SIES

College of Arts, Science & Commerce

RISE WITH EDUCATION

Sion (West), Mumbai – 400022.

Autonomous

Department of Chemistry

Program: M.Sc.

Course: Chemistry

Syllabus for M.Sc. Semester I & II

(Implemented from 2018 – 2019)

Credit Based Semester and Grading System

SEMESTER - I

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SIPSCHE22.4	:	Bioinorganic Chemistry
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SIPSCHE23.1	:	Alkylation of Nucleophilic Carbon Intermediates and Reaction of carbon nucleophiles with carbonyl groups
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SIPSCHE24.3	:	Surface Analytical Techniques and Atomic Spectroscopy
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Practical		
SIPSCHE2P1	:	Physical Chemistry Practical
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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 **LEARNING OBJECTIVES:** *1) To learn the concept of exact differentials in relation to thermodynamics.* *2) Importance of third law of thermodynamics.* *3) Application of standard molar entropies.*		
1 Thermodynamics - 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 **LEARNING OBJECTIVES:** *1. To learn the need for quantum mechanics.* *2. Application of Schrodinger wave equation.* 3. *To study different types of operators and harmonic oscillator.*		
2 Quantum 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, 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.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHE11.3 **LEARNING OBJECTIVES:** *1. To study the kinetics of polymerisation reaction and reaction in gas phase.*		
3 Chemical Dynamics - I		**15L**
3.1	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.	
3.2	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.	
3.3	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 **LEARNING OBJECTIVES:** *1.To understand Debye Huckel, Onsager equation and its applications to aqueous and non-*		

aqueous solution. *2.To study different kinds of fuel cells and its applications.* *3.To introduce the learner to concept in Bio*-electrochemistry.		
4. Electrochemistry		**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, 7th Edn., 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, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, Physical Chemistry, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, Physical Chemistry, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, Text Book of Physical Chemistry, 2nd 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, 2nd 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, 3rd Edn., Pearson Education Limited 2013.
15. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st 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, 2nd Edn

Course Code: SIPSCHE12

Paper II: Inorganic Chemistry

CREDITS: 4 **LECTURES: 60**

UNIT- I , 1L/week		
Course Code: SIPSCHE12.1 **LEARNING OBJECTIVES:** *1) To study the concept of hybridization and molecular orbital theory.* *2) Application 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 σ bonding for SF_6, CO_2, B_2H_6, I_3^- 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 **LEARNING OBJECTIVES:** *1. To study the primary understanding of Group Theory and Molecular Symmetry.*		
2 Molecular 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_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.	
UNIT III, 1L/week		
Course Code: SIPSCHE12.3 **LEARNING 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 Materials 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_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)	
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 **LEARNING OBJECTIVES:** 1. *To study the spectral properties Coordination compound.* 2. *To learn spectral calculations*		

4 Characterization of Coordination compounds		15L
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 Δ, β, 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 Eastern Ltd., 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 **LEARNING 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.*	

1 Physical Organic Chemistry		**15L**
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 *vs* selectivity, Curtin-Hammett Principle, microscopic reversibility, kinetic *vs* 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 **LEARNING 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 Nucleophilic 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, σ- and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. S_NcA, 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 **OBJECTIVES:**		

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

3 Stereochemistry:		**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

OBJECTIVES:

1. *To study general mechanism, selectivity, and important applications of oxidation and reduction reactions using different reagents.*

4 Oxidation and Reduction		**15L**
4.1	Oxidation: General mechanism, selectivity, and important applications of the following: 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). 4.1.2. Oxidation of alcohols to aldehydes and ketones: Chromium reagents such as $K_2Cr_2O_7/H_2SO_4$ (Jones reagent), CrO_3-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. 4.1.3. Oxidation involving C-C bonds cleavage: Glycols using HIO_4, cycloalkanones using	

	CrO_3; carbon-carbon double bond using ozone, $KMnO_4$, CrO_3, $NaIO_4$ and OsO_4; aromatic rings using RuO_4 and $NaIO_4$. 4.1.4. Oxidation involving replacement of hydrogen by oxygen: oxidation of CH_2 to CO by SeO_2, oxidation of arylmethanes by CrO_2Cl_2 (Etard oxidation). 4.1.5. Oxidation of aldehydes and ketones: with H_2O_2 (Dakin reaction), with peroxy acid (Baeyer-Villiger oxidation)	
4.2	Reduction: General mechanism, selectivity, and important applications of the following reducing reagents: 4.2.1. Reduction of CO to CH_2 in aldehydes and ketones- Clemmensen reduction, Wolff-Kishner reduction and Huang-Minlon modification. 4.2.2. Metal hydride reduction: Boron reagents ($NaBH_4$, $NaCNBH_3$, diborane, 9-BBN, $Na(OAc)_3BH$, aluminium reagents ($LiAlH_4$, DIBAL-H, Red Al, L and K- selectrides). 4.2.3. NH_2NH_2 (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_3 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.

Course Code: SIPSCHE14

Paper IV: Analytical Chemistry

CREDITS: 4 **LECTURES: 60**

UNIT- I , 1L/week		
COURSE CODE: SIPSCHE14.1 **LEARNING OBJECTIVES:** 1. *To understand the language of analytical chemistry.* 2. *To learn basic concept of safety in laboratories.* 3. *To give learner an idea of good laboratory practice.*		
1 Language 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. 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 Laboratories: 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		**15L**
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**

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 **LEARNING OBJECTIVES:** 1. *To study the various thermal methods and it application.* 2. *To understand the need for automation in chemical analysis.*		
4 Thermal 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).	

	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.	
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, 5th Edition, Ch: 1.
3. Fundamentals of Analytical Chemistry, By Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Edition, 2004, Ch: 5.
4. Undergraduate Instrumental Analysis, 6th 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 andCh: 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, 5th 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
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, 7th Edition, Willard, Merrit, Dean: Chapter 25.
4. Instrumental Analysis, 5th Edition, Skoog, Holler and Nieman: Chapter 31.
5. Quantitative Chemical Analysis, 6th 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, 7th Edition, Willard, Merrit, Dean: Chapter 26.
8. Instrumental Analysis, 5th 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 (ΔH) 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 $CaSO_4$ at room temperature. 3. To investigate the reaction between acetone and iodine. 4. To study the variation in the solubility of $Ca(OH)_2$ in presence of NaOH and hence to determine the solubility product of $Ca(OH)_2$ 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, 3rd Edn., Longman Group Ltd., 1974. 3 Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Course Code: SIPSCHE1P2

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:** 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhur and 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. by: Dr Deepak Pant.

Course Code: SIPSCHE1P3

Practical Paper III : Organic Chemistry Practical

CREDITS: 2

	(4L/Week)
1	**One step preparations (1.0 g scale)** 1. Bromobenzene to *p*-nitrobromobenzene. 2. Anthracene to anthraquinone. 3. Benzoin to benzyl. 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. **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

CREDITS: 2

(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 by A. I. Vogels, 3rd Ed. 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. 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 Chemical Thermodynamics - II		**15L**
1.1	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		
COURSE CODE: SIPSCHE21.2 **LEARNING OBJECTIVES:** 1. *To understand the concept of quantum chemistry with respect to rigid rotor, quantization of rotational energy, spherical harmonics.* 2. *To study the applications of Schrondiger equation for electron system*		
2 Quantum 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	Hydrogen atom, the two particle problem, separation of the energy as translational and potential, separation of variables, the R the θ* and the ϕ equations, solution of the requation, 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.	
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.	
2.4	Hückel Molecular Orbitals theory for ethylene, 1, 3-butadiene and benzene.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHE21.3 **LEARNING OBJECTIVES:** 1. *To study the principles of chemical kinetics at molecular reaction dynamics.*		
3 Chemical Kinetics and Molecular Reaction Dynamics		**15L**
3.1	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	Kinetics of reactions catalyzed by enzymes - Michaelis-Menten analysis, Lineweaver - Burk and Eadie Analysis.	
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.	
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 **LEARNING OBJECTIVES:** 1. *To understand the principle involved in solid state chemistry at phase equilibria.*		
4. Solid State Chemistry and Phase Equilibria		**15L**
4.1	Solid State Chemistry 4.1.1. Recapitulation: Structures and Defects in solids.	

	Types of Defects and Stoichiometry a) Zero dimensional (point) Defects. b) One dimensional (line) Defects. c) Two dimensional (Planar) Defects. d) Thermodynamics of formation of defects (Mathematical derivation to find concentration 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. Three component system Type-I : Formation of one pair of partially miscible liquids. Type-II: Formation of two pairs of partially miscible liquids. Type-III: Formation of three pairs of partially miscible liquids.	

SUGGESTED REFERENCE SIPSCHE21

1. Peter Atkins and Julio de Paula, Atkin's *Physical Chemistry*, 7th Edn., 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*, 3rd Edn., John Wiley and Sons (Asia) Pte. Ltd., 2002.
4. Ira R. Levine, *Physical Chemistry*, 5th Edn., Tata McGraw-Hill New Delhi, 2002.
5. G.W. Castellan, *Physical Chemistry*, 3rd Edn., Narosa Publishing House, New Delhi, 1983.
6. S. Glasstone, *Text Book of Physical Chemistry*, 2nd Edn., McMillan and Co. Ltd., London, 1962.
7. Principles of Chemical Kinetics, 2nd 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*, 2nd 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, 3rd Edn., Pearson Education Limited 2013.
16. D.N. Bajpai, Advanced Physical Chemistry, S. Chand 1st 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 5th 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		
Course Code: SIPSCHE22.1 **LEARNING 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	Ligand substitution reactions of: a. Octahedral complexes without breaking of metal-ligand bond (Use of isotopic labelling method) b. Square planar complexes, trans-effect, its theories and applications. Mechanism and factors affecting these substitution reactions.	

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 **LEARNING OBJECTIVES:** *1. To study Organometallic Chemistry of Transition metals in details.*	
2 Organometallic 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) $[Pt(PPh_3)_2(HC{\equiv}CPh)_2]$, diallylnickel(II), ferrocene and bis (arene) chromium (0), tricarbonyl (η^2-butadiene) iron (0).	
	UNIT III, 1L/week	
	Course Code: SIPSCHE22.3 **LEARNING OBJECTIVES:** 1. *To understand the harmful effect of heavy metals on environment and their toxicity.* 2. *To do case studies of specific metal toxicity.*	
3 Environmental Chemistry		**15L**
3.1	Conception of Heavy Metals: Critical discussion on heavy metals.	
3.2	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.	

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

LEARNING OBJECTIVES:

1.To study the principle of Bioinorganic Chemistry.

4 Bioinorganic Chemistry		**15L**
4.1	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.	
4.2	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.	
4.3	Copper containing enzymes- superoxide dismutase, tyrosinase and laccase: catalytic reactions and the structures of the metal binding site.	
4.4	Nitrogen fixation - nitrogenase, hydrogenases.	
4.5	Metal ion transport and storage:Ionophores, transferrin, ferritin and metallothionins.	
4.6	Medicinal applications of cis - platin and related compounds.	

SUGGESTED REFERENCE SIPSCHE12.2

Unit I

1. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Inorganic Chemistry, 5th 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, 8th 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, 2nd Ed., Kluwer Academic/ Plenum Publishers, 2002

6. Gurdeep Raj, Advanced Inorganic Chemistry-Vol.II, 12th 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, 2nd 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, 2nded, New Age International Pvt Ltd, 2000.
3. R.H Crabtree, The Organometallic Chemistry of the Transition Metals, 5th edition, Wiley International Pvt, Ltd 2000.
4. B.Doughlas, D.H McDaniel and J.J Alexander. Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons. 1983.
5. Organometallic Chemistry by G.S Sodhi. Ane Books Pvt Ltd.

Unit III

1. Environmental Chemistry 5th edition, Colin Baird Michael Cann, W. H. Freeman and Company, New York, 2012.
2. Environmental Chemistry 7th edition, Stanley E. Manahan, CRC Press Publishers,
3. Environmental Contaminants, Daniel A. Vallero, ISBN: 0-12-710057-1, Elsevier Inc., 2004.
4. Environmental Science 13th 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 4th edition, Stanley E. Manahan, ISBN: 978-1-4665-5317-0, CRC Press Taylor and Francis Group, 2013.
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
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 6th 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.
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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 **LEARNING OBJECTIVES:** *1. To study the alkylation of nucleophilic carbon intermediates.*		
1 Physical 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 **LEARNING OBJECTIVES:** *1. To study and understand the principals involved in reactions and rearrangements with respect to their mechanism and stereochemistry.*		
2 Reactions 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	**15L**
3.1	Introduction to Molecular Orbital Theory for Organic Chemistry: 3.1.1. Molecular orbitals: Formation of σ- and π-MOs by using LCAO method. Formation of π MOs of ethylene, butadiene, 1, 3, 5-hexatriene, allyl cation, anion and radical. Concept of nodal planes and energies of π-MOs 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 (π and π* 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. 3.1.3. Application of FMO concepts in (a) S_N^2 reaction, (b) Lewis acid base adducts (BF_3-NH_3 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 NMR 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	^{13}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^{th} 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.

Course Code: SIPSCHE24

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.*		
1 Chromatography		**15L**
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 **LEARNING OBJECTIVES:** *1. To understand and study the principle involved in Surface Analytical Techniques.* *2. To study the principles, instrumentation and applications of atomic spectroscopy.*		
3 Surface 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 **LEARNING OBJECTIVES:** *1. To study the Electroanalytical technique involving Ion Selective Potentiometry, Polarography, Electrogravimetry and Coulometry.*		
4 Thermal 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, 2nd 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, 5th 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.

Course Code: SIPSCHE2P1

Practical Paper I: Physical Chemistry Practical

CREDITS: 2

	(4L/Week)
1	**Non – instrumental:** 1. Polar plots of atomic orbitals such as 1*s*, 2*s*,*p* and 3*s*,*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. 4. To determine the Michaelis – Menten's constant value (Km) 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, 3rd Edition, Longman Group Ltd., 1974. 3. Experimental Physical Chemistry, V.D. Athawale and P. Mathur, New Age International Publishers, 2001.

Course Code: SIPSCHE2P2

Practical Paper II: Inorganic Chemistry Practical

CREDITS: 2

	(4L/Week)
1	**Inorganic Preparations (Synthesis and Characterization)** 1) Bis-(tetraethylammonium) tetrachloro Cuprate (II) $(Et_4\ N)_2[CuCl4]$ 2) Bis-(tetraethylammonium) tetrachloro Nickelate (II) $(Et_4\ N)_2\ [NiCl_4]$ 3) Bis-(tetraethylammonium) tetrachloro Cobaltate (II) $(Et_4\ N)_2[CoCl_4]$ (**Any two** from the above preparations) 4) Tetrammine monocarbanato Cobalt (III) Nitrate $[Co(NH_3)_4CO_3]NO_3$ 5) Bis (ethylenediammine) Copper (II) Sulphate $[Cu(en)_2]SO_4$ 6) Hydronium dichloro bis(dimethylglyoximato) Cobaltate(III) $H[Co(dmgH)_2Cl_2]$ **Instrumentation** 1) Determination of equilibrium constant by Slope intercept method for Fe^{+3}/ SCN^- system. 2) Determination of Electrolytic nature of inorganic compounds by Conductance measurement. **Reference:** 1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N. Dhur and 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.

Course Code: SIPSCHE2P3

Practical Paper III : Organic Chemistry Practical

CREDITS: 2

	(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. (ii) Non-volatile liquid-Non-volatile liquid (chemical separation). (iii) Water insoluble solid-Non-volatile liquid. **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.

Course Code: SIPSCHE2P4

Practical Paper IV: Analytical Chemistry Practical

CREDITS: 2

(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 $BaCl_2$. 8. To determine amount of potassium in the given sample of fertilizer using flame photometer by standard addition method. **References:** 1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogel's, 3rd 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. 6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals", Part- II, 4th 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 1st and 2nd 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	P3	P4	
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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SIES

College of Arts, Science & Commerce

RISE WITH EDUCATION

Sion (West), Mumbai – 400022.

Autonomous

Program: M.Sc.

Course: Organic Chemistry

Syllabus for M. Sc. Semester III and IV

(Implemented from 2018 – 2019)

Credit Based Semester and Grading System

SEMESTER III

Contents:		
Paper I	:	**Theoretical organic chemistry-I**
SIPSCHEO31.1	:	Organic reaction mechanisms
SIPSCHEO31.2	:	Pericyclic reactions
SIPSCHEO31.3	:	Stereochemistry-I
SIPSCHEO31.4	:	Photochemistry
Paper II	:	**Synthetic Organic Chemistry-I**
SIPSCHEO32.1	:	Name reactions with mechanism and application
SIPSCHEO32.2	:	Radicals in organic synthesis
SIPSCHEOO2.3	:	Enamines, ylides and α-C-H functionalization
SIPSCHEO32.4	:	Metals / non-metals in organic synthesis
Paper III	:	**Natural products and Spectroscopy**
SIPSCHEO33.1	:	Natural products-I
SIPSCHEO33.2	:	Natural products-II
SIPSCHEO33.3	:	Advanced spectroscopic techniques-I
SIPSCHEO33.4	:	Advanced spectroscopic techniques-II
Paper IV	:	**Medicinal , Biogenesis and green chemistry**
SIPSCHEOE-I-34.1	:	Drug discovery, design and development
SIPSCHEOE-I-34.2	:	Drug design, development and synthesis
SIPSCHEOE-I-34.3	:	Biogenesis and biosynthesis of natural products
SIPSCHEOE-I-34.4	:	Green chemistry
Practical		
SIPSCHEO3P1	:	Separation of a solid ternary mixture using micro-scale technique
SIPSCHEO3P2	:	Estimation of drugs
SIPSCHEO3P3	:	Organic preparations (1.0 g scale)
SIPSCHEO3P4	:	Single step organic preparation (1.0 g scale) involving, techniques of purification and green methods of synthesis

SEMESTER IV

Contents:		
Paper I	:	**Theoretical organic chemistry-II**
SIPSCHEO41.1	:	Physical organic chemistry
SIPSCHEO41.2	:	Supramolecular chemistry
SIPSCHEO41.3	:	Stereochemistry-II
SIPSCHEO41.4	:	Asymmetric synthesis
Paper II	:	**Synthetic Organic Chemistry-II**
SIPSCHEO42.1	:	Designing organic synthesis-I
SIPSCHEO42.2	:	Designing organic synthesis-II
SIPSCHEO42.3	:	Electro-organic chemistry and selected methods of organic synthesis
SIPSCHEO42.4	:	Transition and rare earth metals in organic synthesis
Paper III	:	**Natural products and heterocyclic chemistry**
SIPSCHEO43.1	:	Natural products-III
SIPSCHEO43.2	:	Natural products-IV
SIPSCHEO43.3	:	Heterocyclic compounds-I
SIPSCHEO43.4	:	Heterocyclic compounds-II
Paper IV	:	**Intellectual property rights and cheminformatics**
SIPSCHEOE-I-44.1	:	Introduction to intellectual property
SIPSCHEOE-I-44.2	:	Trade secrets
SIPSCHEOE-I-44.3	:	Introduction to cheminformatics
SIPSCHEOE-I-44.4	:	Applications
Practical		
SIPSCHEO4P1	:	Separation of solid-liquid/ liquid-liquid ternary mixture using micro-scale technique
SIPSCHEO4P2	:	Identification of any unknown organic compound with preparation, purification and physical constant of derivative. (minimum 8 organic compounds)
SIPSCHEO4P3	:	Isolation / estimation of natural products
SIPSCHEO4P4	:	Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and mass spectra).

M.Sc. Organic Chemistry
Semester-III

Course Code: SIPSCHEO31 Credits: 04
Paper - I
Theoretical organic chemistry-I

Learning Objectives:

1. *To learn the reactive intermediates and mechanism in organic synthesis.*
2. *To study pericyclic reactions and their types with mechanism.*
3. *To understand the stereochemistry of reactants, intermediates and products.*
4. *To study various types of photochemical reactions with mechanism.*

Unit 1	**ORGANIC REACTION MECHANISMS**	**[15L]**
1.1	Organic reactive intermediates, methods of generation, structure, stability and important reactions involving carbocations, nitrenes, carbenes, arynes and ketenes**.**	**[5L]**
1.2	Neighbouring group participation**:** Mechanism and effects of anchimeric assistance, NGP by unshared/ lone pair electrons, π-electrons, aromatic rings, σ-bonds with special reference to norbornyl and bicyclo[2.2.2]octyl cation systems (formation of non-classical carbocation)	**[3L]**
1.3	Role of FMOs in organic reactivity**:** Reactions involving hard and soft electrophiles and nucleophiles, ambident nucleophiles, ambident electrophiles and α effect.	**[2L]**
1.4	Pericyclic reactions: Classification of pericyclic reactions; thermal and photochemical reactions. Three approaches: Evidence for the concertedness of bond making and breaking Symmetry-Allowed and Symmetry-Forbidden Reactions – • The Woodward-Hoffmann Rules-Class by Class • The generalised Woodward-Hoffmann Rule Explanations for Woodward-Hoffmann Rules • The Aromatic Transition structures [Huckel and Mobius] • Frontier Orbitals • Correlation Diagrams, FMO and PMO approach Molecular orbital symmetry, Frontier orbital of ethylene, 1,3 butadiene, 1,3,5 hexatriene and allyl system.	**[5L]**

Unit 2	**PERICYCLIC REACTIONS**	**[15L]**
2.1	Cycloaddition reactions: Supra and antra facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes. Diels-Alder reactions, 1, 3-Dipolar cycloaddition and cheletropic reactions, ene reaction, retro-Diels-Alder reaction, regioselectivity, periselectivity, torquoselectivity, site selectivity and effect of substituents in Diels-Alder reactions. Other Cycloaddition Reactions- [4+6] Cycloadditions, Ketene Cycloaddition, Allene Cycloadditions, Carbene Cycloaddition, Epoxidation and Related Cycloadditions. Other Pericyclic reactions: Sigmatropic Rearrangements, Electrocyclic Reactions, Alder 'Ene' Reactions.	**[7L]**
2.2	Electrocyclic reactions: Conrotatory and disrotatary motions, 4nπ and [4n+2]π electron and allyl systems.	**[3L]**
2.3	Sigmatropic rearrangements: H-shifts and C-shifts, supra and antarafacial migrations, retention and inversion of configurations. Cope (including oxy-Cope and aza-Cope) and Claisen rearrangements. Formation of Vitamin D from 7-dehydrocholesterol, synthesis of citral using pericyclic reaction, conversion of Endiandric acid E to Endiandric acid A.	**[5L]**
Unit 3:	**STEREOCHEMISTRY-I**	**[15L]**
3.1	Classification of point groups based on symmetry elements with examples (nonmathematical treatment).	**[2L]**
3.2	Conformational analysis of medium rings: Eight to ten membered rings and their unusual properties**,** I-strain, transannular reactions.	**[3L]**
3.3	Stereochemistry of fused ring and bridged ring compounds: decalins, hydrindanes, perhydroanthracenes, steroids, and Bredt's rule.	**[5L]**
3.4	**Anancomeric systems,** Effect of conformation on reactivity of cyclohexane derivatives in the following reactions (including mechanism): electrophilic addition, elimination, molecular rearrangements, reduction of cyclohexanones **(with $LiAlH_4$, selectride and MPV reduction)** and oxidation of cyclohexanols**.**	**[5L]**

Unit 4	PHOTOCHEMISTRY	[15L]
4.1	Principles of photochemistry: quantum yield, electronic states and transitions, selection rules, modes of dissipation of energy (Jablonski diagram), electronic energy transfer: photosensitization and quenching process.	**[3L]**
4.2	Photochemistry of carbonyl compounds: $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions, Norrish-I and Norrish-II cleavages, Paterno-Buchi reaction. Photoreduction, calculation of quantum yield, photochemistry of enones, photochemical rearrangements of α, β-unsaturated ketones and cyclohexadienones. Photo Fries rearrangement, Barton reaction.	**[8L]**
4.3	Photochemistry of olefins: cis-trans isomerizations, dimerizations, hydrogen abstraction, addition and Di- π- methane rearrangement including aza-di- π -methane. Photochemical Cross-Coupling of Alkenes, Photodimerisation of alkenes.	**[2L]**
4.4	Photochemistry of arenes**:** 1, 2- , 1, 3- and 1, 4- additions. Photocycloadditions of aromatic Rings.	**[1L]**
4.5	Singlet oxygen and photo-oxygenation reactions. Photochemically induced Radical Reactions. Chemiluminescence.	**[1L]**

REFERENCES:

1. March's Advanced Organic Chemistry, Jerry March, sixth edition, 2007, John Wiley and sons.
2. Advanced organic chemistry, Jagdamba Singh L. D. S. Yadav, Pragati Prakashan, 2011
3. A guide to mechanism in Organic Chemistry, 6th edition, 2009, Peter Sykes, Pearson education, New Delhi.
4. Advanced Organic Chemistry: Reaction Mechanisms, R. Bruckner, Academic Press (2002).
5. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers
6. Crown ethers and analogous compounds, M. Hiraoka, Elsevier, 1992.
7. Carbenes, Nitrenes and Arynes. Von T. L. Gilchrist, C. W. Rees. Th. Nelson and Sons Ltd., London 1969.
8. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
9. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
10. Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
11. Mechanism and theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.
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Course Code: SIPSCHEO32 **Credits: 04**

Paper-II

Synthetic Organic Chemistry-I

Learning Objectives:

1. *To learn various name reactions in organic synthesis.*
2. *To study organic free radical and their importance in organic synthesis.*
3. *To understand the applications of enamines, ylides and α C-H functionalization in organic synthesis.*

4.	*To know the applications of organometallic compounds in organic synthesis.*	
Unit 1:	**NAME REACTIONS WITH MECHANISM AND APPLICATION**	**[15L]**
1.1	Mukaiyama esterification, Mitsunobu reaction, Darzen's Glycidic Ester syntheis, Ritter reaction, Yamaguchi esterification, Peterson olefination.	**[5L]**
1.2	**Domino reactions**: Characteristics; Nazerov cyclization	**[3L]**
1.3	**Multicomponent reactions**: Strecker Synthesis, Ugi 4CC, Biginelli synthesis, Hantzsch synthesis, Pictet-Spengler synthesis	**[5L]**
1.4	**Click Reactions**: Characteristics, Huisgen 1,3-Dipolar Cycloaddition.	**[2L]**
Unit 2:	**RADICALS IN ORGANIC SYNTHESIS**	**[15L]**
2.1	**Introduction:** Generation, stability, reactivity structural and stereochemical properties of free radicals, Persistent and charged radicals, Electrophilic and nucleophilic radicals.	[3L]
2.2	**Radical Initiators**: azobisisobutyronitrile (AIBN) and dibenzoyl peroxide.	[1L]
2.3	**Characteristic reactions** - Free radical substitution, addition to multiple bonds. Radical chain reactions, radical halogenation of hydrocarbons (Regioselectivity), radical cyclizations, autoxidations: synthesis of cumene hydroperoxide from cumene.	[4L]
2.4	**Radicals in synthesis**: Inter and intra molecular C-C bond formation via mercuric hydride, tin hydride, thiol donors. Cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds. Oxidative coupling, C-C bond formation in aromatics: S_NAr reactions.	[4L]
2.5	Hunsdiecker reaction, Pinacol coupling, McMurry coupling, Sandmeyer reaction, Acyloin condensation.	[3L]
Unit 3:	**ENAMINES, YLIDES AND A-C-H FUNCTIONALIZATION**	**[15]**
3.1	**Enamines:** Generation and application in organic synthesis with mechanistic pathways, Stork enamine reaction. Reactivity, comparison between enamines and enolates. Synthetic reactions of enamines including asymmetric reactions of chiral enamines derived from chiral secondary amines.	[4L]

3.2	**Phosphorus, Sulfur and Nitrogen Ylides:** Preparation and their synthetic applications along with their stereochemical aspects. Wittig reaction, Horner-Wadsworth-Emmons Reaction, Barton-Kellogg olefination.	[6L]
3.3	**α-C-H functionalization:** By nitro, sulfoxide, sulfone and phosphonate groups: generation of carbanions by strong bases (LDA/n-butyl lithium) and applications in C-C bond formation. Bamford-Stevens reaction, Julia olefination and its modification, Seyferth–Gilbert homologation, Steven's rearrangement.	[5L]
Unit 4:	**METALS / NON-METALS IN ORGANIC SYNTHESIS**	**[15]**
4.1	**Mercury in organic synthesis:** Mechanism and regiochemistry of oxymercuration and demercuration of alkenes, mercuration of aromatics, transformation of aryl mercurials to aryl halides. Organomercurials as carbene transfer reagents.	[3L]
4.2	**Organoboron compounds:** Mechanism and regiochemistry of hydroboration of alkenes and alkynes, asymmetric hydroboration using chiral boron reagents, 9-BBN hydroboration, oxazaborolidine (CBS catalyst) and functional group reduction by diborane.	[3L]
4.3	**Organosilicons:** Salient features of silicon governing the reactivity of organosilicons, preparation and important bond-forming reactions of alkyl silanes, alkenyl silanes, aryl silanes and allyl silanes. β-silyl cations as intermediates. Iodotrimethylsilane in organic synthesis.	[3L]
4.4	**Silyl enol ethers:** Application: As nucleophiles (Michael reaction, Mukaiyama aldol reaction), in ring contraction reactions.	[2L]
4.5	**Organotin compounds**: Preparation of alkenyl and allyl tin compounds; application in C-C bond formation, in replacement of halogen by H at the same C atom.	[2L]
4.6	**Selenium in organic synthesis:** Preparation of selenols/selenoxide, selenoxide elimination to create unsaturation, selenoxide and seleno acetals as α-C-H activating groups.	[2L]

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Course Code: SIPSCHEO33 Credits: 04

Paper-III

Natural products and Spectroscopy

Learning Objectives:

1. *To learn the basic concepts involved in natural products.*
2. *To study the multi-step synthesis of various natural products.*
3. *To learn the advance spectroscopic technique for analysis of organic compound.*
4. *To understand advance instrumental techniques for compound interpretation and identification.*

Unit 1:	**NATURAL PRODUCTS-I**	**[15L]**
1.1	**Carbohydrates:** Introduction to naturally occurring sugars: Deoxysugars, aminosugars, branched sugars. Structure elucidation of lactose and D-glucosamine (synthesis not expected).Structural features and applications of inositol, starch, cellulose, chitin and heparin**.**	[5L]
1.2	**Natural pigments:** General structural features, occurrence, biological importance and applications of: carotenoids, anthocyanins, quinones, flavones, pterins and porphyrins (chlorophyll). Structure elucidation of β-carotene and Cyanin (with synthesis). Synthesis of ubiquinone from 3, 4, 5-trimethoxyacetophenone.	[5L]
1.3	**Insect pheromones:** General structural features and importance. Types of pheromones (aggregation, alarm, releaser, primer, territorial, trail, sex pheromones etc.), advantage of pheromones over conventional pesticides. Synthesis of bombykol from acetylene, disparlure from 6-methylhept-1-ene, grandisol from 2-methyl-1, 3-butadiene**.**	[3L]

1.4	**Alkaloids:** Occurrence and physiological importance of morphine and atropine. Structure elucidation, spectral data and synthesis of coniine.	[2L]
Unit 2:	**NATURAL PRODUCTS-II**	**[15L]**
2.1	**Multi-step synthesis of natural products:** Synthesis of the following natural products with special reference to reagents used, stereochemistry and functional group transformations:	[8L]
	a) Woodward synthesis of Reserpine from benzoquinone	
	b) Corey synthesis of Longifoline from resorcinol	
	c) Gilbert-Stork synthesis of Griseofulvin from phloroglucinol	
	d) Corey's Synthesis of Caryophyllene from 2-Cyclohexenone and Isobutylene	
	e) Synthesis of Juvabione from Limonene	
	f) Synthesis of Taxol.	
2.2	**Prostaglandins:** Classification, general structure and biological importance. Structure elucidation of **PGE_1**.	[2L]
2.3	**Lipids:** Classification, role of lipids, Fatty acids and glycerol derived from oils and fats.	[2L]
2.4	**Insect growth regulators:** General idea, structures of JH_2 and JH_3 .	[1L]
2.5	**Plant growth regulators:** Structural features and applications of arylacetic acids, gibberellic acids and triacontanol. Synthesis of triacontanol (synthesis of stearyl magnesium bromide and 12-bromo-1 tetrahydropyranyloxydodecane expected).	[2L]
Unit 3:	**ADVANCED SPECTROSCOPIC TECHNIQUES-I**	**[15L]**
3.1	**Proton NMR spectroscopy:** Recapitulation, chemical and magnetic equivalence of protons, first order, second order, Spin system notations (A_2, AB, AX, AB_2, AX_2, AMX and A_2B_2-A_2X_2 spin systems with suitable examples). Long range coupling (Allylic coupling, 'W' coupling and Coupling in aromatic and heteroaromatic systems), Temperature effects, Simplification of complex spectra, nuclear magnetic double resonance, chemical shift reagents.	[7L]

3.2	**^{13}C –NMR spectroscopy:** Recapitulation, equivalent and non-equivalent carbons (examples of aliphatic and aromatic compounds), **^{13}**C- chemical shifts, calculation of ^{13}C- chemical shifts of aromatic carbons, heteronuclear coupling of carbon to ^{19}F and **^{31}**P.	[4L]
3.3	Spectral problems based on UV, IR, ^{1}HNMR and ^{13}CNMR and Mass spectroscopy.	[4L]
Unit 4:	**ADVANCED SPECTROSCOPIC TECHNIQUES-II**	**[15L]**
4.1	**Advanced NMR techniques:** DEPT experiment, determining number of attached hydrogens (Methyl/methylene/methine and quaternary carbons), two dimensional spectroscopic techniques, COSY and HETCOR spectra, NOE, NOESY and ROESY techniques.	[10L]
4.2	Spectral problems based on UV, IR, ^{1}HNMR, ^{13}CNMR (Including 2D technique) and Mass spectroscopy	[5L]

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Course Code: SIPSCHEOE-I-34 Credits: 04

Paper-IV

Medicinal , Biogenesis and green chemistry

Learning Objectives:

1. *To learn the basic terminology involved in medicinal organic chemistry.*
2. *To study quantitative structure activity relationship in drug discovery, designing.*
3. *To learn primary and secondary metabolites and their importance in biogenesis.*
4. *To learn basic principles of green chemistry and its applications.*

Unit 1:	**DRUG DISCOVERY, DESIGN AND DEVELOPMENT**	**[15L]**
1.1	Introduction, important terms used in medicinal chemistry: receptor, therapeutic index, bioavailability, drug assay and drug potency. General idea of factors affecting bioactivity: Resonance, inductive effect, bioisosterism, spatial considerations. Basic pharmacokinetics: drug absorption, distribution, metabolism (biotransformation) and elimination. Physical and chemical parameters like solubility, lipophilicity, ionization, pH, redox potential, H-bonding, partition coefficient and isomerism in drug distribution and drug-receptor binding.	[7L]
1.2	Procedures in drug design: Drug discovery without a lead: Penicillin, Librium. Lead discovery: random screening, non-random (or targeted) screening. Lead modification: Identification of the pharmacophore, Functional group modification. Structure-activity relationship, Structure modification to increase potency and therapeutic index: Homologation, chain branching, ring-chain transformation, bioisosterism, combinatiorial synthesis (basic idea).	[8L]
Unit 2:	**DRUG DESIGN, DEVELOPMENT AND SYNTHESIS**	**[15L]**
2.1	Introduction to quantitative structure activity relationship studies. QSAR parameters: - steric effects: The Taft and other equations; Methods used to correlate regression parameters with biological activity: Hansch analysis- A linear multiple regression analysis.	[5L]
2.2	Introduction to modern methods of drug design and synthesis- computer-aided molecular graphics based drug design, drug design via enzyme inhibition (reversible and irreversible), bioinformatics and drug design.	[3L]
2.3	Concept of prodrugs and soft drugs. (a) Prodrugs: Prodrug design, types of	[3L]

	prodrugs, functional groups in prodrugs, advantages of prodrug use. (b) Soft drugs: concept and properties.	
2.4	Synthesis and application of the following drugs: Fluoxetine, cetrizine, esomeprazole, fluconazole, zidovudine, methotrexate, diclofenac, labetalol, fenofibrate.	[4L]
Unit 3:	**BIOGENESIS AND BIOSYNTHESIS OF NATURAL PRODUCTS**	**[15L]**
3.1	Primary and secondary metabolites and the building blocks, general pathway of amino acid biosynthesis.	[3L]
3.2	Acetate pathway: Biosynthesis of malonylCoA, saturated fatty acids, prostaglandins from arachidonic acid, aromatic polyketides.	[4L]
3.3	Shikimic Acid pathway: Biosynthesis of shikimic acid, aromatic amino acids, cinnamic acid and its derivatives, lignin and lignans, benzoic acid and its derivatives, flavonoids and isofalvonoids.	[4L]
3.4	Mevalonate pathway: Biosynthesis of mevalonic acid, monoterpenes – geranyl cation and its derivatives, sesquiterpenes – farnesyl cation and its derivatives and diterpenes.	[4L]
Unit 4:	**GREEN CHEMISTRY**	**[15L]**
4.1	Introduction, basic principles of green chemistry. Designing a green synthesis: Green starting materials, green reagents, green solvents and reaction conditions, green catalysts.	[1L]
4.2	Use of the following in green synthesis with suitable examples:	[9L]
	a) Green reagents: dimethylcarbonate, polymer supported reagents.	
	b) Green catalysts: Acid catalysts, oxidation catalysts, basic catalysts, phase transfer catalysts [Aliquot 336, benzyltrimethyl ammonium chloride (TMBA), Tetra-n-butyl ammonium chloride, crown ethers], biocatalysts.	
	c) Green solvents: water, ionic liquids, deep eutectic solvents, supercritical carbon dioxide.	
	d) Solid state reactions: solid phase synthesis, solid supported synthesis	
	e) Microwave assisted synthesis: reactions in water, reactions in organic solvents, solvent free reactions.	

	f) Ultrasound assisted reactions.	
4.3	Comparison of traditional processes versus green processes in the syntheses of ibuprofen, adipic acid, 4-aminodiphenylamine, p-bromotoluene and benzimidazole.	[3L]
4.4	Green Catayst: Nanocatalyst, Types of nanoctalysts, Advantages and Disadvantages of nanocatalysts, Idea of Magnetically separable nanocatalysts.	[2L]

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Course Code: SIPSCHEOE-II-34 **Credits: 04**

Paper-IV

Bioorganic chemistry

Learning Objectives:

1. *To know the biomolecules, their structure and importance in life.*
2. *To study organic biomolecular synthesis and metabolic reaction pathways.*
3. *To learn the importance of enzymes and co-enzymes in biological system.*

Unit 1:	**BIOMOLECULES-I**	**[15L]**
1.1	Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure of protein: folding and	[2L]

	domain structure. Quaternary structure.	
1.2	Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.	[3L]
1.3	Structure: Purine and pyrimidine bases, ribose, deoxyribose, nucleosides and nucleotides (ATP, CTP, GTP, TTP, UTP) formation of polynucleotides strand with its shorthand representation**.**	[3L]
1.4	RNAs (various types in prokaryotes and eukaryotes) m- RNA and r- RNA – general account , t- RNA-clover leaf model, Ribozymes**.**	[2L]
1.5	DNA: Physical properties – Effect of heat on physical properties of DNA (Viscosity, buoyant density and UV absorption), Hypochromism, Hyperchromism and Denaturation of DNA. Reactions of nucleic acids (with DPA and Orcinol).	[2L]
1.6	Chemical synthesis of oligonucleotides: Phosphodiester, Phosphotriester, Phosphoramidite and H- phosphonate methods including solid phase approach.	[3L]
Unit 2:	**BIOMOLECULES-II**	**[15L]**
2.1	Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalyzed by enzymes. Properties of enzymes: a) enzyme efficiency/ catalytic power b) enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site.	[6L]
2.2	Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition.	[4L]
2.3	Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalyzed hydrolysis of a peptide bond.	[5L]
Unit 3:	**BIOMOLECULES - III**	**[15L]**
3.1	Chemistry of coenzymes. Structure, mechanism of action and bio-modeling studies of the following coenzymes: nicotinamide adenine dinucleotide, flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate,	[12L]

	Vitamin B12, biotin, lipoic acid, Coenzyme A.	
3.2	Oxidative phosphorylation, chemiosmosis, rotary model for ATP synthesis and role of cytochrome in oxygen activation.	[3L]
Unit 4:	**BIOMOLECULES – IV**	**[15L]**
4.1	Role of main enzymes involved in the synthesis and breakdown of glycogen.	[2L]
4.2	Enzyme catalyzed organic reactions: Hydrolysis, hydroxylation, oxidation and reduction.	[6L]
4.3	Enzymes in organic synthesis. Fermentation: Production of drugs/drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde) and immobilized form (production of 6-aminopenicillanic acid).	[7L]

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Course Code: SIPSCHEO3P1

Credits: 02 **Practical**

Paper-I

Learning Objectives:

1. *To learn separation techniques of ternary mixture.*
2. *To identify the organic compounds and to prepare their respective derivatives.*

SEPARATION OF A SOLID TERNARY MIXTURE USING MICRO-SCALE TECHNIQUE

1. Separation of solid components of a ternary mixture (water insoluble/soluble including carbohydrates) based upon differences in the physical and the chemical properties of the components.
2. Purification of the three components, measurement of their mass and determination of their physical constants.
3. Calculation of percentage yields of the individual components. (Identification of the components is not expected).

Course Code: SIPSCHEO3P2

Credits: 02 **Practical**

Paper-II

Learning Objectives:

1. *To estimate the actual quantity of the biologically active compound in the drugs.*
2. *To know the importance of spectrophotometer in quantitative analysis.*

ESTIMATION OF DRUGS

1. Estimation of penicillin by iodometric titrations.
2. Estimation of streptomycin using uv-visible spectrophotometer.
3. Estimation of paracetamol by hydrolysis.
4. Estimation of aspirin in the given tablet using uv-visible spectrophotometer.
5. Estimation of diazepam by non-aqueous titrations.
6. Estimation of vitamin C by iodometric titrations.

Course Code: SIPSCHEO3P3

Credits: 02 **Practical**

Paper-III

Learning Objectives:

1. To implement various organic reactions in synthetic organic chemistry.
2. To study the planning and purification techniques involved in organic synthesis.

ORGANIC PREPARATIONS (1.0 G SCALE)

1. Benzilic acid rearrangement: Benzilic acid from benzil
2. Sandmeyer reaction: p-Nitroiodobenzene from p-nitroaniline
3. Heterocyclic compound: 7-Hydroxy-4-methylcoumarin from resorcinol
4. Acetylation: Mannitol hexaacetate from mannitol
5. Claisen-Schmidt reaction: Dibenzalacetone from benzaldehyde
6. Oxidation: Fluorenone from fluorene
7. Acetylation: Acetylferrocene from ferrocene

Note:

Students are expected to know (i) the planning of synthesis, effect of reaction parameters including stoichiometry, and safety aspects including MSDS (ii) the possible mechanism, expected spectral data (IR and NMR) of the starting material and final product.

Students are expected to purify the product by Steam distillation / Vacuum distillation or Column chromatography, measure its mass or volume, check the purity by TLC, determine physical constant and calculate percentage yield.

Course Code: SIPSCHEO3P4

Credits: 02 **Practical**

Paper-IV

Learning Objectives:,

1. To know greener techniques (microwave oven) for organic compound synthesis.

SINGLE STEP ORGANIC PREPARATION (1.0 G SCALE) INVOLVING Techniques of purification and green methods of synthesis

Set I: Techniques of purification:

1. Steam distillation
2. Vacuum distillation
3. Column chromatography

Set II: Green methods of synthesis (microwave induced)

1. Synthesis of Schiff's base from aniline and p-anisaldehyde in the presence of lime juice
2. Synthesis of coumarin by Knoevenagel reaction using salicylaldehyde, and ethyl acetoacetate in presence of a base.
3. Synthesis of dihydropyrimidones- Biginelli reaction: acid-catalyzed three component reaction between vanillin, ethyl acetoacetate and thiourea.
4. Synthesis of acetanilide from aniline.

Learning points:

Set I: Techniques of purification

1. Students are expected to perform a purification technique using a known mass or volume of the given substance.

2. Check the purity of the purified compound by TLC, measure its mass and physical constant.

Set II: Green methods of synthesis (Microwave induced)

Students are expected to purify the product by recrystallization, measure its mass, determine physical constant and calculate percentage yield.

References for Practicals:

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Note:

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with

such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Semester-IV

Course Code: SIPSCHEO41 Credits: 04

Paper - I

Theoretical organic chemistry-II

Learning Objectives:

1. *To learn physical organic chemistry aspects (structural effects and reactivity) for organic chemistry.*
2. *To study supramolecular chemistry and its applications in organic synthesis*
3. *To understand the stereo-chemical aspects and its applications in organic synthesis*
4. *To study principles of asymmetric synthesis and chiral auxiliaries in asymmetric synthesis.*

Unit 1:	**PHYSICAL ORGANIC CHEMISTRY**	**[15L]**
1.1	Structural effects and reactivity**:** Linear free energy relationship (LFER) in determination of organic reaction mechanism, The Hammett equation, substituent constants, theories of substituent effects, interpretation of σ-values, reaction constants ρ, Yukawa-Tsuno equation**.**	**[7L]**
1.2	Uses of Hammett equation, deviations from Hammett equation. Dual parameter correlations, Inductive substituent constants. The Taft model, σ_I and σ_R scales, steric parameters Es and β. Solvent effects, Okamoto-Brown equation, Swain-Scott equation, Edward and Ritchie correlations, Grunwald-Winstein equation, Dimroth's E_T parameter, Solvatochromism Z-scale, Spectroscopic Correlations, Thermodynamic Implications.	**[8L]**
Unit 2	**SUPRAMOLECULAR CHEMISTRY**	**[15L]**
2.1	Principles of molecular associations and organizations as exemplified in biological macromolecules like nucleic acids, proteins and enzymes.	**[3L]**
2.2	Synthetic molecular receptors: receptors with molecular cleft, molecular tweezers, receptors with multiple hydrogen sites.	**[3L]**
2.3	Structures and properties of crown ethers, cryptands, cyclophanes, calixarenes, rotaxanes and cyclodextrins. Synthesis of crown ethers, cryptands and calixarenes.	**[5L]**
2.4	Molecular recognition and catalysis, molecular self-assembly. Supramolecular Polymers, Gelsand Fibres.	**[4L]**

Unit 3	**STEREOCHEMISTRY- II**	**[15L]**
3.1	Racemisation and resolution of racemates including conglomerates: Mechanism of racemisation, methods of resolution: mechanical, chemical, kinetic and equilibrium asymmetric transformation and through inclusion compounds.	**[3L]**
3.2	Determination of enantiomer and diastereomer composition: enzymatic method, chromatographic methods. Methods based on NMR spectroscopy: use of chiral derivatising agents (CDA), chiral solvating agents (CSA) and Lanthanide shift reagents (LSR).	**[3L]**
3.3	Correlative method for configurational assignment: chemical, optical rotation and NMR spectroscopy.	**[4L]**
3.4	Molecular dissymmetry and chiroptical properties: Linearly and circularly polarized light. Circular birefringence and circular dichroism. ORD and CD curves. Cotton effect and its applications. The octant rule and the axial α–haloketone rule with applications.	**[5L]**
Unit 4:	**ASYMMETRIC SYNTHESIS**	**[15L]**
4.1	Principles of asymmetric synthesis: Introduction, the chiral pool in Nature, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions.	**[3L]**
4.2	Synthesis of L-DOPA [Knowles's Mosanto process]. Asymmetric reactions with mechanism: Aldol and related reactions, Cram's rule, Felkin-Anh model, Sharpless enantioselective epoxidation, hydroxylation, aminohydroxylation, Diels-Alder reaction, reduction of prochiral carbonyl compounds and olefins.	**[9L]**
4.3	Use of chiral auxiliaries in diastereoselective reductions, asymmetric amplification. Use of chiral BINOLs, BINAPs and chiral oxazolines asymmetric transformations.	**[3L]**

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30. Large ring compounds, J.A.Semlyen, Wiley-VCH, 1997.
31. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji, Wiley- Eastern
32. Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Sciertific Publication.
33. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
34. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
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36. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.

37. Molecular Orbitals and Organic Chemical Reactions by Ian Fleming (Wiley – A john Wiley and Sons, Ltd., Publication)

Course Code: SIPSCHEO42 Credits: 04

Paper - II

Synthetic organic chemistry-II

Learning Objectives:

1. *To learn the synthetic planning and designing in various organic synthesis.*
2. *To understand the methodology, basics, and applications of electro-organic chemistry.*
3. *To study applications of organometallics (transition and rare earth elements) in organic synthesis.*

Unit 1:	**DESIGNING ORGANIC SYNTHESIS-I**	**[15L]**
1.1	**Protecting groups in Organic Synthesis:** Protection and deprotection of the hydroxyl, carbonyl, amino and carboxyl functional groups and its applications.	[3L]
1.2	**Concept of umpolung (Reversal of polarity):** Generation of acyl anion equivalent using 1,3-dithianes, methyl thiomethyl sulfoxides, cyanide ions, cyanohydrin ethers, nitro compounds and vinylated ethers.	[3L]
1.3	**Introduction to Retrosynthetic analysis and synthetic planning:** Linear and convergent synthesis; Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions (FGI), functional group addition (FGA), functional group removal (FGR) importance of order of events in organic synthesis, one and two group C-X disconnections (1,1; 1,2; 1,3 difunctionalized compounds), selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity.	[9L]
Unit 2:	**DESIGNING ORGANIC SYNTHESIS-II**	**[15L]**
2.1	**General strategy:** Choosing a disconnection-simplification, symmetry, high yielding steps and recognisable starting material.	[3L]
2.2	**One group C-C Disconnections:** Alcohols (including stereoslectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.	[6L]
2.3	**Two group C-C Disconnections:** 1,2- 1,3- 1,4- 1,5- and 1,6-difunctionalized compounds, Diels-Alder reactions, α, β-unsaturated	[6L]

	compounds, control in carbonyl condensations, Michael addition and Robinson annulation.	
Unit 3:	**ELECTRO-ORGANIC CHEMISTRY AND SELECTED METHODS OF ORGANIC SYNTHESIS**	**[15L]**
3.1	**Electro-organic chemistry:**	[7L]
3.1.1	Introduction: Electrode potential, cell parameters, electrolyte, working electrode, choice of solvents, supporting electrolytes.	
3.1.2	Cathodic reduction: Reduction of alkyl halides, aldehydes, ketones, nitro compounds, olefins, arenes, electro-dimerization.	
3.1.3	Anodic oxidation: Oxidation of alkylbenzene, Kolbe reaction, Non-Kolbe oxidation, Shono oxidation.	
3.2	**Selected Methods of Organic synthesis**	[8L]
	Applications of the following in organic synthesis:	
3.2.1	Crown ethers, cryptands, micelles, cyclodextrins, catenanes.	
3.2.2	Organocatalysts: Proline, Imidazolidinone.	
3.2.3	Pd catalysed cycloaddition reactions: Stille reaction, Saeguse-Ito oxidation to enones, Negishi coupling.	
3.2.4	Use of Sc(OTf), and Yb(OTf) as water tolerant Lewis acid catalyst in aldol condensation, Michael reaction, Diels-Alder reaction, Friedel – Crafts reaction.	
Unit 4:	**TRANSITION AND RARE EARTH METALS IN ORGANIC SYNTHESIS**	**[15L]**
4.1	**Introduction to basic concepts:** 18 electron rule, bonding in transition metal complexes, C-H activation, oxidative addition, reductive elimination, migratory insertion.	[3L]
4.2	**Palladium in organic synthesis:** π-bonding of Pd with olefins, applications in C-C bond formation, carbonylation, alkene isomerisation, cross-coupling of organometallics and halides. Representative examples: Heck reaction, Suzuki-Miayura coupling, Sonogashira reaction and Wacker oxidation. Heteroatom coupling for bond formation between aryl/vinyl groups and N,	[5L]

	S or P atoms.	
4.3	**Olefin metathesis** using Grubb's catalyst.	[1L]
4.4	**Application of Ni, Co, Fe, Rh, and Cr carbonyls** in organic synthesis.	[4L]
4.5	**Application of samarium iodide** including reduction of organic halides, aldehydes and ketones, α-functionalised carbonyl and nitro compounds.	[1L]
4.6	**Application of Ce (IV)** in synthesis of heterocyclic quinoxaline derivatives and its role as a de-protecting agent**.**	[1L]

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14. Name Reactions, Jie Jack Lie, 3rd Edn., Springer
15. Organic Electrochemistry, H. Lund, and M. Baizer, 3rd Edn., Marcel Dekker.

Course Code: SIPSCHEO43 Credits: 04

Paper - III

Natural products and heterocyclic chemistry

Learning Objectives:

1. *To learn the importance of steroids, vitamins and terpenoids in natural products.*
2. *To study the heterocyclic chemistry (3-6 membered rings) and their applications in organic synthesis.*

Unit 1:	**NATURAL PRODUCTS-III**	**[15L]**
1.1	**Steroids:** General structure, classification. Occurrence, biological role, important structural and stereochemical features of the following: corticosteroids, steroidal hormones, steroidal alkaloids, sterols and bile acid	[5L]
1.2	Synthesis of 16-DPA from cholesterol and plant sapogenin.	[2L]
1.3	Synthesis of the following from 16-DPA: androsterone, testosterone, oestrone, oestriol, oestradiol and progesterone.	[5L]
1.4	Synthesis of cinerolone, jasmolone, allethrolone, exaltone and muscone.	[3L]
Unit 2:	**NATURAL PRODUCTS-IV**	**[15L]**
2.1	**Vitamins:** Classification, sources and biological importance of vitamin B_1, B_2, B_6, folic acid, B_{12}, C, D_1, E (α-tocopherol), K_1, K_2, H (β- biotin).	[5L]
	Synthesis of the following:	
	Vitamin A from β-ionone and bromoester moiety.	
	Vitamin B_1 including synthesis of pyrimidine and thiazole moieties	
	Vitamin B_2 from 3, 4-dimethylaniline and D(-)ribose	
	Vitamin B_6 from: 1) ethoxyacetylacetone and cyanoacetamide, 2) ethyl ester of N-formyl-DL-alanine (Harris synthesis)	
	Vitamin E (α-tocopherol) from trimethylquinol and phytyl bromide	
	Vitamin K_1 from 2-methyl-1, 4-naphthaquinone and phytol.	
2.2	**Antibiotics:** Classification on the basis of activity. Structure elucidation, spectral data of penicillin-G, cephalosporin-C and chloramphenicol. Synthesis of chloramphenicol (from benzaldehyde and β-nitroethanol) penicillin-G and phenoxymethylpenicillin from D-penicillamine and t-butyl phthalimide malonaldehyde (synthesis of D-penicillamine and t-butyl phthalimide malonaldehyde expected).	[6L]
2.3	**Naturally occurring insecticides:** Sources, structure and biological properties of pyrethrums (pyrethrin I), rotenoids (rotenone). Synthesis of pyrethrin I.	[2L]
2.4	**Terpenoids**: Occurrence, classification, structure elucidation,	[2L]

	stereochemistry, spectral data and synthesis of zingiberene.	
Unit 3:	**HETEROCYCLIC COMPOUNDS-I**	**[15L]**
	Heterocyclic compounds: Introduction, classification, Nomenclature of heterocyclic compounds of monocyclic (3-6 membered) (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
	Structure, reactivity, synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazines, pyrimidine, pyrazines and oxazines.	
Unit 4:	**HETEROCYCLIC COMPOUNDS-II**	**[15L]**
	Nomenclature of heterocyclic compounds of bicyclic/tricyclic (5-6 Membered) fused heterocycles (up to three hetero atoms)**.** (Common, systematic (Hantzsch-Widman) and replacement nomenclature)	
	Nucleophilic ring opening reactions of oxiranes, aziridines, oxetanes and azetidines.	
	Structure, reactivity, synthesis and reactions of coumarins, quinoxalines, cinnolines, indole, benzimidazoles, benzoxazoles, benzothiazoles, Purines and acridines.	

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Course Code: SIPSCHEOE-I-44 Credits: 04

Paper-IV

Intellectual property rights and cheminformatics

Learning Objectives:

1. *To learn various terms and terminology involved in intellectual property rights*
2. *To study trade secrets and economic value of intellectual property.*
3. *To know the evolution of cheminformatics and its application.*

Unit 1:	**Introduction to Intellectual Property**	**[15L]**
1.1	**Introduction to Intellectual Property:**	[2L]
	Historical Perspective, Different types of IP, Importance of protecting IP.	
1.2	**Patents:**	[5L]
	Historical Perspective, Basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India.	
1.3	**Industrial Designs:**	[2L]
	Definition, how to obtain, features, International design registration.	
1.4	**Copyrights:**	[2L]
	Introduction, how to obtain, Differences from Patents.	
1.5	**Trade Marks**	[2L]
	Introduction, how to obtain, Different types of marks – Collective marks, certification marks, service marks, trade names etc.	
1.6	**Geographical Indications**	[2L]

	Definition, rules for registration, prevention of illegal exploitation, importance to India.	
Unit 2:	**Trade Secrets**	[15L]
2.1	Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection.	[2L]
2.2	**IP Infringement issue and enforcement:**	[2L]
	Role of Judiciary, Role of law enforcement agencies – Police, Customs etc.	
2.3	**Economic Value of Intellectual Property:**	[2L]
	Intangible assests and their valuation, Intellectual Property in the Indian context – Various Laws in India Licensing and Technology transfer.	
2.4	**Different International agreements:**	
	a) World Trade Organization (WTO):	[5L]
	i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement	
	ii) General Agreement on Trade Related Services (GATS) Madrid Protocol.	
	iii) Berne Convention.	
	iv) Budapest Treaty.	
	b) Paris Convention	[6L]
2.5	**WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.	
Unit III:	**Cheminformatics**	[15L]
3.1	**Introduction to Cheminformatics:**	[5L]
	History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modeling and structure elucidation.	
3.2	**Representation of molecules and chemical reactions:**	[5L]
	Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Molfiles and Sdfiles, Libraries and toolkits,	

	Different electronic effects, Reaction classification.	
3.3	**Searching Chemical Structures:**	[5L]
	Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.	
Unit IV:	**APPLICATIONS:**	[15L]
	Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure – Property Relations, Descriptor Analysis, Model Building, Modeling Toxicity, Structure – Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.	

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2. Gasteiger, J. & Engel, T. (2003) *Cheminformatics: A textbook.* Wiley–VCH
3. Gupta, S. P. *QSAR and Molecular Modeling.* Springer-Anamaya Pub.: New Delhi.

Course Code: SIPSCHEOE-II-44 Credits: 04

Paper-IV

Research Methodology

Learning Objectives:

1. *To learn research methodology for research data analysis and scientific writing.*
2. *To study the chemical safety and ethical handling of chemicals.*
3. *To learn the writing skills in scientific research project/ practical work.*

Unit 1:	**SOURCES**	[15L]
1.1	**Print**	[5L]
	Primary, Secondary and Tertiary sources.	

1.2	**Journals:**	
	Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.	
1.3	**Digital:**	[5L]
	Web sources, E-journals, Journal access, TOC alerts, Hot articles, Citation Index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki-databases, ChemSpider, Science Direct, SciFinder, Scopus.	
1.4	**Information Technology and Library Resources:**	[5L]
	The Internet and World wide web, Internet resources for Chemistry, finding and citing published information.	
Unit II:	**DATA ANALYSIS**	[15L]
2.1	**The Investigative Approach:**	
	Making and recording Measurements, SI units and their use, Scientific methods and design of experiments.	
2.2	**Analysis and Presentation of Data:**	
	Descriptive statistics, choosing and using statistical tests, Chemometrics, Analysis of Variance (ANOVA), Correlation and regression, curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, general polynomial fitting, linearizing transformations, exponential function fit, r and its abuse, basic aspects of multiple linear regression analysis.	
Unit III:	**METHODS OF SCIENTIFIC RESEARCH AND WRITING SCIENTIFIC PAPERS**	[15L]
	Reporting practical and project work, Writing literature surveys and reviews, organizing a poster display, giving an oral presentation.	
3.1	**Writing Scientific Papers:**	

	Justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work, writing ethics, avoiding plagiarism.	
Unit IV:	**CHEMICAL SAFETY & ETHICAL HANDLING OF CHEMICALS**	[15L]
	Safe working procedure and protective environment, protective apparel, emergency procedure, first aid, laboratory ventilation, safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric pressur, safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.	

REFERENCES:

1. Chemical Safety matters – IUPAC-IPCS, (1992) Cambridge University Press. OSU Safety manual 1.01
2. Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J., & Jones, A., (2011), *Practical skills in Chemistry*, 2nd Ed., Prentice Hall, Harlow.
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4. Harris, D. C. (2007) *Quantative Chemical Analysis* 6th Ed., Freeman Chapters 3-5
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Course Code: SIPSCHEO4P1

Credits: 02 **Practical**

Paper-I

Learning Objectives:

1. *To learn separation techniques and miscibility criteria of ternary mixture.*
2. *To identify the organic compounds and to prepare their respective derivatives.*

SEPARATION OF SOLID-LIQUID/ LIQUID-LIQUID TERNARY MIXTURE USING MICRO-SCALE TECHNIQUE

1. Separation of components of ternary mixtures (solid-liquid or liquid-liquid) based upon differences in the physical and the chemical properties of the components.
2. Purification of the three components, measurement of their mass and determination of their physical constants.
3. Calculation of percentage yield of the individual components. (Identification of the components is not expected). (Minimum 6 experiments)

Course Code: SIPSCHEO4P2

Credits: 02 **Practical**

Paper-II

Learning Objectives:

1. *To learn the solubility and miscibility criteria for identification of unknown organic compounds.*

IDENTIFICATION OF ANY UNKNOWN ORGANIC COMPOUND WITH PREPARATION, PURIFICATION AND PHYSICAL CONSTANT OF DERIVATIVE. (MINIMUM 8 ORGANIC COMPOUNDS)

(Minimum 8 experiments)

Course Code: SIPSCHEO4P3

Credits: 02 **Practical**

Paper-III

Learning Objectives:

1. *To learn isolation/extraction of biologically active ingredients in natural products by qualitative methods.*

ISOLATION / ESTIMATION OF NATURAL PRODUCTS

1. Extraction of clove oil from cloves.
2. Extraction of nicotine dipicrate from tobacco.
3. Estimation of proteins by Biuret method using spectrophotometer.
4. Estimation of glucose by Folin Wu method.
5. Estimation of citral using hydroxylamine hydrochloride.
6. Estimation of saponification value of oil.

Course Code: SIPSCHEO4P4

Credits: 02 **Practical**

Paper-IV

Learning Objectives:

1. *To learn the interpretation of the organic compounds by various spectroscopic techniques (UV, IR, PMR, CMR and Mass spectra).*

INTERPRETATION OF SPECTRAL DATA OF ORGANIC COMPOUNDS (UV, IR, PMR, CMR AND MASS SPECTRA).

Interpretation of spectral data of organic compounds (UV, IR, PMR, CMR and Mass spectra). A student will be given UV, IR, PMR, CMR, and Mass spectra of a compound from which preliminary information should be reported within first half an hour of the examination without referring to any book/reference material. The complete structure of the compound may then be elucidated by referring reference material etc. (Minimum 8 spectral analysis)

Note:

1. The candidate is expected to submit a journal and project certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

REFERENCES FOR PRACTICALS:

1. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis- V.
2. K. Ahluwalia and Renu Aggarwal, Universities Press India Ltd., 2000
3. Advanced Practical Organic Chemistry – N. K. Vishnoi, Third Addition, Vikas Publishing House PVT Ltd
4. Systematic Laboratory Experiments in Organic Synthesis- A. Sethi, New Age International Publications
5. Systematic Identification of Organic compounds, 6th edition, R. L. Shriner, R. C. Fuson and D.Y. Curtin Wiley, New York.
6. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
7. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
8. Macro-scale and Micro-scale Organic Experiments, K. L. Williamson, D. C. Heath.
9. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
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11. Vogel's Textbook of Practical Organic Chemistry, Fifth edition,2008, B.S.Furniss, A. J.Hannaford, P. W. G. Smith, A. R. Tatchell, Pearson Education.
12. Laboratory Manual of Organic Chemistry, Fifth edition, R K Bansal, New Age Publishers.
13. Organic structures from spectra, L. D. Field, S. Sternhell, John R. Kalman, Wiley, 4th ed., 2011.

MODALITY OF ASSESSMENT

1. The candidate is expected to submit a journal certified by the Head of the Department /institution at the time of the practical examination.

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3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Scheme of examination for M.Sc. Organic Chemistry Semester III and IV. Internal Theory examination (40 Marks)

1. One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners).

a) Selection of the topic, introduction, write up, references. …….20 marks

b) Presentation. ……. 20 marks

There will not be any internal examination for practical.

External Theory Examination (60 Marks)

Paper	Time allotted in hours	Maximum marks
Paper- I	**2.5**	**60**
Paper- II	**2.5**	**60**
Paper- III	**2.5**	**60**
Paper- IV	**2.5**	**60**

It is recommended that a total of five questions be set, based on the syllabus with due weightage to the number of lectures allotted per topic.
The candidates are expected to answer all five questions.
Question 5 will be based on all four units and the remaining questions will be based on each unit.

Semester End Practical Examination	**(50 Marks)**
Laboratory Work	**40 Marks**
Journal	**05 Marks**
Viva	**05 Marks**

The practical examination will be held for two days as described below. The candidates will be examined practically and orally on each day.

Paper	**Experiments**	**Time duration in hours**	**Maximum marks**
Paper- I	**1**	**3.5**	**50**
Paper- II	**1**	**3.5**	**50**
Paper- III	**1**	**3.5**	**50**
Paper- IV	**1**	**3.5**	**50**

SIES

College of Arts, Science & Commerce

RISE WITH EDUCATION

Sion (West), Mumbai – 400022.

(Autonomous)

Department of Chemistry

Program: M.Sc.

Course: Inorganic Chemistry

Syllabus for M.Sc. Semester III & IV

(Implemented from 2018 – 2019)

Credit Based Semester and Grading System

SEMESTER III

Contents:		
Paper I	:	**Chemistry of Inorganic Solids**
SIPSCHEI31.1	:	Descriptive Crystal Chemistry
SIPSCHEI31.2	:	Imperfection in crystals and Non-stoichiometry
SIPSCHEI31.3	:	Methods of Preparations
SIPSCHEI31.4	:	Behaviour of Inorganic Solids
Paper II	:	**Bioinorganic and Coordination Chemistry.**
SIPSCHEI32.1	:	Bioinorganic Chemistry
SIPSCHEI32.2	:	Reactivity of Chemical Species – I
SIPSCHEI32.3	:	Reactivity of Chemical Species – II
SIPSCHEI32.4	:	Structure, Bonding, and Stereochemistry of Coordination Compounds
Paper III	:	**Spectral Methods in Inorganic Chemistry**
SIPSCHEI33.1	:	Diffraction Methods – I
SIPSCHEI33.2	:	Diffraction Methods – II
SIPSCHEI33.3	:	Electron Spin Resonance Spectroscopy
SIPSCHEI33.4	:	Mossbauer Spectroscopy
Paper IV	:	**Applied Chemistry (Elective)**
SIPSCHEI34.1	:	Inorganic Materials
SIPSCHEI34.2	:	Nuclear Chemistry and Inorganic Pharmaceuticals
SIPSCHEI34.3	:	Advances in Nanomaterials
SIPSCHEI34.4	:	Some Selected Topics
Practical		
SIPSCHEI3P1	:	Analysis of ores/alloys
SIPSCHEI3P2	:	Solvent Extraction
SIPSCHEI3P3	:	Inorganic Preparations
SIPSCHEI3P4	:	Analysis of the following samples

SEMESTER IV

Contents:		
Paper I	:	**Properties of Inorganic Solids and Group Theory.**
SIPSCHEI41.1	:	Electrical Properties.
SIPSCHEI41.2	:	Magnetic Properties.
SIPSCHEI41.3	:	Thermal and Optical Properties.
SIPSCHEI41.4	:	Applications of group theory to Electronic structures
Paper II	:	**Organometallics and main group Chemistry.**
SIPSCHEI42.1	:	Organometallic Chemistry.
SIPSCHEI42.2	:	Applications of Organometallic Compounds.
SIPSCHEI42.3	:	Inorganic cluster and cage compounds.
SIPSCHEI42.4	:	Inorganic ring and chain compounds
Paper III	:	**Instrumental methods in Inorganic Chemistry.**
SIPSCHEI43.1	:	Spectroscopy.
SIPSCHEI43.2	:	Microscopy of Surfaces – I.
SIPSCHEI43.3	:	Microscopy of Surfaces – II.
SIPSCHEI43.4	:	Thermal Methods.
Paper IV	:	**Intellectual Property Rights and Cheminformatics**
SIPSCHEI44.1	:	Introduction to Intellectual Property.
SIPSCHEI44.2	:	Trade Secrets.
SIPSCHEI44.3	:	Introduction to Cheminformatics.
SIPSCHEI44.4	:	Applications.
Practical		
SIPSCHEI4P1	:	Analysis of ores.
SIPSCHEI4P2	:	Coordination Chemistry.
SIPSCHEI4P3	:	Analysis of the following samples.
SIPSCHEI4P4	:	Spectral interpretation.

Course Code: SIPSCHEI31

Paper I

Chemistry of Inorganic Solids

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEIN31 CREDITS: 4 LECTURES: 60

Chemistry of Inorganic Solids		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI31.1 **LEARNING OBJECTIVES:** *4) To study the structure of different types of crystals such as oxide, perovskite, spinel, etc.* *5) To study the imperfection in crystals such as Frenkel, Schottky and surface defects.* *6) To study the different methods of synthesis of single crystals, thin film and alloys.* *7) To study the behavior of inorganic solids.*		
1 Chemistry of Inorganic Solids		**15L**
1.1	**Descriptive Crystal Chemistry** **(a) Simple structures** Structures of AB type compounds (PbO and CuO), AB_2 type (β cristobalite, CaC_2 and Cs_2O), A_2B_3 type (Cr_2O_3 and Bi_2O_3), AB_3 (ReO_3, Li_3N), ABO_3 type, relation between ReO_3 and perovskite $BaTiO_3$ and its polymorphic forms, Oxide bronzes, ilmenite structure, AB_2O_4 type, normal, inverse, and random spinel structures. **(b) Linked Polyhedra** (i) Corner sharing: tetrahedral structure (silicates) and octahedral structure (ReO_3) and rotation of ReO_3 resulting in VF_3, RhF_3 and calcite type structures. (ii) Edge sharing: tetrahedral structures (SiS_2) and octahedral structures (BiI_3 and $AlCl_3$). pyrochlores, octahedral tunnel structures and lamellar structures.	
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI31.2		
2 Imperfection in Crystals and Non-Stoichiometry		**15L**

2.1	**Imperfection in Crystals and Non-Stoichiometry** (a) **Point defects**: Point defects in metals and ionic Crystal – Frenkel defect and Schottky defect. Thermodynamics formation of these defects (mathematical derivation to find defect concentration), Defects in Non-Stoichiometric compounds, colour centres. (b) **Line defects**: Edge and Screw Dislocations. Mechanical Properties and Reactivity of Solids. (c) **Surface Defects**: Grain Boundary and Stacking Fault, Dislocation and Grain Boundaries, Vacancies and Interstitial Space in Non-Stoichiometric Crystals, Defect Clusters, Interchangeable Atoms and Extended Atom.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI31.3		
3 Methods of Preparations		**15L**
3.1	**Methods of Preparations** **(**a) Methods of Synthesis: Chemical Method, High Pressure Method, Arc Technique and Skull Method (with examples). (b) Different methods for single crystal growth: (i) Crystal Growth from Melt: Bridgman and Stockbargar, Czochralski and Vernuil methods. (ii) Crystal growth from liquid solution: Flux growth and temperature gradient methods. (iii) Crystal growth from vapour phase: Epitaxial growth methods. (c) Thin film preparation: Physical and Chemical methods. (d) Solid Solutions: Formation of Substitutional, Interstitial and Complex Solid Solutions, Mechanistic Approach, Study of Solid solutions by X-ray Powder Diffraction and Density Measurement.	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI31.4		
4	**Behaviour of Inorganic Solids**	**15L**
4.1	**Behaviour of Inorganic Solids** **(a) Diffusion in Solids:** Fick's Laws of Diffusion, Kirkendall Effect, Wagner mechanism, Diffusion and Ionic Conductivity, Applications of Diffusion in Carburizing and non-Carburizing Processes in Steel Making. **(b) Solid state reactions:** General principles and factors influencing reactions of solids, Reactivity of solids. **(c) Liquid Crystals:** Introduction and classification of thermotropic liquid crystals, Polymorphism in liquid crystal, Properties and applications of liquid crystals.	**15L**

SUGGESTED REFERENCE SIPSCHEI31

1. L. E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005.
2. A.R. West, Solid State Chemistry and Its Applications, John Wiley and sons, 1987.
3. C.N.R. Rao and J. Gopalkrishnan, New Directions in Solid State Chemistry, 2nd Edition, Cambridge University Press. 1997
4. L.V. Azaroff, Introduction to solids, Tata-McGraw Hill Book Co. New Delhi, 1977.
5. D.W. Bruce and Dermont O Hare, Inorganic Chemistry, 2nd Edition, Wiley and sons, New York, 1966.
6. J.M. Hollas, Symmetry in Molecules, Chapman and Hall Ltd., 1972.
7. Rebert L Carter, Molecular Symmetry and Group John Wiley and Sons, New York, 1988.
8. Ulrich Muller, Inorganic structural Chemistry, 2nd edition, John Wiley and Sons, Chichester, 1993.
9. R.N. Kutty and J.A.K. Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.
10. H.V. Keer, Principles of the Solid state, Wiley Eastern Ltd., 1993.Gary L. Miessler and Donald A. Tarr, Inorganic Chemistry, 3rd edition , Pearson Education, Inc., 2004.
11. D.K. Chakrabarty, Solid State Chemistry, New Age International Publishers, 1996.
12. A. Earnshaw, Introduction to Magnetochemistry, Acad. Press, N.Y. (1966).

Course Code: SIPSCHEI32

Paper II

Bioinorganic and Coordination Chemistry

Credits: 4 Credits (60 Lectures)

Bioinorganic and Coordination Chemistry.		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI32.1 **LEARNING OBJECTIVES:** *3) To study the principles involved in bioinorganic and coordinate compounds.* *4) To understand the reaction of chemical species.* *5) To study structure, bonding and stereochemistry of coordination compounds using Molecular Orbital Theory and Angular Overlap Model.*		
1 Bioinorganic Chemistry		**15L**
1.1	**Bioinorganic Chemistry** (i) Coordination geometry of the metal ion and functions. (ii) Zinc in biological systems: Carbonic anhydrase, protolytic enzymes, e.g. carboxy peptidase, Zinc finger. (iii) Role of metal ions in biological electron transfer processes: iron sulphur proteins, (iv) Less common ions in biology e.g. Manganese (arginase: structure and reactivity), Nickel (urease : structure and reactivity) (v) Biomineralization.	
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI32.2		
2 Reactivity of Chemical Species – I		**15L**
2.1	**Reactivity of Chemical Species** **2.2.1** Recapitulation of the definition of Lewis acids and bases, Classification of Lewis acids and bases based on frontier Molecular orbital topology, Reactivity matrix of Lewis acids and bases. **2.2.2** Group Characteristic of Lewis acids (Group – 1, 13-17). **2.2.3** Pauling rules to determine the strength of oxoacids, classification and structural anomalies.	

UNIT III, 1L/week		
COURSE CODE: SIPSCHEI32.3		
3 Reactivity of Chemical Species – II		**15L**
3.1	**Reactivity of Chemical Species – II** **3.3.1** Pourbaix Diagrams. **3.3.2** Amphoteric behavior, Periodic trends in amphoteric properties of p-block and d-block elements **3.3.3** Oxoanions and oxocations. **3.3.4** Measures of hardness and softness of acids and bases, Drago-Wayland equation. **3.3.5** Applications of acid-base Chemistry: Super acids and super bases, heterogeneous acid-base reactions.	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI32.4		
4 Structure, Bonding, and Stereochemistry of Coordination Compounds		**15L**
4.1	Structure, Bonding, and Stereochemistry of Coordination Compounds (a) Structure and Bonding: i) Molecular Orbital Theory for Complexes with coordination number 4 and 5 for the central ion (sigma as well as pi bonding) (ii) Angular Overlap Model for octahedral and tetrahedral complexes for sigma and pi bond. (b) Stereochemistry of Coordination Compounds: (i) Chirality and Fluxionality of coordination compounds with higher coordination numbers. (ii) Geometries of coordination compounds from coordination number 6 to 9.	

SUGGESTED REFERENCE SIPSCHEI32

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2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3rd edition.
3. James E. Huheey, Inorganic Chemistry, 3rd edition, Harper and Row, Publishers, Asia, Pte Ltd., 1983.
4. W.W. Porterfield, Inorganic Chemistry - A Unified Approach, Academic press (1993).
5. D.F. Shriver, P.W. Atkins and Tina Overton, Inorganic Chemistry, 5th edition Oxford University.

6. Asim K. Das, Fundamental Concepts of Inorganic Chemistry, (Volumes -I, II and III) CBS Pub. (2000).

7. N.N. Greenwood and A. Earnshaw, Chemistry of Elements, Pergamon, 1984.

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11. H. Sisler, Chemistry in Non-aqueous Solvents: New York Reinhold Publ. 1965.

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13. C.M. Day and Joel Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 1985.

14. L.E. Orgel, An Introduction to Ligand Field Theory, Methuen and Co. Ltd., London, 1960.

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16. J.D. Lee, Concise Inorganic Chemistry, 5th edition, Blackwell Science Ltd., 2005.

17. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals, Wiley-Interscience, New York, 1988.

18. G.W. Parshall and S.D. Ittel, Homogeneous Catalysis, 2nd edition, John Wiley and sons, Inc., New York, 1992.

19. Gary O. Spessard and Gary L. Miessler, Organometallic Chemistry, Prentice-Hall, (1997).

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21. B. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons,1983.

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23. F. A. Cotton, G. Wilkinson, C. Murillo and M. Bochmann, Advanced Inorganic Chemistry, 6th ed., John Wiley, New York, 1999.

24. F.A. Cotton and R.A. Walton, Multiple Bonds between Metal Atoms, 2nd edition, Claranden Press, Oxford, 1993.

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Course Code: SIPSCHEI33

Paper III

Spectral Methods in Inorganic Chemistry

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI33 CREDITS: 4 LECTURES: 60

Spectral Methods in Inorganic Chemistry		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI33.1 **LEARNING OBJECTIVES:** *4. To study in detail the different spectral methods in inorganic compounds.* *5. To study the principle undergoing spectroscopic technique like ESR, Mossbauer spectroscopy.*		
1 Diffraction Methods – I		**15L**
1.1	**Diffraction Methods – I** X-Ray Diffraction: Bragg Condition, Miller Indices, Laue Method, Bragg Method, Debye Scherrer Method of X-Ray, Structural Analysis of Crystals.	
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI33.2.		
2 Diffraction Methods – II		**15L**
2.1	**Diffraction Methods – II** **(a) Electron Diffraction:** Scattering of electrons, Scattering Intensity versus Scattering Angle, Weird Measurement Technique and Elucidation of structures of simple gas phase molecules. **(b) Neutron Diffraction:** Scattering of Neutrons: Scattering of neutrons by Solids and Liquids, Magnetic Scattering, Measurement Technique.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI33.3		
3 Electron Spin Resonance Spectroscopy		**15L**

3.1	**Electron Spin Resonance Spectroscopy** (a) Electron behaviour, interaction between electron spin and magnetic field. (b) Instrumentation: Source, sample cavity, magnet and modulation coils, microwave bridge, Sensitivity. (c) Relaxation processes and Line width in ESR transitions: (i) ESR relaxation and chemical bonding. (ii) Interaction between nuclear spin and electron spin (hyperfine coupling). (iii) Spin polarization for atoms and transition metal ions. (iv) Spin-orbit coupling and significance of 'g' tensors. (v) Application to transition metal complexes (having one unpaired electron).	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI33.4		
4 Mossbauer Spectroscopy		**15L**
4.1	**Mossbauer Spectroscopy** **4.4.1** Basic principle, recoil energy and Doppler shift. **4.4.2** Instrumentation: sources and absorber, motion devices, detection, reference substances and calibration. **4.4.3** Isomer shift, quadrupole interaction, magnetic interaction, electronegativity and chemical shift. **4.4.4 Applications:** *Iron compounds* - low spin and high spin Fe(II) and Fe(III) compounds and complexes, effect of pi-bonding, mono and polynuclear Iron complexes, spinel oxides and iron-sulphur proteins, *Tin compounds* - tin halides and tin oxides, organotin compounds, *Iodine compounds* - I_2 and alkali metal iodide compounds.	**15L**

SUGGESTED REFERENCE SIPSCHEI33

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis Fifth edition, (1996), ELBS Publication. Chapter 2, 3, 11.

2. W.H. Zachariasen. Theory of X-Ray Diffration in Crystals. JohnWiley. New York. 1946.

3. B.D. Cality, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954.

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6. H.H. Willard, L.L. Merrit, J.A. Dean and F.A. Settle, Instrumental Methods of Analysis, C.B.S. Publishers and Distributors, New Delhi, 1986.

7. P.J. Horne, Nuclear Magnetic Resonance. Oxford University Press, Oxford, 1995.

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15. Haissilsky, Nuclear Chemistry and its Application, 1962.

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21. Graham Smith; David Keeble. Introduction to Modern EPR Spectroscopy CRC Press 2013.

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23. K. Veera Reddy, Symmetry and Spectroscopy,

24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell; edition (2007).

25. Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E. Horwood, (1990).

Course Code: SIPSCHEI34

Paper IV

Applied Chemistry (Elective)

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI34 CREDITS: 4 LECTURES: 60

Applied Chemistry (Elective)		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI34.1 **LEARNING OBJECTIVES:** *4. To study the Classification, synthesis and application of magnetic material.* *5. To study the nuclear phenomenon involve in fusion by using the PUREX process, radiopharmaceuticals and their applications.* *6. To study the different advances made in Nanomaterials.* *7. To study some selective topics involving supramolecular chemistry and intercalation compounds.*		
1 Inorganic Materials		**15L**
1.1	**Inorganic Materials** (a) Classification, manufacture and applications of (i) Inorganic fibers (ii) Biofibers and (iii) Inorganic fillers. Study of (i) Condensed phosphates and (ii) Coordination polymers. (b) Preparation, properties and uses of industrially important chemicals – potassium permanganate, sodium thiosulphate, bleaching powder, hydrogen peroxide, potassium dichromate.	
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI34.2		
2 Nuclear Chemistry and Inorganic Pharmaceuticals		**15L**
2.1	**Nuclear Chemistry and Inorganic Pharmaceuticals** **(a) Nuclear Chemistry :** Introduction to of nuclear fuels and separation of fission products from Spent fuel rods by PUREX process. Super heavy element, discovery, Preparation, position in the periodic table. **(b) Inorganic Pharmaceuticals :**	

	Radiopharmaceuticals containing Technetium and Bismuth, contrast agents for X-ray and NMR imaging. Gastrointestinal agents viz. (i) Antacids (Aluminium hydroxide, Milk of magnesia, Sodium bicarbonate and (ii) Cathartics (Magnesium sulphate and Sodium phosphate). Topical agents viz. (iii) Protectives and adsorbents (Talc, Calamine), (iv) Antimicrobial agents (Potassium permanganate, Tincture iodine, Boric acid) and astringents (Potash alum).	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI34.2		
3 Advances in Nanomaterials		**15L**
3.1	**(a) Types of nanomaterials:** e.g. nanotubes, nanorods, solid spheres, core-shell in a nanoparticles, mesoporous materials, isolation of nanomaterials. **(b) Some important properties of nanomaterials:** optical properties of metal and semiconductor nanoparticles, magnetic properties. **(c) Some special nanomaterials: Carbon nanotubes:** Types, synthesis using various methods, growth mechanism and electronic structure. Porous silicon: Preparation and mechanism of porous silicon formation, Factors affecting porous structure and properties of porous silicon. Aerogels: Types of aerogels, properties and applications of aerogels. **(d)** Applications of nanomaterials in electronics, energy, automobiles, sports and toys, textile, cosmetics, medicine, space and defense. Environmental effects of nanotechnology.	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI34.4		
4 Some Selected Topics		**15L**
4.1	**Some Selected Topics:** i) Isopoly and Heteropoly acids. ii) Supramolecular chemistry. iii) Inorganic pesticides. iv) Intercalation compounds.	**15L**

SUGGESTED REFERENCE SIPSCHEI34

1. G.M. Masters, Introduction to Environmental Engineering and Science, Prentice-Hall of India Pvt. Ltd. New Delhi, 1995.

2. Sulabha K. Kulkarni, Nanotechnology-Principles and Practices, Capital Publishing Co., 2007.

3. K. R. Mahadik and B. S. Kuchekar, Concise Inorganic Pharmaceutical Chemistry, Nirali Prakashan, Pune.

4. D. A. Skoog, D. M. West, and F. J. Holler, Fundamentals of Analytical Chemistry, 7th Edition, (printed in India in 2001), ISBN Publication.

5. B. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, 2nd edition, John Wiley and Sons, 1983.

Course Code: SIPSCHEI3P1

Practical Paper I

Analysis of ores/alloys

COURSE CODE: SIPSCHEI3P1 CREDITS: 2

Course Code: SIPSCHEI3P1 (4L/Week)	
1	1. **Analysis of Brass alloy:** (i) Cu content by iodometric method, (ii) Zn content by complexometric method. **2. Analysis of Mangelium alloy:** (i) Al content by gravimetric method as basic succinate. (ii) Mg content by complexometric method. **3. Analysis of Bronze alloy:** (i) Cu content by complexometric method. (ii) Sn content by gravimetric method. **4. Analysis of steel nickel alloy:** (i) Ni content by homogeneous precipitation method.

Course Code: SIPSCHEI3P2

Practical Paper II

Solvent Extraction

COURSE CODE: SIPSCHEI3P2 CREDITS: 2

Course Code: SIPSCHEI3P2 (4L/Week)	
1	1. Separation of Mn and Fe using isoamyl alcohol and estimation of Mn. 2. Separation of Co and Ni using n-butyl alcohol and estimation of Co. 3. Separation of Al and Fe using ethyl acetate determination of Fe by redox titration. 4. Separation of Fe and Mo using isoamyl alcohol and estimation of Mo. 5. Separation of Cu and Fe using n-butyl acetate and estimation of Cu.

Course Code: SIPSCHEI3P3

Practical Paper III

Inorganic Preparations

COURSE CODE: SIPSCHEI3P3 CREDITS: 2

Inorganic Preparations (4L/Week)	
1	1. Preparation of $V(oxinate)_3$. 2. Preparation of Sn(IV) Iodide. 3. Preparation of Co(α -nitroso- β -naphthol)$_3$. 4. Preparation of $Ni(salicylaldoxime)_2$. 5. Preparation of Hexamine cobalt (III) chloride. 6. Preparation of Trans-bis(glycinato) copper(II).

Course Code: SIPSCHEI3P4

Practical Paper IV

Analysis of the following samples

COURSE CODE: SIPSCHEI3P4 CREDITS: 2

Course Code: SIPSCHEI3P4 (4L/Week)	
1	1. Calcium tablet for its calcium content by complexometric titration. 2. Bleaching powder for its available chlorine content by iodometric method. 3. Iron tablet for its iron content colorimetry by 1,10-phenanthroline method. 4. Nycil powder for its Zinc content complexometrically.

Reference books for practical's

1. A. I. Vogel's, *Quantitative Inorganic Analysis.*

2. J. D. Woolins, *Inorganic Experiments.*

3. Palmer, *Inorganic Preparations.*

4. Gurdeep Raj, *Advanced Practical Inorganic Chemistry*

5. James E. House, Inorganic chemistry, Academic press, 2nd edition, (2013).

SEMESTER IV

Course Code: SIPSCHEI41

Paper I

Properties of Inorganic Solids and Group Theory

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI41 CREDITS: 4 LECTURES: 60

Properties of Inorganic Solids and Group Theory.		
UNIT- I, 1L/week		
COURSE CODE: SIPSCHEI41.1 **LEARNING OBJECTIVES:** *1) To study the properties of Inorganic solid, electrical properties like Thomson and Seebeck effect and their applications.* *2) To study the magnetic behavior of substance and mechanism of ferromagnetic and antiferromagnetic ordering, hard and soft magnets.* *3) To study the thermal properties of material like ceramics, polymers and optical properties of laser, phosphor.* *4) To understand the principle involved in group theory and their application to tetrahedral molecules, Ligand field theory.*		
1 Electrical Properties		**15L**
1.1	**Electrical Properties** (a) Electrical properties of solids: (i) Conductivity: Solid Electrolytes, Fast Ion Conductors, Mechanism of Conductivity, Hopping Conduction. (b) Other Electrical Properties: Thomson and Seebeck effects, Thermocouples and their Applications, Hall Effect, Dielectric, Ferroelectric, Piezoelectric and Pyrroelectric Materials and their Inter-relationships and Applications.	
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI41.2		
2 Magnetic Properties.		**15L**

2.1	**Magnetic Properties.** Behaviour of substances in magnetic field, mechanism of ferromagnetic and antiferromagnetic ordering, superexchange, hysteresis, hard and soft magnets, structures and magnetic Properties of Metals and Alloys, Transition metal oxides, Spinels, garnets, Ilmenites, Perovskite and Magneto plumbites, Application in transformer cores, information storage, magnetic bubble memory devices and as permanent magnets.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI41.3		
3 Thermal and Optical Properties		**15L**
3.1	**Thermal and Optical Properties** **a) Thermal Properties:** Introduction, Heat Capacity and its Temperature Dependence, Thermal Expansion of Metals, Ceramics and Polymers and Thermal Stresses. **b) Optical properties:** Colour Centres and Birefringence, Luminescent and Phosphor Materials, Coordinate Model, Phosphor Model, Anti Stokes Phosphor, Ruby Laser, Neodymium Laser.	**15L**
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI41.4		
4 Applications of group theory to Electronic structures		**15L**
4.1	**Applications of group theory to Electronic structures** (a) Recapitulation of Points groups and Character tables. (b) Transformation Properties of Atomic Orbitals. (c) Sigma and pi- molecular orbitals for AB_4 (tetrahedral) and AB_6 (octahedral) molecules. (d) Ligand Field Theory : Electronic structures of free atoms and ions, Splitting of levels and terms in a chemical environment, Construction of energy level diagrams, Direct product, Correlation diagrams for d^2 ions in octahedral and tetrahedral ligand field, Methods of Ascending and Descending Symmetry, Hole formalism.	**15L**

SUGGESTED REFERENCE SIPSCHEI41

1. Leslie E. Smart and E. A. Moore, Solid State Chemistry-An introduction, 3rd edition, Taylor and Francis, 2005.

2. A.R. West, Solid State Chemistry and Its Applications, John Wiley and sons, 1987.

3. C.N.R. Rao and J. Gopalakrishnan New Directions in Solid State Chemistry, 2nd Ed., Cambridge University Press. 1997.

4. L.V. Azaroff, Introduction to solids, Tata-McGraw Hill Book Co. New Delhi, 1977.

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9. R.N. Kutty and J.A.K. Tareen, Fundamentals of Crystal Chemistry, Universities Press (India) Ltd., 2001.

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Course Code: SIPSCHEI42

Paper II

Organometallics and main group Chemistry

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI42 CREDITS: 4 LECTURES: 60

Organometallics and main group Chemistry		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI42.1 **LEARNING OBJECTIVES:** *1) To study the chemistry of organometallic and main group element with its application.* *2) To understand the concept of inorganic cluster cage compounds.* 3) *To study inorganic ring and chain compounds.*		
1 Organometallic Chemistry		**15L**
1.1	**Organometallic Chemistry** (a) Metal-Metal Bonding and Metal Clusters. (b) Electron Count and Structures of Clusters. (c) Isolobal Analogy. (d) Organo Palladium and Organo Platinum Complexes (preparations, properties and applications).	**15L**
UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI42.2		
2 Applications of Organometallic Compounds		**15L**
2.1	**Applications of Organometallic Compounds** **(a)** Catalysis-Homogenous and Heterogenous Catalysis: Comparison, Fundamental Reaction Steps. **(b)** Organometallics as Catalysts in Organic Reactions: (i) Hydrosilylation (ii) Hydroboration (iii) Water gas Shifts reaction (iv) Wacker process (oxidation of alkenes) (v) Alcohol carbonylation.	**15L**

	(c) Coupling reactions: (i) Heck reaction (ii) Suzuki reaction.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI42.3		
3 Inorganic cluster and cage compounds		**15L**
3.1	**Inorganic cluster and cage compounds** (i) Introduction (ii) Bonding in boranes (iii) Heteroboranes (iv) Carboranes (v) Cluster compounds (vi) Electron precise compounds and their relation to clusters.	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI42.4		
4 Inorganic ring and chain compounds		**15L**
4.1	**Inorganic ring and chain compounds** (a) Silicates, polysilicates and aluminosilicates. (b) Phosphazenes and phosphazene polymers. (c) Polyanionic and polycationic compounds.	

SUGGESTED REFERENCE SIPSCHEI42

1. Gary Wulfsberg, Inorganic Chemistry; Viva Books PA Ltd., New Delhi; 2002.
2. F.A. Cotton and Wilkinson, Advanced Inorganic Chemistry, 3rd edition.
3. James E. Huheey, Inorganic Chemistry, 3rd edition, Harper and Row, Publishers, Asia, Pte Ltd., 1983.
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Course Code: SIPSCHEI43

Paper III

Instrumental methods in Inorganic Chemistry.

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI43 CREDITS: 4 LECTURES: 60

Instrumental methods in Inorganic Chemistry.		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI43.1 **LEARNING OBJECTIVES:** *1) To introduce the basics of Infrared spectroscopy, Raman spectroscopy, NMR spectroscopy.* *2) To interpret IR and Raman Spectra of molecules.* *3) To study surface spectroscopy, microscopy and understand problems of surface analysis* *4) To study the application of TGA, DSC, DTA, TMA, EGA (Evolved gas analyser) thermomechanical analysis.*		
1 Spectroscopy		**15L**
1.1	**Spectroscopy** **(a) Infrared spectroscopy:** Fundamental modes of vibrations, selection rules, IR absorption bands of metal - donor atom, effect of complexation on the IR spectrum of ligands formations on the IR of ligands like NH_3, CN^-, CO, olefins (C=C) and $C_2O_4^{2-}$. **(b) Raman spectroscopy:** Raman spectroscopy for diatomic molecules. Determination of molecular structures like diatomic and triatomic molecules. **(c) Applications of Group theory in Infrared and Raman spectroscopy.** Molecular Vibrations: Introduction; The Symmetry of Normal Vibrations; Determining the Symmetry Types of the Normal Modes; symmetry based Selection Rules of IR and Raman; Interpretation of IR and Raman Spectra for molecules such as H_2O, BF_3, N_2F_2, NH_3 and CH_4. **(d) Nuclear Magnetic Resonance Spectroscopy :** Introduction to basic principles and instrumentation. Use of ^1H, ^{19}F, ^{31}P, ^{11}B NMR spectra in structural elucidation of inorganic compounds; Spectra of paramagnetic materials: Contact shift, application of contact shift, lanthanide shift reagent.	

UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI43.2		
2 Microscopy of Surfaces – I		**15L**
2.1	**Microscopy of Surface – I:** Introduction to surface spectroscopy, microscopy, problems of surface analysis, distinction of surface species, sputter etching and depth profile and chemical imaging, instrumentations, Ion Scattering Spectra (ISS), Secondary Ion Mass Spectroscopy (SIMS),Auger Emission Spectroscopy (AES).	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI43.3		
3 Microscopy of Surfaces – II		**15L**
3.1	**Microscopy of Surface – II:** ESCA, Scanning Electron Microscopy (SEM), Atomic force microscopy (AFM) and transmission electron microscopy (TEM): Instrumentation and applications.	
Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI43.4		
4 Thermal Methods		**15L**
4.1	**Thermal Methods:** **3.4.1** Application of TGA in Thermal characterization of polymers, quantitative analysis of mixture of oxalates, moisture content in coal, study of oxidation state of alloys etc. **3.4.2** Application of DSC and DTA in determination of thermodynamic parameters such as heat capacity and standard enthalpy of formation of the compounds, investigation of phase transitions, thermal stability of polymeric materials, purity of pharmaceuticals samples, Melting point of organic compounds etc. **3.4.3** Basic principle, instrumentation and applications to other thermal methods like Thermomechanical analysis (TMA) and evolved gas analysis (EGA).	**15L**

SUGGESTED REFERENCE SIPSCHEI43

1. G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, Vogel's Textbook of Quantitative Chemical Analysis 5th edition, (1996), ELBS Publication. Chapter 2, 3, 11.
2. W.H. Zachariasen. Theory of X-Ray Diffraction in Crystals. John Wiley. New York, 1946.
3. B.D. Cullity, Elements of X-Ray Diffraction Procedures. John Wiley and Sons. New York, 1954.
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14. M.T.R. Series, The Superheavy Elements.

15. M. Haissinsky, Nuclear Chemistry and its Application, 1962.

16. S. Glasstone, Sourcebook of Atomic Energy, East-West Publisher, 1969.

17. D. Harvey, Modern Analytical Chemistry, The McGraw-Hill Pub, 1st Ed. 2000.

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22. C.N.R. Rao, Chemical Applications of Infrared Spectroscopy Academic Press, N.Y. (1963

23. K. Veera Reddy, Symmetry and Spectroscopy,

24. Paul Gabbott Principles and Applications of Thermal Analysis Wiley-Blackwell; edition (2007)

25. Richard Vernon Parish, NMR, NQR, EPR, and Mössbauer spectroscopy in inorganic chemistry, Publisher, E. Horwood, (1990).

Course Code: SIPSCHEI44

Paper IV Applied Chemistry (Elective)

Credits: 4 Credits (60 Lectures)

COURSE CODE: SIPSCHEI44 CREDITS: 4 LECTURES: 60

INTELLECTUAL PROPERTY RIGHTS AND CHEMINFORMATICS		
UNIT- I , 1L/week		
COURSE CODE: SIPSCHEI44.1 **LEARNING OBJECTIVES:** *1) To understand the concept of 'IP', Industrial designs, copy rights, Trader Marks* *2) To Study Trade secrets Economic value of Zp* *3) To understand the Genre of 'Cheminformatics' representation of molecule chemical reaction.* 4) *To Study the application of linear free energy relationship, quantitative structure, drug design.*		
1 INTELLECTUAL PROPERTY RIGHTS and CHEMINFORMATICS		**15L**
1.1	**Introduction to Intellectual Property:** **1.1.1** Introduction to Intellectual Property. **1.1.2** Historical perspective, Different types of IP, Importance of protecting IP. **1.1.3** Patents. **1.1.4** Historical perspective, basic and associated right, WIPO, PCT system, Traditional Knowledge, Patents and Health care-balancing promoting innovation with public health, Software patents and their importance for India. **1.1.5** Industrial Designs: Definition, How to obtain, features, International design registration. **1.1.6 Copyrights:** Introduction, How to obtain, Differences from Patents. **1.1.7 Trade Marks:** Introduction, How to obtain, Different types of marks - Collective marks, certification marks, service marks, trade names etc. **1.1.8 Geographical Indications:** Definition, rules for registration, prevention of illegal exploitation, importance to India. Recycling and recovery of metals with reference to silver, lead, cobalt, nickel and chromium, Laboratory Wastes Disposal Management in Chemical Laboratories.	

UNIT- II, 1L/week		
COURSE CODE: SIPSCHEI44.2		
2 Trade Secrets		**15L**
2.1	**Manufacture and Applications of Inorganic Compounds – I** **Trade Secrets:** Introduction and Historical Perspectives, Scope of Protection, Risks involved and legal aspects of Trade Secret Protection. **IP Infringement issue and enforcement:** Role of Judiciary, Role of law enforcement agencies - Police, Customs etc. **Economic Value of Intellectual Property:** Intangible assets and their valuation, Intellectual Property in the Indian context - Various Laws in India Licensing and Technology transfer. **Different International agreements:** **(a) World Trade Organization (WTO):** (i) General Agreement on Tariffs and Trade (GATT), Trade Related Intellectual Property Rights (TRIPS) agreement (ii) General Agreement on Trade Related Services (GATS) Madrid Protocol. (iii) Berne Convention (iv) Budapest Treaty **(b) Paris Convention**, **WIPO** and **TRIPS, IPR** and Plant Breeders Rights, IPR and Biodiversity.	
UNIT III, 1L/week		
COURSE CODE: SIPSCHEI44.3		
3 Introduction to Cheminformatics		**15L**
3.1	**Introduction to Cheminformatics:** History and evolution of cheminformatics, Use of Cheminformatics, Prospects of cheminformatics, Molecular modelling and structure elucidation. **Representation of molecules and chemical reactions:** Nomenclature, Different types of notations, SMILES coding, Matrix representations, Structure of Mol files and Sd files, Libraries and toolkits, Different electronic effects, Reaction classification. **Searching Chemical Structures:** Full structure search, sub-structure search, basic ideas, similarity search, three dimensional search methods, basics of computation of physical and chemical data and structure descriptors, data visualization.	

Unit – IV, 1L/week		
COURSE CODE: SIPSCHEI44.4		
4 Applications		**15L**
4.1	Prediction of Properties of Compound, Linear Free Energy Relations, Quantitative Structure - Property Relations, Descriptor Analysis, Model Building, Modelling Toxicity, Structure - Spectra correlations, Prediction NMR, IR and Mass spectra, Computer Assisted Structure elucidations, Computer assisted Synthesis Design, Introduction to drug design, Target Identification and Validation, Lead Finding and Optimization, analysis of HTS data, Virtual Screening, Design of Combinatorial Libraries, Ligand-based and Structure based Drug design, Application of Cheminformatics in Drug Design.	

SUGGESTED REFERENCE SIPSCHEI44

1. Andrew R. Leach and Valerie J. Gillet (2007) *An Introduction to Cheminformatics.* Springer: The Netherlands.

2. Gasteiger, J. and Engel, T. (2003) *Chemoinformatics: A textbook*. Wiley–VCH

3. Gupta, S. P. *QSAR and Molecular Modelling.* Springer-Anamaya Pub.: New Delhi.

Course Code: SIPSCHEI4P1

Practical Paper I

Analysis of ores

COURSE CODE: SIPSCHEI4P1 CREDITS: 2

Course Code: SIPSCHEI4P1 (4L/Week)	
1	1. Analysis of galena ore: (i) Pb content as $PbCrO_4$ by gravimetric method using 5% potassium chromate. (ii) Fe content by colorimetrically using 1,10-phenanthroline. 2. Analysis of Zinc blend ore: (i) Zn content by complexometric method. (ii) Fe content by colorimetric method (Azide method). 3. Analysis of Pyrolusite ore: (i) Mn content by complexometric method. (ii) Acid insoluble residue by gravimetric method.

Course Code: SIPSCHEI4P2

Practical Paper II

Coordination Chemistry

COURSE CODE: SIPSCHEI4P2 CREDITS: 2

Course Code: SIPSCHEI4P2	
LEARNING OBJECTIVES 1. *To learn to calibrate volumetric apparatus.* 2. *To learn to perform experiments that has specific aims with correct techniques.* 3. *To develop skills of observation, recording and analyzing data.* 4. *To learn to present the experimental work in a systematic manner.* 5. *To understand miscibility concept of various organic compounds.*	
Course Code: SIPSCHEI4P2 (4L/Week)	
1	1. Determination of Stability constant of $[Zn(NH_3)_4]^{2+}$ by potentiometry. 2. Determination of Stability constant of $[Ag(en)]^{+}$ by potentiometry. 3. Determination of Stability constant of $[Fe(SCN)]^{2+}$ by slope ratio method. 4. Determination of CFSE values of hexa-aqua complexes of Ti^{3+} and Cr^{3+}. 5. Determination of Racah parameters for complex $[Ni(H_2O)_6]^{2+}$ and $[Ni(en)_3]^{2+}$.

Course Code: SIPSCHEI4P3

Practical Paper III

Analysis of the following samples

COURSE CODE: SIPSCHEI4P3 CREDITS: 2

Course Code: SIPSCHEI4P3 (4L/Week)	
1	1. Electral powder for Na/K content flame photometrically. 2. Fasting salt for chloride content conductometrically. 3. Sea water for percentage salinity by Volhard's method. 4. Soil for mixed oxide content by gravimetric method. 5. Fertilizer for potassium content by flame photometry.

Course Code: SIPSCHEI4P4

Paper IV

Spectral interpretation

COURSE CODE: SIPSCHEI4P4 CREDITS: 2

Course Code: SIPSCHEI4P4 (4L/Week)	
1	Spectral interpretation

SUGGESTED REFERENCE SIPSCHEI4P4

1. A. I. Vogel's, *Quantitative Inorganic Analysis.*
2. J. D. Woolins, *Inorganic Experiments.*
3. Palmer, *Inorganic Preparations.*
4. G. Raj, Advanced *Practical Inorganic Chemistry.*
5. J. E. House, Inorganic chemistry, Academic press, 2nd edition, (2013).

MODALITY OF ASSESSMENT

1. The candidate is expected to submit a journal certified by the Head of the Department /institution at the time of the practical examination.
2. A candidate will not be allowed to appear for the practical examination unless he/she produces a certified journal or a certificate from the Head of the institution/department stating that the journal is lost and the candidate has performed the required number of experiments satisfactorily. The list of the experiments performed by the candidate should be attached with such certificate.
3. Use of non-programmable calculator is allowed both at the theory and the practical examination.

Scheme of examination for M.Sc. Inorganic Chemistry Semester III and IV.

Internal Theory examination (40 Marks)

One seminar based on curriculum / publication of a research paper/ presentation of a research paper in seminar or conference (to be assessed by teacher of the institution teaching PG learners).

a) Selection of the topic, introduction, write up, references ……. 20 marks

b) Presentation ……. 20 marks

There will not be any internal examination for practical.

External Theory Examination (60 Marks)

Paper	Time allotted in hours	Maximum marks
I	**2.5**	**60**
II	**2.5**	**60**
III	**2.5**	**60**
IV	**2.5**	**60**

It is recommended that a total of five questions be set, based on the syllabus with due weightage to the number of lectures allotted per topic. The candidates are expected to answer all five questions. Question 5 will be based on all four units and the remaining questions will be based on each unit.

Semester End Practical Examination (50 Marks)

Laboratory Work : 40 Marks

Journal : 05 Marks

Viva : 05 Marks

The practical examination will be held for two days as described below. The candidates will be examined practically and orally on each day.

Paper	Experiments	Time duration in hours	Maximum marks
I	**1**	**3.5**	**50**
II	**1**	**3.5**	**50**
III	**1**	**3.5**	**50**
IV	**1**	**3.5**	**50**
