearson Education, 2006.
- 2. D. Banerjea, Coordination Chemistry
- 3. Geary Coordination reviews
- 4. P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong; Shriver and Atkins:Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
- 5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced InorganicChemistry, 6th ed. Wiley, 1999,
- 6. B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of InorganicChemistry(3rd edn.), John Wiley and Sons (1994).

### **Course Code: SIPSCHE13**

### **Paper III: Organic Chemistry**

### **CREDITS: 4**

### **LECTURES: 60**

	UNIT- I, 1L/week	
	COURSE CODE: SIPSCHE13.1	
LE	ARNING OBJECTIVES:	
1.	Understand the principles of kinetics and thermodynamics as applied to rates and equilibrium positions of chemical reactions.	
2.	To describe how experimental verification in the presence of an intermediate or a product in a chemical reaction helps in determining a given reaction mechanism.	
3.	Understand the basic concept of acidity and basicity.	

SIES M.SC. CHEMISTRY SEMESTER I & II SYLLABUS

1 Phy	1 Physical Organic Chemistry	
1.1	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 <i>vs</i> selectivity, Curtin-Hammett Principle, microscopic reversibility, kinetic <i>vs</i> thermodynamic control of organic reactions.	
1.2	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 stereo-chemical evidence.	
1.3	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.	
	UNIT- II, 1L/week	
	COURSE CODE: SIPSCHE13.2	
LEA	RNING OBJECTIVES:	
1.	To study different types of substitution reactions in aliphatic and aromatic substrates.	
2.	To understand the concept of aromaticity, anti-aromaticity and homoaromaticity in annulenes, charged rings, fused ring systems and heterocycles.	
2 Nu	cleophilic substitution reactions and Aromaticity	15L
2.1	Nucleophilic substitution reactions: Aliphatic nucleophilic substitution: $S_N1$ , $S_N2$ , $S_N^{i}$ reactions, mixed $S_N1$ and $S_N2$ and SET mechanisms. $S_N$ reactions involving NGP - participation by aryl rings, $\sigma$ - and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. $S_N cA$ , $S_N1$ and $S_N2$ reactions. $S_N$ at $sp^2$ (vinylic) carbon.	
2.2	Aromatic nucleophilic substitution: $S_NAr$ , $S_N1$ , benzyne mechanisms. Ipso, cine, tele and vicarious substitution. Ester hydrolysis: Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples.	
2.3	Aromaticity: Structural, thermochemical and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel's $(4_{n+2})$ and $4n$ rules. Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene $(C_{60})$ .	
	UNIT III, 1L/week	
	COURSE CODE: SIPSCHE13.3	
OBJI	ECTIVES:	

SIES M.SC. CHEMISTRY SEMESTER I & II SYLLABUS

1. To study the Stereochemistry of different organic molecule with chirality.

3 Ster	eochemistry:	15L	
3.1	Concept of Chirality: Recognition of symmetry elements.		
3.2	Molecules with tri- and tetra-coordinate centers: Compounds with carbon, silicon, nitrogen, phosphorous and sulphur chiral centers, relative configurational stabilities.		
3.3	Molecules with two or more chiral centers: 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 pseudoasymmetric centres. R-S nomenclature for chiral centres in acyclic and cyclic compounds.		
3.4	Axial and planar chirality: Principles of axial and planar chirality. 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, trans-cyclooctenes.		
3.5	Prochirality: 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 stereoheterotopic ligands and faces. Symbols for stereoheterotopic 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.		
	Unit – IV, 1L/week		
	COURSE CODE: SIPSCHE13.4		
OBJE	CTIVES:		
1.	1. To study general mechanism, selectivity, and important applications of oxidation and reduction reactions using different reagents.		
4 Oxi	dation and Reduction	15L	
4.1	Oxidation: General mechanism, selectivity, and important applications of the following:		
C	4.1.1. Dehydrogenation: Dehydrogenation of C-C bonds including aromatization of six membered rings using metal (Pt, Pd, Ni) and organic reagents (chloranil, DDQ).		
	<ul> <li>4.1.2. Oxidation of alcohols to aldehydes and ketones: 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.</li> </ul>		
	4.1.3. Oxidation involving C-C bonds cleavage: Glycols using HIO <sub>4</sub> , cycloalkanones using	L	

	<ul> <li>CrO<sub>3</sub>; carbon-carbon double bond using ozone, KMnO<sub>4</sub>, CrO<sub>3</sub>, NaIO<sub>4</sub> and OsO<sub>4</sub>; aromatic rings using RuO<sub>4</sub> and NaIO<sub>4</sub>.</li> <li>4.1.4. Oxidation involving replacement of hydrogen by oxygen: oxidation of CH<sub>2</sub> to CO by SeO<sub>2</sub>, oxidation of arylmethanes by CrO<sub>2</sub>Cl<sub>2</sub> (Etard oxidation).</li> <li>4.1.5. Oxidation of aldehydes and ketones: with H<sub>2</sub>O<sub>2</sub> (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)</li> </ul>	
4.2	Reduction: General mechanism, selectivity, and important applications of the following reducing reagents:	
	4.2.1. Reduction of CO to CH <sub>2</sub> in aldehydes and ketones- Clemmensen reduction, Wolff- Kishner reduction and Huang-Minlon modification.	
	4.2.2. Metal hydride reduction: Boron reagents (NaBH4, NaCNBH3, diborane, 9-BBN,	
	Na(OAc) <sub>3</sub> BH, aluminium reagents (LiAlH <sub>4</sub> , DIBAL-H, Red Al, L and K- selectrides).	
	4.2.3. NH <sub>2</sub> NH <sub>2</sub> (diimide reduction) and other non-metal based agents including organic reducing agents (Hantzsch dihydropyridine).	
	4.2.4. Dissolving metal reductions: 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.	

#### SUGGESTED REFERENCE SIPSCHE13

- 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 mechamism, 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, Pragati Prakashan.

### Paper IV: Analytical Chemistry

### **CREDITS: 4**

**LECTURES: 60** 

	UNIT- I, 1L/week	
	COURSE CODE: SIPSCHE14.1	
LEA	ARNING OBJECTIVES:	
j	. To understand the language of analytical chemistry.	
2	2. To learn basic concept of safety in laboratories.	
Ĵ	3. To give learner an idea of good laboratory practice.	
1 L	anguage of Analytical Chemistry	15L
1.1	Language of Analytical Chemistry:	
	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.	
Ċ	1.1.4 Quantitative methods of analysis: calibration curve, standard addition and internal standard method.	
1.2	Quality in Analytical Chemistry:	
	1.2.1 Quality Management System (QMS):	
	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 and 5S), quality audits and quality reviews, responsibility of laboratory staff for quality and problems.	

1.2.2 Safety in Lab	oratories:
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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).

### 1.2.3 Accreditations:

Accreditation of Laboratories, Introduction to ISO series, Indian Government Standards (ISI, Hallmark, AGMARK).

1.2.4 Good Laboratory Practices (GLP)

Principle, Objective, OECD guidelines, The US FDA 21CFR58, Klimisch score.

#### UNIT- II, 1L/week

### **COURSE CODE: SIPSCHE14.2**

### **LEARNING OBJECTIVES:**

1. To improve the fundamental concept of numerical calculations in analytical chemistry.

2. To equip the learner for quality control in industry.

### 2 Calculations based on Chemical Principles

- 2.1 The following topics are to be covered in the form of numerical problems only.
  - a) Concentration of a solution based on volume and mass units.
  - b) Calculations of ppm, ppb and dilution of the solutions, concept of mmol.
  - c) Stoichiometry of chemical reactions, concept of kg / mol, limiting reactant, theoretical and practical yield.
  - d) Solubility and solubility equilibria, effect of presence of common ion.
  - e) Calculations of pH of acids, bases, acidic and basic buffers.
  - f) Concept of formation constants, stability and instability constants, stepwise formation constants.
  - g) 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).

### UNIT III, 1L/week

### COURSE CODE: SIPSCHE14.3

### **LEARNING OBJECTIVES:**

- 1. To study the various optical methods in analytical chemistry.
- 2. To get an insight in the various applications of spectroscopy.

### **3** Optical Methods

15L

15L

3.1	Recapitulation and FT Technique				
	3.1.1 Recapitulation of basic concepts, Electromagnetic spectrum, Sources, Detectors, sample containers.				
	3.1.2 Laser as a source of radiation, Fibre optics.				
	3.1.3 Introduction of Fourier Transform.				
3.2	Molecular Ultraviolet and Visible Spectroscopy (Numericals are expected)				
	3.2.1 Derivation of Beer- Lambert's Law and its limitations, factors affecting molecular absorption, types of transitions [emphasis on charge transfer absorption], pH, temperature, solvent and effect of substituents.				
	3.2.2 Applications of Ultraviolet and Visible spectroscopy:				
	1) On charge transfer absorption.				
	2) Simultaneous spectroscopy.				
	3) Derivative Spectroscopy.				
	3.2.3 Dual spectrometry – Introduction, Principle, Instrumentation and Applications.				
3.3	Infrared Absorption Spectroscopy				
	3.1.1 Instrumentation: Sources, Sample handling, Transducers, Dispersive, non- dispersive instrument.				
	3.1.2 FTIR and its advantages.				
	3.1.3 Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on "Finger print" region, Quantitative analysis, Advantages and Limitations of IR.				
	3.1.4 Introduction and basic principles of diffuse reflectance spectroscopy.				
	Unit – IV, 1L/week				
	COURSE CODE: SIPSCHE14.4				
LEA	ARNING OBJECTIVES:				
1.	To study the various thermal methods and it application.				
2.	To understand the need for automation in chemical analysis.				
4 TI	nermal Methods	15L			
4.1	Thermal Methods:				
	4.1.1 Introduction, Recapitulation of types of thermal methods, comparison between TGA and DTA.				
	4.1.2 Differential Scanning Calorimetry- Principle, comparison of DTA and DSC, Instrumentation, Block diagram, Nature of DSC Curve, Factors affecting curves (sample size, sample shape, pressure).				

	<ul> <li>4.1.3 Applications - Heat of reaction, Specific heat, Safety screening, Polymers, liquid crystals, Percentage crystallinity, oxidative stability, Drug analysis, Magnetic transition. e.g. Analysis of Polyethylene for its crystallinity.</li> </ul>	
4.2	Automation in chemical analysis: Need for automation, Objectives of automation, An overview of automated instruments and instrumentation, process control analysis, flow injection analysis, discrete automated systems, automatic analysis based on multilayered films, gas monitoring equipments, Automatic titrators.	

### SUGGESTED REFERENCE SIPSCHE14

#### Unit I

- 1. Modern Analytical Chemistry by David Harvey, McGraw-Hill Higher Education
- 2. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5<sup>th</sup> Edition, Ch: 1.
- 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.
- 4. Undergraduate Instrumental Analysis, 6<sup>th</sup> Edition, J W Robinson, Marcel Dekker, Ch:1.
- 5. ISO 9000 Quality Systems Handbook, Fourth Edition, David Hoyle. (Chapter: 3 and 4) (Free download).
- 6. Quality in the Analytical Laboratory, Elizabeth Pickard, Wiley India, Ch: 5, Ch: 6 and Ch: 7.
- 7. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
- 8. Quality in Totality: A Manager's Guide To TQM and ISO 9000, Parag Diwan, Deep and Deep Publications, 1st Edition, 2000.
- 9. Quality Control and Total Quality Management P.L. Jain-Tata McGraw-Hill (2006) Total Quality Management Bester field Pearson Education, Ch:5.
- 10. Industrial Hygiene and Chemical Safety, M H Fulekar, Ch:9, Ch:11 and Ch:15.
- 11. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 and Ch:19.
- 12. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
- 13. OECD Principles of Good Laboratory Practice (as revised in 1997)".
- 14. OECD Environmental Health and Safety Publications. OECD. 1. 1998.

### Unit II

1. 3000 solved problems in chemistry, Schaums Solved problem series, David E. Goldbers, Mc Graw Hill international Editions, Chapter 11,15,16,21,22

### Unit III

- 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.
- 2. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 3. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 8.

- 4. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 13, 14.
- 5. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, Instrumental Methods of Analysis,6 th Edition, CBS Publisher. Chapter 2.
- 6. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher. Chapter 5.
- 7. G. W. Ewing, Instrumental Methods of Chemical Analysis, 5 th Edition, McGraw Hill Publisher, Chapter 3.
- 8. M. Ito, The effect of temperature on ultraviolet absorption spectra and its relation to hydrogen bonding, J. Mol. Spectrosc. 4 (1960) 106-124.
- 9. A. J. Somnessa, The effect of temperature on the visible absorption band of iodine inseveral solvents, Spectrochim. Acta. Part A: Molecular Spectroscopy, 33 (1977) 525- 528.
- 10. D. A. Skoog, F. J. Holler, T. A. Nieman, Principles of Instrumental Analysis, 5 th Edition, Harcourt Asia Publisher. Chapter 16, 17.
- 11. R. D. Braun, Introduction to Instrumental Analysis, McGraw Hill Publisher, Chapter 12
- Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. Theophanides Theophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech, (open access)

### Unit IV

- 1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27.
- 2. Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications.
- 3. Instrumental methods of analysis, 7<sup>th</sup> Edition, Willard, Merrit, Dean: Chapter 25.
- 4. Instrumental Analysis, 5<sup>th</sup> Edition, Skoog, Holler and Nieman: Chapter 31.
- 5. Quantitative Chemical Analysis, 6<sup>th</sup> Edition, Vogel: Chapter 12.
- 6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd and Amp; Kenneth H. Tonge.
- 7. Instrumental methods of analysis, 7<sup>th</sup> Edition, Willard, Merrit, Dean: Chapter 26.
- 8. Instrumental Analysis, 5<sup>th</sup> Edition, Skoog, Holler and Nieman: Chapter 33.
- 9. Introduction to instrumental methods of analysis by Robert D. Braun, McGraw Hill (1987): Chapter 28

# 10.Course Code: SIPSCHE1P1 Practical Paper I : Physical Chemistry Practical CREDITS: 2

	(4L/Week)
1	Non – Instrumental:
	1. To determine the heat of solution ( $\Delta$ H) of a sparingly soluble acid (benzoic /salicylic acid) from solubility measurement at three different temperature.
	2. To study the variation of calcium sulphate with ionic strength and hence determine the thermodynamic solubility product of CaSO <sub>4</sub> at room temperature.
	3. To investigate the reaction between acetone and iodine.
	4. To study the variation in the solubility of Ca(OH) <sub>2</sub> in presence of NaOH and hence to determine the solubility product of Ca(OH) <sub>2</sub> at room temperature.
	5. Graph Plotting of mathematical functions - linear, exponential and trigonometry and identify whether functions are acceptable or non-acceptable?
	Instrumental:
	1. To determine the mean ionic activity coefficient of an electrolyte by e.m.f. measurement.
	2. To study the effect of substituent on the dissociation constant of acetic acid conductometrically.
	3. To determine pKa values of phosphoric acid by potentiometric titration with sodium hydroxide using glass electrode.
	4. To verify Ostwald's dilution law and to determine the dissociation constant of a weak mono-basic acid conductometrically.
	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> Edn., Longman Group Ltd., 1974.
	3 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

### **Practical Paper II : Inorganic Chemistry Practical**

### **CREDITS: 2**

	(4L/Week)
1	Ores and Alloys
	1) Analysis of Devarda's alloy.
	2) Analysis of Cu – Ni alloy.
	3) Analysis of Tin Solder alloy.
	4) Analysis of Limestone.
	Instrumentation
	1) Estimation of Copper using Iodometric method Potentiometrically.
	2) Estimation of $Fe^{+3}$ solution using Ce(IV) ions Potentiometrically.
	Reference:
	<ol> <li>Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1<sup>st</sup> Edn., 2010., U.N.Dhur and Sons Pvt Ltd</li> </ol>
	2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly.
	3. Inorganic Chemistry Practical under UGC Syllabus for M.Sc. by: Dr Deepak Pant.

### **Course Code:** SIPSCHE1P3

### **Practical Paper III : Organic Chemistry Practical**

		(4L/Week)
1	One s	tep preparations (1.0 g scale)
	1.	Bromobenzene to <i>p</i> -nitrobromobenzene.
	2.	Anthracene to anthraquinone.
	3.	Benzoin to benzyl.
	4.	Anthracene to Anthracene maleic anhydride adduct.
	5.	2-Naphthol to BINOL.
	6.	<i>p</i> -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.

### Learning points:

- 1. Planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS should be learnt.
- 2. Purify the product by crystallization. Formation and purity of the product should be checked by TLC.
- 3. Report mass and melting point of the purified product.

### **Course Code:** SIPSCHE1P4

### Practical Paper IV: Analytical Chemistry Practical

	(4L/Week)				
1	1.	To carry out assay of the sodium chloride injection by			
		Volhard's method. Statistical method.			
	2.	To determine (a) the ion exchange capacity (b) exchange efficiency of the			
		given cation exchange resin.			
	3.	To determine 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 lead and tin content of a solder alloy by titration with EDTA.			
	6.	To determine amount of Cu(II) present in the given solution containing a			
		mixture of Cu(II) and Fe(II).			
	7.	To determine number of nitro groups in the given compound using $TiCl_3$ .			
	References:				
	1.	Quantitative Inorganic Analysis including Elementary Instrumental Analysis			
	Ċ	by A. I. Vogels, 3 <sup>rd</sup> Ed. ELBS.			
	2.	Yogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham,			
		Denny, Barnes, Thomas, Pearson education			
	3.	Standard methods of chemical analysis, F. J. Welcher			
	4.	Standard Instrumental methods of Chemical Analysis, F. J. Welcher			
	5.	W.W. Scott "Standard methods of Chemical Analysis", Vol. I, Van			
		Nostrand Company.			
	6.	E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of			
		Metals", Part- II, 4th Ed., A Wiley Interscience Publication, New York, 1978.			

# **SEMESTER - II**

### **Course Code: SIPSCHE21**

### **Paper I : Physical Chemistry**

**CREDITS: 4** 

**LECTURES: 60** 

UNIT-I, 1L/week

### COURSE CODE: SIPSCHE21.1

### **LEARNING OBJECTIVES:**

1. To study the thermodynamic parameter like fugacity, real solution, surfaces, bioenergetics.

1 Che	emical Thermodynamics - II	15L			
1.1	<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.				
1.2	Real solutions: Chemical potential in non-ideal solutions excess functions of non-ideal solutions calculation of partial molar volume and partial molar enthalpy, Gibbs Duhem Margules equation.				
1.3	Thermodynamics of surfaces, Pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET isotherm (derivations expected).				
1.4	Bioenergetics: Standard free energy change in biochemical reactions, exergonic, endergonic. Hydrolysis of ATP, synthesis of ATP from ADP.				
	UNIT- II, 1L/week				
LEAF	COURSE CODE: SIPSCHE21.2 LEARNING OBJECTIVES:				
C	<ol> <li>To understand the concept of quantum chemistry with respect to rigid rotor, quantization of rotational energy, spherical harmonics.</li> <li>To study the applications of Schrondiger equation for electron system</li> </ol>				
2 Qua	antum Chemistry II	15L			
2.1	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.				

2	2.2	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 requation, introductio of the four quantum numbers and their interdependence on the basis of the solutions of the thre equations, total wave function, expression for the energy, probability density function, distance 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.	l, n e s 7,			
2	2.3 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.					
2	2.4	Hückel Molecular Orbitals theory for ethylene, 1, 3-butadiene and benzene.				
		UNIT III, 1L/week				
		COURSE CODE: SIPSCHE21.3				
L	EAR	RNING OBJECTIVES:				
	j	1. To study the principles of chemical kinetics at molecular reaction dynamics.				
3 Chemical Kinetics and Molecular Reaction Dynamics			15L			
3.1	El inf rel	Elementary Reactions in Solution: Solvent Effects on reaction rates, Reactions between ions- influence of solvent Dielectric constant, influence of ionic strength, Linear free energy relationships Enzyme action.				
3.2	Ki an	Kinetics of reactions catalyzed by enzymes - Michaelis-Menten analysis, Lineweaver - Burk and Eadie Analysis.				
3.3	Inl Ef	Inhibition of Enzyme action: Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes.				
3.4	Ki	netics of reactions in the Solid State: - Factors affecting reactions in solids.				
3.5	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.					
		Unit – IV, 1L/week				
	(	COURSE CODE: SIPSCHE21.4				
LEA	RN	ING OBJECTIVES:				
Ì	l. T	o understand the principle involved in solid state chemistry at phase equilibria.				
4. So	olid S	State Chemistry and Phase Equilibria	15L			
4.1	Solid State Chemistry					

4.1.1. Recapitulation: Structures and Defects in solids.

		Туре	es of Defects and Stoichiometry	
	a)	Ze	ero dimensional (point) Defects.	
	b)	Or	ne dimensional (line) Defects.	
	c)	Τv	vo dimensional (Planar) Defects.	
	d)	Th	nermodynamics of formation of defects (Mathematical derivation to find	
		co	ncentration of defects and numerical problems based on it)	
4.2	Phase equilibria			
	4.2.1 Recapitulation: Introduction and definition of terms involved in phase rule. Thermodynamic derivation of Gibbs Phase rule.			
	4.2.2 Two component system:			
		a)	Solid –Gas System : Hydrate formation, Amino compound formation	
		b)	Solid – Liquid System: Formation of a compound with congruent melting point, Formation of a compound with incongruent melting point. (with suitable examples)	
	4.2.3.	Th	ree component system	
		ſ	Type-I : Formation of one pair of partially miscible liquids.	
		ſ	Type-II: Formation of two pairs of partially miscible liquids.	
		ſ	Type-III: Formation of three pairs of partially miscible liquids.	

### SUGGESTED REFERENCE SIPSCHE21

- 1. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7<sup>th</sup> Edn., Oxford University Press, 2002.
- 2. K.J. Laidler and J.H. Meiser, *Physical Chemistry*, 2<sup>nd</sup> Ed., CBS Publishers and Distributors, New Delhi, 1999.
- 3. Robert J. Silby and Robert A. Alberty, *Physical Chemistry*, 3<sup>rd</sup> Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
- 4. Ira R. Levine, *Physical Chemistry*, 5<sup>th</sup> Edn., Tata McGraw-Hill New Delhi, 2002.
- 5. G.W. Castellan, *Physical Chemistry*, 3<sup>rd</sup> Edn., Narosa Publishing House, New Delhi, 1983.
- 6. S. Glasstone, *Text Book of Physical Chemistry*, 2<sup>nd</sup> Edn., McMillan and Co. Ltd., London, 1962.
- 7. Principles of Chemical Kinetics, 2<sup>nd</sup> Ed., James E. House, ELSEVIER, 2007.
- 8. B.K. Sen, Quantum Chemistry including Spectroscopy, Kalyani Publishers, 2003.
- 9. A.K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
- 10. R.K. Prasad, *Quantum Chemistry*, 2<sup>nd</sup> Edn., New Age International Publishers, 2000.
- 11. S. Glasstone, Thermodynamics for Chemists, Affiliated East-West Press, New Delhi, 1964.
- 12 W.G. Davis, Introduction to Chemical Thermodynamics A Non Calculus Approach, Saunders, Philadelphia, 19772.
- 13. Peter A. Rock, *Chemical Thermodynamics*, University Science Books, Oxford University Press, 1983.
- 14. Ira N. Levine, Quantum Chemistry, 5th Edn., Pearson Education (Singapore) Pte. Ltd., Indian

Branch, New Delhi, 2000.

- 15. Thomas Engel and Philip Reid, Physical Chemistry, 3<sup>rd</sup> Edn., Pearson Education Limited 2013.
- 16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1<sup>st</sup> Edn., 1992.
- 17. Solid State Chemistry [An Introduction], 3rd Ed., Lesley E. Smart and Elaine A. Moore, Taylor and Francis, 2010.
- 18 The Physics and 'Chemistry of Solids, Stephen Elliott, Willey India, 2010
- 19. Principles of the Solid State, H.V. Keer, New Age International Publishers, 2011.
- 20. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 1996.
- 21. Principles of physical Chemistry , Marrown and Prutton 5<sup>th</sup> edition
- 22. Essentials of Physical Chemistry, Arun Bahl, B. S Bahl, G. D. Tulli, S Chand and Co. Ltd, 2012 Edition.
- 23. Introduction of Solids L.V Azaroff, Tata McGraw Hill.
- 24. A Text book of physical Chemistry ; Applications of thermodynamics vol III, Mac Millan Publishers India Ltd ,2011
- 25. New directions in solid state Chemistry, C.N.R. Rao and J Gopalkrishnan, Cambridge University Press.

### **Course Code: SIPSCHE22**

### Paper II: Inorganic Chemistry

### **CREDITS: 4**

### **LECTURES: 60**

	UNIT- I, 1L/week	
LEA	Course Code: SIPSCHE22.1 RNING OBJECTIVES: 1. To study inorganic reaction mechanism involving octahedral and square planar complexes and their stereochemistry.	
1 Inorganic Reaction Mechanism		15L
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).	
1.2	<ul> <li>Ligand substitution reactions of:</li> <li>a. Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method)</li> <li>b. Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.</li> </ul>	

1.3	Redox reactions: Inner and outer sphere mechanisms, complimentary and non- complimentary reactions.	
1.4	Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)	
	UNIT- II, 1L/week	
	Course Code: SIPSCHE22.2	
LEA	RNING OBJECTIVES:	
1	. To study Organometallic Chemistry of Transition metals in details.	
2 OI	ganometallic Chemistry of Transition metals	15L
2.1	Eighteen and sixteen electron rule and electron counting with examples.	
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 Fe, Cr and Half Sandwich compounds of Cr and Mo.	
2.3	Structure and bonding on the basis of VBT and MOT in the following	
	organometallic compounds:	
	Zeise's salt, bis (triphenylphosphine) diphenylacetylene platinum (0)	
	[Pt(PPh <sub>3</sub> ) <sub>2</sub> (HC=CPh) <sub>2</sub> ], diallylnickel(II), ferrocene and bis (arene) chromium (0), tricarbonyl	
	$(\eta^2$ -butadiene) iron (0).	
	UNIT III, 1L/week	
	Course Code: SIPSCHE22.3	
LEA	RNING OBJECTIVES:	
1	. To understand the harmful effect of heavy metals on environment and their toxicity.	
2	2. To do case studies of specific metal toxicity.	
3 Envi	ronmental Chemistry	15L
31 0	Conception of Heavy Metals: Critical discussion on heavy metals.	

	Toxicity of metallic species: Mercury lead cadmium arsenic copper and chromium with	
3.2	respect to their sources distribution speciation biochemical effects and toxicology control and	
	treatment	
3.3	Case Studies:	
	(a) Itai-itai disease for Cadmium toxicity,	
	(b) Arsenic Poisoning in the Indo-Bangladesh region.	
3.4	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.	
	Unit – IV, 1L/week	
	Course Code: SIPSCHE22.4	
LEA	RNING OBJECTIVES:	
	1.To study the principle of Bioinorganic Chemistry.	
4 Bi	1. To study the principle of Bioinorganic Chemistry.         oinorganic Chemistry	15L
4 Bi	1. To study the principle of Bioinorganic Chemistry.         oinorganic Chemistry         Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- structure of metal active	15L
4 Bi 4.1	1.To study the principle of Bioinorganic Chemistry.         oinorganic Chemistry         Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- structure of metal active center and differences in mechanism of oxygen binding, Differences between hemoglobin and	15L
4 Bi 4.1	1.To study the principle of Bioinorganic Chemistry.         oinorganic Chemistry         Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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	15L
4 Bi 4.1	1.To study the principle of Bioinorganic Chemistry. oinorganic Chemistry Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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.	15L
4 Bi 4.1 4.2	1.To study the principle of Bioinorganic Chemistry. <b>oinorganic Chemistry</b> Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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. Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases-structure of the metal center and mechanism of oxygen activation by these enzymes	15L
4 Bi 4.1 4.2	1.To study the principle of Bioinorganic Chemistry. oinorganic Chemistry Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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. Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases-structure of the metal center and mechanism of oxygen activation by these enzymes.	15L
4 Bi 4.1 4.2 4.3	1.To study the principle of Bioinorganic Chemistry. oinorganic Chemistry Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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. Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases-structure of the metal center and mechanism of oxygen activation by these enzymes. Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site.	15L
4 Bi 4.1 4.2 4.3 4.4	1.To study the principle of Bioinorganic Chemistry.          oinorganic Chemistry         Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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.         Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases-structure of the metal center and mechanism of oxygen activation by these enzymes.         Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site.         Nitrogen fixation - nitrogenase, hydrogenases.	15L
4 Bi 4.1 4.2 4.3 4.4 4.5	<ul> <li>1.To study the principle of Bioinorganic Chemistry.</li> <li>oinorganic Chemistry</li> <li>Biological oxygen carriers; hemoglobin, hemerythrene and hemocyanine- 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.</li> <li>Activation of oxygen in biological system with examples of mono-oxygenases, and oxidases-structure of the metal center and mechanism of oxygen activation by these enzymes.</li> <li>Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site.</li> <li>Nitrogen fixation - nitrogenase, hydrogenases.</li> <li>Metal ion transport and storage: Ionophores, transferrin, ferritin and metallothionins.</li> </ul>	15L

### SUGGESTED REFERENCE SIPSCHE12.2

### Unit I

- 1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5<sup>th</sup> Ed., Oxford University Press, 2010.
- 2. D. Banerjea, Coordination Chemistry, Tata McGraw Hill, 1993.
- 3. W. H. Malik, G. D./ Tuli and R. D. Madan, Selected Topics in Inorganic Chemistry, 8<sup>th</sup> Ed., S. Chand and Company ltd.
- 4. M. L. Tobe and J. Burgess, Inorganic Reaction Mechanism, Longman, 1999.
- 5. S. Asperger, Chemical kinetics and Inorganic Reaction Mechanism, 2<sup>nd</sup> Ed., Kluwer Academic/

Plenum Publishers, 2002

- 6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12<sup>th</sup> Edition, Goel publishing house, 2012.
- 7. B. R. Puri, L. R. Sharma and K. C. Kalia, Principles of Inorganic Chemistry, Milestone Publishers, 2013-2014.
- 8. F. Basalo and R. G. Pearson, Mechanism of Inorganic Reactions, 2<sup>nd</sup> Ed., Wiley, 1967.
- 9. R. Gopalan and V. Ramlingam, Concise Coordination chemistry, Vikas Publishing house Pvt Ltd., 2001.
- 10. Robert B. Jordan, Reaction Mechanisms of Inorganic and Organometallic Systems, 3rd Ed., Oxford University Press 2008.

#### Unit II

- 1. D. Banerjea, Coordination chemistry. Tata McGrew Hill, New Delhi, 1993.
- 2. R.C Mehrotra and A.Singh, Organometallic Chemistry- A unified Approach, 2<sup>nd</sup>ed, New Age International Pvt Ltd, 2000.
- 3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5<sup>th</sup> edition, Wiley International Pvt, Ltd 2000.
- 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.
- 5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

### Unit III

- 1. Environmental Chemistry 5<sup>th</sup> edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
- 2. Environmental Chemistry 7<sup>th</sup> edition, Stanley E. Manahan, CRC Press Publishers,
- 3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
- 4. Environmental Science 13<sup>th</sup> edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN- 10: 0-495-56016-2, Brooks/Cole, Cengage Learning, 2010.
- 5. Fundamentals of Environmental and Toxicological Chemistry 4<sup>th</sup> edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor and Francis Group, 2013.
- 6. Living in the Environment 17<sup>th</sup> edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN-10: 0-538-49414-X, Brooks/Cole, Cengage Learning, 2011
- 7. Poisoning and Toxicology Handbook, Jerrold B. Leikin, Frank P. Paloucek, ISBN: 1- 4200-4479-6, Informa Healthcare USA, Inc.
- 8. Casarett and Doull's Toxicology- The Basic Science of Poisons 6<sup>th</sup> edition, McGraw- Hill, 2001.

#### Unit IV

- 1. R. W. Hay, *Bioinorganic Chemistry*, Ellis Harwood, England, 1984.
- 2. I. Bertini, H.B.Gray, S. J. Lippard and J.S. Valentine, Bioinorganic Chemistry, First South Indian Edition, Viva Books, New Delhi, 1998.
- 3. J. A. Cowan, *Inorganic Biochemistry-An introduction*, VCH Publication, 1993.
- 4. S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Publications, Mill Valley, Caligronic, 1994.
- 5. G.N. Mukherjee and A. Das, Elements of Bioinorganic Chemistry, Dhuri and Sons, Calcutta, 1988.
- 6. J.Chem. Educ. (Special issue), Nov, 1985.
- 7. E.Frienden, J.Chem. Educ., 1985, 62.
- 8. Robert R.Crechton, Biological Inorganic Chemistry An Introduction, Elsevier
- 9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.
- 10. JM. D. Yudkin and R. E. Offord A Guidebook to Biochemistry, Cambridge University Press, 1980.

# Course Code: SIPSCHE23 Paper III: Organic Chemistry

### **CREDITS: 4**

### **LECTURES: 60**

	UNIT-I, 1L/week	
	COURSE CODE: SIPSCHE23.1	
LEA	ARNING OBJECTIVES:	
<i>1. T</i>	o study the alkylation of nucleophilic carbon intermediates.	
1 Ph	ysical Organic Chemistry	15L
1.1	Alkylation of Nucleophilic Carbon Intermediates:	
	1.1.1.Generation of carbanion, kinetic and thermodynamic enolate formation, regioselectivity in enolate formation, alkylation of enolates.	
	1.1.2.Generation and alkylation of dianion, medium effects in the alkylation of enolates, oxygen versus carbon as the site of alkylation.	
	1.1.3. Alkylation of aldehydes, ketones, esters, amides and nitriles.	
	1.1.4. Nitrogen analogs of enols and enolates- Enamines and Imines anions, alkylation of enamines and imines.	
	1.1.5. Alkylation of carbon nucleophiles by conjugate addition (Michael reaction).	
1.2	Reaction of carbon nucleophiles with carbonyl groups	
	1.2.1 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.	
	1.2.2 Addition reactions with amines and iminium ions; Mannich reaction.	
	1.2.3 Amine catalyzed condensation reaction: Knoevenagel reaction.	
	1.2.4 Acylation of carbanions.	
	UNIT- II, 1L/week	
	COURSE CODE: SIPSCHE23.2	
LEA	RNING OBJECTIVES:	
	1. To study and understand the principals involved in reactions and rearrangements with respect to their mechanism and stereochemistry.	
2 R	eactions and Rearrangements	15L

2.1	Mechanisms, stereochemistry (if applicable) and applications of the following		
	Reactions: Baylis - Hilman reaction, McMurry Coupling, Corey-Fuchs reaction, Nef reaction, Passerini reaction.		
2.2	Concerted rearrangements: Hofmann, Curtius, Lossen, Schmidt, Wolff, Boulton-Katritzky.		
2.3	Cationic rearrangements: Tiffeneau-Demjanov, Pummerer, Dienone-phenol, Rupe, Wagner-Meerwein.		
2.4	Anionic rearrangements: Brook, Neber, Von Richter, Wittig, Gabriel–Colman, Payne,		
	UNIT III, 1L/week		
COURSE CODE: SIPSCHE23.3			
LEARNING OBJECTIVES:			

- 1. To study the MOT in organic molecules using LCAO method and introduction to FMO and its application.
- 2. To understand the basic concept of ultraviolet and infrared spectroscopy and its application for structural determination of organic compounds.

3 Introduction to Molecular Orbital Theory for Organic Chemistry and Applications of

UV and IR spectroscopy

3.1	Introduction to Molecular Orbital Theory for Organic Chemistry:					
	3.1.1.Molecular orbitals: Formation of $\sigma$ - and $\pi$ -MOs by using LCAO method. Formation of $\pi$ MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of $\pi$ -MOs					
0	3.1.2.Introduction to FMOs: HOMO and LUMO and significance of HOMO-LUMO gap in absorption spectra as well as chemical reactions. MOs of formaldehyde: The effect of electronegativity perturbation and orbital polarization in formaldehyde. HOMO and LUMO ( $\pi$ and $\pi^*$ orbitals) of formaldehyde. A brief description of MOs of nucleophiles and electrophiles. Concept of 'donor-acceptor' interactions in nucleophilic addition reactions on formaldehyde. Connection of this HOMO- LUMO interaction with 'curved arrows' used in reaction mechanisms. The concept of hardness and softness and its application to electrophiles and nucleophiles. Examples of hard and soft nucleophiles/ electrophiles. Identification of hard and soft reactive sites on the basis of MOs.					
	3.13.Application of FMO concepts in (a) $S_N^2$ reaction, (b) Lewis acid base adducts (BF <sub>3</sub> -NH <sub>3</sub> complex), (c) ethylene dimerization to butadiene, (d) Diels-Alder cycloaddition, (e) regioselective reaction of allyl cation with allyl anion (f) addition of hydride to formaldehyde.					
3.2	Applications of UV and IR spectroscopy:					
	3.2.1 Ultraviolet spectroscopy: 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).

3.2.2 Infrared spectroscopy: 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.

### Unit – IV, 1L/week

### **COURSE CODE: SIPSCHE23.4**

### **LEARNING OBJECTIVES:**

1. To understand the principle and application of Nuclear Magnetic Resonance and Mass spectroscopy.

4 NM	R spectroscopy and Mass spectrometry	15L
4.1	Proton magnetic resonance spectroscopy: 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.	
4.2	<sup>13</sup> C NMR spectroscopy: 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.	
4.3	Mass spectrometry: Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, 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, ortho - effect.	
4.4	Structure determination involving individual or combined use of the above spectral techniques.	

### SUGGESTED REFERENCE SIPSCHE23

- 1. Organic Chemistry, J. Claydens, N. Greeves, S. Warren and P. Wothers, Oxford University Press.
- 2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Part A and B, Plenum Press.

- 3. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, Michael B. Smith, Jerry March, Wiley.
- 4. Organic Chemistry, R.T. Morrison, R.N. Boyd and S.K. Bhattacharjee, Pearson Publication (7<sup>th</sup> Edition)
- 5. Advanced Organic Chemistry: Reactions and mechanism, B. Miller and R. Prasad, Pearson Education.
- 6. Advanced Organic Chemistry: Reaction mechanisms, R. Bruckner, Academic Press.
- 7. Understanding Organic Reaction Mechanisms, Adams Jacobs, Cambridge University Press.
- 8. Writing Reaction Mechanism in organic chemistry, A. Miller, P.H. Solomons, Academic Press.
- 9. Principles of Organic Synthesis, R.O.C. Norman and J.M Coxon, Nelson Thornes.
- 10. Advanced Organic Chemistry: Reactions and mechanism, L.G. Wade, Jr., Maya Shankar Singh, Pearson Education.
- 11. Mechanism in Organic Chemistry, Peter Sykes, 6th
- 12. Molecular Orbital and Organic chemical reactions, Ian Fleming Reference Edition, Wiley
- 13. Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks.
- 14. Spectrometric Identification of Organic Compounds, R. Silverstein, G.C Bassler and T.C. Morrill, John Wiley and Sons.
- 15. Organic Spectroscopy, William Kemp, W.H. Freeman and Company.
- 16. Organic Spectroscopy-Principles and Applications, Jagmohan, Narosa Publication.
- 17. Organic Spectroscopy, V.R. Dani, Tata McGraw Hill Publishing Co.
- 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. Ellerd, and F.G. Favaloro, John Wiley and Sons.

### Paper IV: Analytical Chemistry

**CREDITS: 4** 

LECTURES: 60

UNIT-I, 1L/week

### COURSE CODE: SIPSCHE24.1

### **LEARNING OBJECTIVES:**

1. To study the concept and theories in chromatography.

2. To explore the learner to gas chromatography and High Performance Liquid Chromatography

### 15L **1** Chromatography 1.1 Recapitulation of basic concepts in chromatography: Classification of chromatographic methods, requirements of an ideal detector, types of detectors in LC and GC, comparative account of detectors with reference to their applications (LC and GC respectively), qualitative and quantitative analysis. 1.2 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. 1.3 Gas Chromatography: 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. 1.4 High Performance Liquid Chromatography (HPLC): Normal phase and reversed phase with special reference to types of commercially available columns (Use of C8 and C18) columns). Diode array type and fluorescence detector, Applications of HPLC. Chiral and ion chromatography. UNIT- II, 1L/week **COURSE CODE: SIPSCHE24.2 LEARNING OBJECTIVES:** 1. To study X-ray spectroscopy, Mass spectrometry and Radioanalytical Methods and its applications. 2 Instrumental methods of Chemical Analysis 15L 2.1 X-ray spectroscopy: principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy. 2.2 Mass spectrometry: recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: Quadrupole, time of flight and ion trap. Applications. 2.3 Radioanalytical Methods – recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications. UNIT III, 1L/week

	COURSE CODE: SIPSCHE24.3	
LEA	ARNING OBJECTIVES:	
1. T	o understand and study the principle involved in Surface Analytical Techniques.	
2. T	o study the principles, instrumentation and applications of atomic spectroscopy.	
3 S	urface Analytical Techniques and Atomic Spectroscopy	15L
3.1	Surface Analytical Techniques: Introduction, Principle, Instrumentation and Applications of	
	3.1.1 Scanning Electron Microscopy (SEM)	
	3.1.2 Scanning Tunneling Microscopy (STM)	
	3.1.3 Transmission Electron Microscopy (TEM)	
	3.1.4 Electron Spectroscopy (ESCA and Auger)	
3.2	Atomic Spectroscopy	
	3.2.1. Advantages and Limitations of AAS.	
	3.2.2 Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.	
	Unit – IV, 1L/week	
	COURSE CODE: SIPSCHE24.4	
LEA	ARNING OBJECTIVES:	
1.T	o study the Electroanalytical technique involving Ion Selective Potentiometry, Polarography, Electrogravimetry and Coulometry.	
4 Tł	nermal Methods	15L
4.1	Ion selective potentiometry: 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.	
4.2	Polarography: Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves.	
4.3	Electrogravimetry: Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications	
4.4	Coulometry: Introduction, principle, instrumentation, coulometry at controlled potential and controlled current.	

### SUGGESTED REFERENCE SIPSCHE24

### Unit I

1. Instrumental Analysis, Skoog, Holler and Amp; Crouch HPLC Practical and Industrial Applications, 2<sup>nd</sup> Ed., Joel K. Swadesh, CRC Press

### Unit II

- 1. Essentials of Nuclear Chemistry, H J Arnikar, New Age Publishers (2005)
- 2. Fundamentals of Radiochemistry D. D. Sood , A. V. R. Reddy and N. Ramamoorthy
- 3. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5th Edition, Ch: 12
- 4. Principles of Instrumental Analysis Skoog, Holler and Nieman, 5th Edition, Ch: 20

### Unit III

- 1. Instrumental Analysis by Douglas A. Skoog F. James Holler Crouch, Publisher: Cengage; Edition, (2003), ISBN-10: 8131505421, ISBN-13: 978-8131505427
- 2. Physical Principles of Electron Microscopy, An Introduction to TEM, SEM, and AEM
- 3. Authors: Ray F. Egerton, ISBN: 978-0- 387-25800- 3 (Print) 978-0- 387-26016- 7 (Online)
- 4. Modern techniques of surface science by D.P. Woodruff, T.A. Delchar, Cambridge Univ. Press, 1994.
- 5. Introduction to Scanning Tunneling Microscopy by C. J. Chen, Oxford University Press, NewYork, 1993.
- 6. 5. Transmission Electron Microscopy: A text book for Material Science, David B Williams and C., Barry Carter, Springer
- 7. Modern Spectroscopy, by J.M. Hollas, 3rd Edition (1996), John Wiley, New York
- 8. Principles of Instrumental Analysis Skoog, Holler, Nieman, 5th ed., Harcourt College Publishers, 1998.
- 9. Instrumental Analysis by Douglas A. Skoog, F. James Holler Crouch, Publisher: Cengage: Edition (2003), ISBN10: 8131505421.

### Unit IV

- 1. Principles of Instrumental Analysis Skoog, Holler, Nieman, 5<sup>th</sup> Edition, Harcourt College Publishers, 1998. Chapters 23, 24, 25.
- 2. Analytical Chemistry Principles John H Kennnedy, 2nd edition, Saunders College Publishing (1990).
- 3. Modern Analytical Chemistry David Harvey; McGraw Hill Higher education publishers, (2000).
- 4. Vogel's Text book of quantitative chemical analysis, 6th edition, Pearson Education Limited, (2007).
- 5. Electrochemical Methods Fundamentals and Applications, Allen J Bard and Larry R Faulkner, John Wiley and Sons, (1980).
- 6. Instrumental Methods of Analysis Willard, Merrit, Dean and Settle, 7th edition, CBS publishers.

# **Practical Paper I: Physical Chemistry Practical**

	(4L/Week)
1	Non – instrumental:
	1. Polar plots of atomic orbitals such as $1s$ , $2s$ , $p$ and $3s$ , $p$ orbitals by using angular part of hydrogen atom wave functions.
	2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.
	3. To study phase diagram of three component system water – chloroform /toluene - acetic acid.
	4. To determine the rate constant of decomposition reaction of diacetone alcohol by dilatometric method.
	Instrumental:
	1. To determine the formula of silver ammonia complex by potentiometric method.
	2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
	3. To determine Hammette constant of m- and p- amino benzoic acid/nitro benzoic acid by pH measurement.
	<ol> <li>To determine the Michaelis – Menten's constant value (Km) of the enzyme Beta Amylase spectrophotometrically.</li> </ol>
	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.
	1

### **Practical Paper II: Inorganic Chemistry Practical**

	(4L/Week)
In	organic Preparations (Synthesis and Characterization)
1)	Bis-(tetraethylammonium) tetrachloro Cuprate (II) (Et <sub>4</sub> N) <sub>2</sub> [CuCl4]
2)	Bis-(tetraethylammonium) tetrachloro Nickelate (II) (Et <sub>4</sub> N) <sub>2</sub> [NiCl <sub>4</sub> ]
3)	Bis-(tetraethylammonium) tetrachloro Cobaltate (II) (Et <sub>4</sub> N) <sub>2</sub> [CoCl <sub>4</sub> ]
	(Any two from the above preparations)
4)	Tetrammine monocarbanato Cobalt (III) Nitrate [Co(NH <sub>3</sub> ) <sub>4</sub> CO <sub>3</sub> ]NO <sub>3</sub>
5)	Bis (ethylenediammine) Copper (II) Sulphate [Cu(en) <sub>2</sub> ]SO <sub>4</sub>
6)	Hydronium dichloro bis(dimethylglyoximato) Cobaltate(III) H[Co(dmgH) <sub>2</sub> Cl <sub>2</sub> ]
In	strumentation
1)	Determination of equilibrium constant by Slope intercept method for Fe <sup>+3</sup> / SCN <sup>-</sup> system.
2)	Determination of Electrolytic nature of inorganic compounds by Conductance measurement.
R	eference:
1.	Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1 <sup>st</sup> Edn., 2010., U.N. Dhur and Sons Pvt. Ltd
2.	The Synthesis and Characterization of Inorganic Compounds by William L. Jolly.
	Inorgania Chemistry Practical under LICC Syllabus for M Sa, in all India Universitia

#### **Practical Paper III : Organic Chemistry Practical**

	(4L/Week)						
1	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:						
	(i) Water soluble/water insoluble solid and water insoluble solid.						
	<ul><li>(ii) Non-volatile liquid-Non-volatile liquid (chemical separation).</li><li>(iii) Water insoluble solid-Non-volatile liquid.</li></ul>						
	Minimum three mixtures from each type and a total of ten mixtures are expected.						
	Reference:						
	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.						

### Practical Paper IV: Analytical Chemistry Practical

		(4L/Week)
1	1.	To determine percentage purity of sodium carbonate in washing soda pH metrically.
	2.	To determine amount of Ti(III) and Fe(II) in a mixture by titration with Ce(IV) potentiometrically.
	3.	To determine the percentage purity of a sample (glycine/sodium benzoate/primary amine) by titration with perchloric acid in a non-aqueous medium using glass calomel system potentiometrically.
	4.	To determine the amount of nitrite present in the given water sample colorimetrically.
	5.	To determine the amount of Fe(II) and Fe(III) in a mixture using 1,10- phenanthroline spectrophotometrically.
	6.	Simultaneous determination of Cr(VI) and Mn(VII) in a mixture spectrophotometrically.
	7.	To determine the percentage composition of HCl and $H_2SO_4$ on weight basis in a mixture of two by conductometric titration with NaOH and BaCl <sub>2</sub> .
	8.	To determine amount of potassium in the given sample of fertilizer using flame photometer by standard addition method.
	Re	eferences:
	1.	Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel's, 3 <sup>rd</sup> edition ELBS
	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.	Standard Instrumental methods of Chemical Analysis, F. J. Welcher
	5.	W.W.Scott" Standard methods of Chemical Analysis", Vol. I, Van Nostrand Company, Inc.
5	6.	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.

#### **MODALITY OF ASSESSMENT**

#### THEORY EXAMINATION PATTERN:

- (A) Semester End Theory Internal Assessment 40 Marks
- (B) Semester End Theory Assessment 60 Marks (Duration These examinations shall be of two and half hours duration).

#### Theory question paper pattern:

- 1. There shall be **four** questions.
- 2. Each unit there will be one question with **15** Marks each.
- 3. All questions shall be **compulsory** with internal choices within the questions.

Question 1 (Unit-1),

Question 2 (Unit-2),

Question 3 (Unit-3) &

Question 4 (Unit-4).

- 4. All Questions may be sub divided into sub questions of **five** marks each.
- 5. Please ensure that the allocation of marks depends on the number of lectures allotted for each topic.

#### Marks distribution pattern for theory examination

Theory Examination	Paper I	Paper II	Paper III	Paper IV	Grand Total
Internal Assessment	40	40	40	40	160
Theory	60	60	60	60	240
Total Marks	100	100	100	100	400

### **II] PRACTICAL EXAMINATION PATTERN:**

### Scheme of examination: There will be no internal assessment for practical.

A candidate will be allowed to appear for the semester end practical examination only if the candidate submits a **certified journal** at the time of practical examination or a certificate from the Head of the Department/Institute to the effect that the candidate has completed the practical course of that semester of M.Sc. - I Chemistry as per the minimum requirement.

The duration of the practical examination will be **three and half hours** per experiment. The questions on slips for the same should be framed in such a way that candidate will be able to complete the task and should be evaluated for its skill and understanding of chemistry.

Note: Minimum 75% experiments of prescribed syllabus should be completed in the 1<sup>st</sup> and 2<sup>nd</sup> semester. Certified journal is a must to be eligible to appear for the semester end practical examination, failing which they will not be allowed to appear for the examination.

Marks distribution pattern for practical examination

Sr. No.	Practical Examination	Papers				Total
		P1	P2	Р3	P4	IUtal
1.	Experiment	40	40	40	40	160
2.	Journal	05	05	05	05	20
3.	Viva Voce	05	05	05	05	20
Practical Marks		50	50	50	50	200

### **Overall Examination and Marks Distribution Pattern**

Semester End Examination	Paper I	Paper II	Paper III	Paper IV	Grand Total
Internal Assessment	40	40	40	40	160
Theory	60	60	60	60	240
Practical	50	50	50	50	200
Total Marks	150	150	150	150	600

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