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Deccan Education Society's

Kirti M. Doongursee College of Arts, Science and Commerce (AUTONOMOUS)

Affiliated to

UNIVERSITY OF MUMBAI

Syllabus for

Program: Master of Science

Course: M.Sc. Part-I (NEP)

Subject: Chemistry

with effect from

Academic Year 2023-2024

Deccan Education Society's

Kirti M. Doongursee College (autonomous)

Proposed Curriculum as per NEP 2020

Year of implementation- 2023-24

Name of the Department: Chemistry

Semester	Course Code	Course Title	Vertical	Credit
I	K23PSCHEMJ111	Physical Chemistry	Major	4
	K23PSCHEMJ112	Inorganic Chemistry	Major	4
	K23PSCHEMJ113	Organic Chemistry	Major	4
	K23PSCHEMJP111	Practical Inorganic + Organic	Major	2
	K23PSCHEL131	Analytical Chemistry	Elective	2
	K23PSCHEP131	Practical Physical + Analytical	Elective Practical	2
	K23PSCHERM141	Research Methodology For Chemistry	RM	4
II	K23PSCHEMJ211	Physical Chemistry	Major	4
	K23PSCHEMJ212	Inorganic Chemistry	Major	4
	K23PSCHEMJ213	Organic Chemistry	Major	2
	K23PSCHEMJP211	Practical Inorganic + Organic	Elective Practical	2

	K23PSCHEOE231	Analytical Chemistry	Elective	2
	K23PSCHEP231	Physical + Analytical	Elective Practical	2
	K23PSCHEOJ251		OJT/FP	4

Semester-I

Course Code	Course Title	Credits	Lectures /Week
K23PSCHEMJ111	**Paper I (Physical Chemistry)**	**4**	**4**

About the Course:

CO1	After successfully completing this course on **Thermodynamics** ,Learners will be able to understand principles of thermodynamics, Maxwell equation and its application to ideal gases. Joule Thomson effect and its applications. Learners will also understand laws of thermodynamics, especially the third law in detail , entropy change for phase transition, absolute entropy, residual entropy etc.
CO2	By studying the course on **Basics of Quantum Mechanics,** the learner will understand the limitations of classical mechanics and how it is possible to explain the behaviour of subatomic particles with the application of quantum mechanics . They will learn about Schrodinger's wave equation and its interpretation, particle waves, wave functions, properties of wave function.They will also be able to learn about Operators,Eigen function and Eigen values and solve problems on it; derive Schrodinger's time independent wave equation. They will be able to understand the concept of particle in one , two and three dimensional box , separation of variables, quantization and introduction of quantum numbers; Harmonic Oscillator, Hermite Polynomials.
CO3	After completing this course on **Chemical Dynamics** students will have knowledge of steady state approximation, microscopic reversibility, detailed balanced chain reaction,some inorganic reactions like decomposition of phosgene, decomposition of ozone etc. they will also understand theories of reaction mechanism, explosion limits, kinetics of polymerisation reactions in details and theories of reactions in gas phase .

CO4	After studying the topic of **Electrochemistry,** the learner will be able to understand the advanced concepts of electrochemistry like Debye Huckel theory of activity coefficient, Debye Huckel limiting law, electrolytic conductance and ionic interaction, Debye-Falkenhagen effect and Wien effect. The learner will be able to derive the Debye Huckel Onsager equation. He will also get knowledge of different types of Fuel cells like alkaline fuel cell, solid -oxide fuel cell etc. The student will also get introduced to Biochemistry . He will be able to understand cells and membranes, membrane potential and theory of membrane potential. interfacial electron transfer in biological systems, enzymes as electrodes. He will be able to derive the Goldmann equation. The student will be able to solve numerical and theoretical problems from all topics of each unit

Unit	Topics	No of Lectures
I	**Thermodynamics-I [15]** 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. **[8L]** 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. **[7L]** [Ref 2 and 1,10,11,12 17]	**15**
II	**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.	**15**

	2.3. Operators and their algebra, linear and Hermitian operators, operators for the dynamic variables of a system such as, position, linear momentum, angular momentum, total energy, eigen functions, eigen values and eigen value equation, Schrödinger wave equation as the eigen value equation of the Hamiltonian operator, average value and the expectation value of a dynamic variable of the system, Postulates of Quantum Mechanics, Schrodinger‟s Time independent wave equation from Schrodinger‟s time dependent wave equation. 2.4. Application of quantum mechanics to the following systems: a) Free particle, wave function and energy of a free particle. b) Particle in a one, two and three dimensional box, separation of variables, Expression for the wave function of the system, expression for the energy of the system, concept of quantization, introduction of quantum number, degeneracy of the energy levels. c) Harmonic oscillator, approximate solution of the equation, Hermite polynomials, expression for wave function, expression for energy, use of the recursion formula. [Ref 7, 8 and 9]	
III	**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	**15**

	average no .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. [Ref. 2 and 15, 17, 18]	
IV	**Electrochemistry [15L]** **Recapitulation – basics of electrochemistry.** 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) [Ref: 14 and 16, 17, 18] **[Note: Numerical and theoretical problems from each unit are expected]**	**15**

REFERENCE BOOKS:

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	Course Title	Credits	Lectures /Week
K23PSCHEMJ112	**Paper II (Inorganic Chemistry)**	**4**	**4**

CO1	After studying Chemical bonding students will get knowledge of hybridization involving sigma bonding, VBT, MOT and importance of weak forces of attraction such as hydrogen bonding etc.
CO2	In Molecular symmetry and Group theory unit students will learn about the symmetry operations and applications of group theory.
CO3	In the Solid state Chemistry unit students will learn about electronic structure of solids, band theory, methods of preparation of inorganic solids and nanomaterials along with applications.
CO4	In characterization of coordination compounds students will get the idea of the preparation of coordination compounds and how their characterization is done.

Unit	Topics	No of Lectures
I	**Chemical Bonding: [15 L]** 1.1 **Recapitulation of hybridization** Derivation of wave functions for *sp*, *sp2*, *sp3* orbital hybridization types considering only sigma bonding. 1.2 Discussion of involvement of *d* orbitals in various types of hybridizations. Concept of resonance, resonance energy derivation expected. Formal charge with examples. 1.3 Critical analysis of VBT. 1.4 Molecular Orbital Theory for diatomic species of First transition Series. 1.5 Molecular Orbital Theory for Polyatomic species considering σ bonding for SF6, CO2, B2H6, I3- molecular species. 1.6 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.	**15**
II	**Molecular Symmetry and Group Theory: [15L]**	**15**

	2.1. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. 2.2. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. 2.3. 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 C2v, C3v and D2h, structure of character tables. 2.4. Applications of Group Theory (a) Symmetry adapted linear combinations (SALC), symmetry aspects of MO theory, sigma bonding in ABn (Ammonia, CH4) 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.	
III	**Materials Chemistry and Nanomaterials: [15 L]** **3.1 Solid State Chemistry** 3.1.1. Electronic structure of solids and band theory, Fermi level, K Space and Brillouin Zones. 3.1.2. Structures of Compounds of the type: AB [nickel arsenide (NiAs)], AB2 [fluorite (CaF2) and anti-fluorite structures, rutile (TiO2) structure and layer structure [cadmium chloride and iodide (CdCl2, CdI2)]. 3.1.3. 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** 3.2.1. Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-	**15**

	precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms. 3.2.2. Applications in the field of semiconductors, solar cells	
IV	**Characterisation 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, B, C, Nephelauxetic ratio. 4.3. Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.	**15**

Reference Books:

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 Education Limited, 2nd Edition 2005.
5. J. Huheey, F. A. Keiter and R. I. Keiter, Inorganic Chemistry–Principles of Structure 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 Benjamin Cummings Publishing Company, 1989.
8. G. Miessler and D. Tarr, Inorganic Chemistry, 3rd Ed., Pearson Education, 2004.
9. R. Sarkar, General and Inorganic Chemistry, Books & Allied (P) Ltd., 2001.
10. C. M. Day and J. Selbin, Theoretical Inorganic Chemistry, Affiliated East West Press 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 & Sons, New York, 1996.

3. R. L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, New York, 1998.
4. K. V. Reddy. Symmetry and Spectroscopy of Molecules, 2nd Edition, New Age International Publishers, New Delhi, 2009.
5. A. Salahuddin Kunju and G. Krishnan, Group Theory and its Applications in Chemistry, PHI Learning, 2012.
6. P. K. Bhattacharya, Group Theory and its Chemical Applications, Himalaya Publishing House. 2014.
7. S. Swarnalakshmi, T. Saroja and R. M. Ezhilarasi, A Simple Approach to Group Theory in Chemistry, Universities Press, 2008.

Unit III

1. Solid State Chemistry Introduction, Lesley E. Smart, Elaine A. Moore, ISBN 0-203-49635-3, Taylor & Francis Group, LLC.
2. Nanomaterials & 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 & Co. KGaA, Weinheim.
4. Nano-Surface Chemistry, 2001, Morton Rosoff, ISBN: 0-8247-0254-9, Marcel Dekker Inc. New York.
5. The Chemistry of Nanomaterials, CNR Rao, Muller Cheetham, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.
6. Semiconductor Nanomaterials, Challa S.S.R. Kumar, ISBN: 978-3-527-32166-7, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2010.

Unit IV

1. J. E. Huheey, E. A. Keiter and R. L. Keiter; Inorganic Chemistry: Principles of Structure 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 & Atkins: Inorganic Chemistry, 4th ed. Oxford University Press, 2006.
5. F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann; Advanced Inorganic Chemistry, 6th ed. Wiley, 1999,
6. B. Douglas, D. McDaniel and J. Alexander. *Concepts and Models of Inorganic Chemistry*(3rd edn.), John Wiley & Sons (1994).

Course Code	Course Title	Credits	Lectures /Week
K23PSCHEMJ113	**Paper III (Organic Chemistry)**	**4**	**4**

About the Course:

CO1	In the topic **Physical Organic Chemistry,** the students will learn about the fundamentals of rate, equilibrium constant, transition state, activated complex and its nature, reactivity, selectivity, Curtin-Hammett principle, microscopic reversibility and kinetic Vs. thermodynamic control of organic reactions; various methods of determining reaction mechanism; factors affecting the acidity and basicity of acids and bases.
CO2	In the topic **Nucleophilic Substitution Reactions**, the students will be able to clear the ideas about SN1, SN2, SNi, SET, NGP participation and the factors affecting these reactions; Aromatic nucleophilic substitution reactions like SN1, Ipso, benzyne, cine, tele and vicarious substitution. Students will also learn about Ester Hydrolysis and their various types.
CO3	In the topic **Aromaticity**, the students shall learn about basics of aromaticity, various criteria for aromaticity, application of HMO Theory, Huckel rules, Frost-Musulin diagram; aromatic, homoaromatic and antiaromatic ; and aromaticity of various types of compounds like metallocenes, azulenes, annulenes, aromatic ions and Fullerenes.
CO4	In the topic **Stereochemistry**, the students will learn about Chirality, Symmetry elements; stereochemistry of- molecules with tri-and tetra-coordinate centers, molecules with two or more chiral centres; axial and planar chirality and the concept of Prochirality.
CO5	In the topic **Oxidation and Reduction**, the students will learn about Oxidation, Dehydrogenation by using metal and organic reagents; Oxidation of alcohols to aldehydes and ketones by using chromium reagents and other name oxidations; Oxidations involving C-C bond cleavage, replacement of H by O; reduction of CO to -CH2 in aldehydes and ketones; Reduction by using metal hydrides, hydrazine, dissolving metals in liq. NH3.

Unit	Topics	No of Lectures
I	**Physical Organic Chemistry: (15 L)** **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 stereochemical 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. *[Reference Books: 1, 2, 3, 16]*	**15**
II	**Nucleophilic substitution reactions and Aromaticity** **2.1. Nucleophilic substitution reactions: (9 L)** **2.1.1. Aliphatic nucleophilic substitution:** SN1, SN2, SNi reactions, mixed SN1 and SN2 and SET mechanisms. SN reactions involving NGP - participation by aryl rings, α-and pi-bonds. Factors affecting these reactions: substrate, nucleophilicity, solvent, steric effect, hard-soft interaction, leaving group. Ambident nucleophiles. SNcA, SN1‟ and SN2‟ reactions. SN at sp2 (vinylic) carbon. **2.1.2. Aromatic nucleophilic substitution:** SNAr, SN1, benzyne mechanisms. Ipso, cine, tele and vicarious substitution. **2.1.3. Ester hydrolysis:** Classification, nomenclature and study of all eight mechanisms of acid and base catalyzed hydrolysis with suitable examples. **2.2. Aromaticity: (6 L)**	**15**

	2.2.1. Structural, thermochemical, and magnetic criteria for aromaticity, including NMR characteristics of aromatic systems. Delocalization and aromaticity. **2.2.2.** Application of HMO theory to monocyclic conjugated systems. Frost-Musulin diagrams. Huckel‟s (4n+2) and 4n rules. **2.2.3.** Aromatic and antiaromatic compounds up-to 18 carbon atoms. Homoaromatic compounds. Aromaticity of all benzenoid systems, heterocycles, metallocenes, azulenes, annulenes, aromatic ions and Fullerene (C60). [Reference Books: 4-15]	
III	**Stereochemistry: (15 L)** **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-pseudoasymmetric centre. Symbols for enantiotopic and diastereotopic faces.	**15**

	[Reference Books: 6-8]	
IV	**Oxidation and Reduction: (15 L)** **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. [Reference Books: 17, 18, 14]	**15**

Reference Books:

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	**Course Title**
K23PSCHEMJP111	**Practicals-Inorganic+ Organic Chemistry**

CO1	In Inorganic preparations students will prepare the metal complexes along with their characterization.
CO2	In Instrumentation conductance measurement is done for the determination of electrolytic nature of inorganic compounds.
CO3	Spectrophotometer is used to measure the optical density for different concentrations of metal and ligand for the determination of equilibrium constant by slope intercept method for Fe^{+3}/SCN^{-}.
CO1	In one-step preparations, the students shall learn about planning of synthesis, its stoichiometry
CO2	Students will also learn Safety aspects of reactants and products including their MSDS study

CO3	Students will learn about the purification of the product.
CO4	Students will clear their ideas about the TLC and its use in checking the formation and the purity of product.
CO5	Students will learn about taking the mass and melting point of the productStudents will learn about taking the mass and melting point of the product

	Inorganic Preparations (Synthesis and Characterization)
1	Bis-(tetraethylammonium) tetrachloro Cuprate (II) (Et4 N) 2[CuCl4]
2	Bis-(tetraethylammonium) tetrachloro Nickelate (II) (Et4 N) 2 [NiCl4]
3	Bis-(tetraethylammonium) tetrachloro Cobaltate (II) (Et4 N) 2 [CoCl4]
	(Any two from above preparations)
4	Tetrammine monocarbanato Cobalt (III) Nitrate [Co(NH3)4CO3]NO3
5	Bis (ethylenediammine) Copper (II) Sulphate [Cu(en)2]SO4
6	Hydronium dichlorobis(dimethylglyoximato) Cobaltate(III) H[Co(dmgH)2Cl2]
	Instrumentation
7	Determination of equilibrium constant by Slope intercept method for Fe+3/ SCN- system
8	Determination of Electrolytic nature of inorganic compounds by Conductance measurement.
	One step preparations (1.0 g scale)
1	Bromobenzene to p-nitrobromobenzene
2	Anthracene to anthraquinone
3	Benzoin to benzil
4	Anthracene to Anthracene maleic anhydride adduct
5	2-Naphthol to BINOL

6	p-Benzoquinone to 1,2,4-triacetoxybenzene
7	Ethyl acetoacetate to 3-methyl-1-phenylpyrazol-5-one
8	*o*-Phenylenediamine to 2-methylbenzimidazole
9	*o*-Phenylenediamine to 2,3-diphenylqunooxaline

Course Code	**Elective Course**	**Credits**	**Lectures /Week**
K23PSCHEEL111	**Analytical Chemistry**	**2**	**2**

About the Course:

CO1	LANGUAGE OF ANALYTICAL CHEMISTRY:outcome:It prepares the learner completely for his entry in industrial and corporate sector .the learner is made fully aware of the common analytical problems faced in production and quality control .The learner is given detailed knowledge of the various instrumental and non instrumental methods used in industries and research analytical laboratories the determinate and indeterminate errors discussed involved and their calculations makes the student full aware of the statistical methods used for quality control in industries the discussion in the topic Accreditation and safety in laboratories prepares the learner to work in analytical laboratories in the industrial sector TQM total quality management is a management topic gives the learner clear idea of the pattern of working in corporate sector the frequently used techniques,in corporates for continuous improvement in quality .processes and systems of 5s .Kaizen and Six sigma are discussed in detail to make the learner aware of the atmosphere and ambience of corporate sector
CO2	CALCULATIONS BASED ON CHEMICAL PRINCIPLES : outcome :the learner will be able to prepare any type of solution required for analysis from ppb ppm to large concentrations, fully understanding the theoretical aspect behind the calculation used in the preparation The theoretical concepts of stoichiometry of the reactions ,formation constant ,stability constant are clearly discussed to give the learner a holistic information about chemical calculations

CO3	OPTICAL METHODS: The main objective of coaching this course is to impart knowledge in students about basic principle, instrumentation, and application of Recapitulation and FT Technique, Molecular Ultraviolet and Visible Spectroscopy, Applications of Ultraviolet and Visible spectroscopy, Infrared Absorption Spectroscopy . This enables learners to understand the function of various instruments and its application in chemical industries.
CO4	THERMAL METHODS: Thermal Methods: The main objective of coaching this course is to impart knowledge in students about basic principle, instrumentation, application , types of thermal methods, comparison between TGA and DTA, Differential Scanning Calorimetry, 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 multi-layered films, gas monitoring equipment and Automatic titrators. This enables learners to understand the function of various instruments and its application in chemical industries.

Unit	**Topics**	**No of Lectures**
I	**1.1 Language of Analytical Chemistry [8 L]** **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: [7 L]** **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 & 5S),	**15**

	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	
II	**Optical Methods [15 L]** **3.1 Recapitulation and FT Technique [3 L]** **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 [6 L]** 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. Applications of Ultraviolet and Visible spectroscopy: 1) On charge transfer absorption 2) Simultaneous spectroscopy **3)** Derivative Spectroscopy **3.2.2** Dual spectrometry – Introduction, Principle, Instrumentation and Applications **3.3 Infrared Absorption Spectroscopy [6 L]** **3.3.1** Instrumentation: Sources, Sample handling, Transducers, Dispersive, non-dispersive instrument**05 L** **3.3.2** FTIR and its advantages **3.3.3** Applications of IR [Mid IR, Near IR, Far IR]: Qualitative with emphasis on “Finger print” region, Quantitative analysis, Advantages and Limitations of IR	**15**

	3.3.4 Introduction and basic principles of diffuse reflectance spectroscopy.	

Reference Books:

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 & 4) (Free download).
6. Quality in the Analytical Laboratory, Elizabeth Pichard, Wiley India, Ch: 5, Ch: 6 &Ch: 7.
7. Quality Management, Donna C S Summers, Prentice-Hall of India, Ch:3.
8. Quality in Totality: A Manager‟s Guide To TQM and ISO 9000, ParagDiwan, Deep & 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 & Ch:15.
11. Safety and Hazards Management in Chemical Industries, M N Vyas, Atlantic Publisher, Ch:4, Ch:5 & Ch:19.
12. Staff, World Health Organization (2009) Handbook: Good Laboratory Practice (GLP)
13. OECD Principles of Good Laboratory Practice (as revised in 1997)". OECD Environmental Health and Safety Publications. OECD. **1**. 1998.
14. Klimisch, HJ; Andreae, M; Tillmann, U (1997). "A systematic approach for evaluating the quality of experimental toxicological and eco-toxicological data". doi:10.1006/rtph.1996.1076. PMID 9056496.

Unit II

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)

CO1	After successfully completing this course, students will be able to: prepare the solution of the desired concentration and the desired volume; Know the principle and handling of pH meter, Potentiometer, conductivity meter and Plot accurate graphs of the desired scale for the calculation
CO2	After performing non instrumental experiments,the students learn about the application of theoretical concepts in practicals. • In the heat of solution experiment the students will be able to understand the relation of temperature and solubility product of sparingly soluble salt. and also will be able to determine the heat of solution of sparingly soluble salt • In the second experiment students will be able to get knowledge about the variation of solubility of calcium sulphate with ionic strength and will also learn to calculate thermodynamic solubility product • In the kinetics experiment, the students learn about dependance of rate on concentration of reactants, rate laws , rate equation; they will also be able to plots graphs and determine order of reaction from graph • After performing this experiment the students understand the variation of solubility of calcium hydroxide in presence of NaOH and also will be able to determine solubility product of calcium hydroxide
CO1	Analytical Chemistry Practical: The main goal of teaching this course is to develop practical skills in students to facilitate them to perform analysis. In this course learner learned, To carry out assay of the sodium chloride injection by Volhard's method
CO2	The main goal of teaching this course is to develop practical skills in students to facilitate them to perform analysis. In this course learner learned,To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin, To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA, and To determine the breakthrough capacity of a cation exchange resin.
CO3	The main goal of teaching this course is to develop practical skills in students to facilitate them to perform analysis. In this course the learner learned To determine the lead and tin content of a solder alloy by titration with EDTA.
CO4	The main goal of teaching this course is to develop practical skills in students to facilitate them to perform analysis. In this course the learner learned To determine the amount of Cu(II) present in the given solution containing a mixture of Cu(II) and Fe(II) And To determine number of nitro groups in the given compound using TiCl3.

Course Code	Course Title	Credits	Lectures /Week
K23PSCHEELP111	**Practicals-Physical +Analytical Chemistry**	**2**	**4**
Course Objectives:			
1	**Non – instrumental:** 1. Polar plots of atomic orbitals such as 1*s*, and 3 orbitals by using angular part of hydrogen atom wave functions.		
2	2. To study the influence of ionic strength on the base catalysed hydrolysis of ethyl acetate.		
3	3. To study phase diagram of three component system water – chloroform /toluene - acetic acid.		
4	4. To determine the rate constant of decomposition reaction of diacetone alcohol by dialtometric method.		
5	**Instrumental:** 1. To determine the formula of silver ammonia complex by potentiometric method.		
6	2. To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.		
7	3. To determine Hammette constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by pH measurement.		
8	4. To determine the Michaelis – Menten‟s constant value (Km) of the enzyme Beta Amylase spectrophotometrically.		

1	To carry out assay of the sodium chloride injection by Volhard‟s method.
	Statistical method.
2	2. To determine (a) the ion exchange capacity (b) exchange efficiency of the given cation exchange resin.
3	3. To determine amount of Cr(III) and Fe(II) individually in a mixture of the two by titration with EDTA.
4	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 TiCl3.

Physical 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.

Analytical References :

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company,Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part-II,4th Ed.,A Wiley Interscience Publication,New York,1978.

Course Code	RESEARCH METHODOLOGY SEM -I	Credits	Lectures /Week
K23PSCHERM141	RESEARCH METHODOLOGY FOR CHEMISTRY	4	4

CO1	Various sources of Information journals indices etc.
CO2	Safe handling of chemicals and fundamentals of electronic credits.
CO3	To write research and scientific papers work safely in Laboratory also use first aid if necessary.
CO4	Using statistical tests, chemo metrics, ANNOVA, regression analysis the student can analyse data for research.

	RESEARCH METHODOLOGY FOR CHEMISTRY	
1	**Literature Survey** 1.1 **Print:** Sources of information: Primary, secondary, tertiary sources; 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. 1.2 **Digital:** Web resources, 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. 1.3 **Information Technology and Library Resources:** The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information.	15
2	**Methods of Scientific Research and Writing Scientific Papers** 2.1 Reporting practical and project work 2.2 Writing literature surveys and reviews	15

	2.3 Organizing a poster display 2.4 Giving an oral presentation 2.5 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.	
3	**Chemical Safety and Ethical Handling of Chemicals** 3.1 Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation 3.2 Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards 3.3 procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals 3.4 recovery, recycling and reuse of laboratory chemicals 3.5 procedure for laboratory disposal of explosives 3.6 identification, verification and segregation of laboratory waste 3.7 disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals	**15**
4	**Data Analysis** 4.1 The Investigative Approach: Making and Recording Measurements. SI Units and their use.Scientific method and design of experiments 4.2 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,	**15**

	linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.	

Reference Books

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011)
  Practical skills in chemistry. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment.* Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis.* Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.
- OSU safety manual 1.01.

Semester-II

Course Code	Major Course	Credits	Lectures /Week
K23PSCHEMJ211	**Paper-I Physical Chemistry**	**4**	**4**

About the Course:

CO1	After studying this module of **Chemical Thermodynamics II** students shall be able to: know the concept of fugacity, determine the coefficient of fugacity, understand the concept of partial molal quantities for real solutions and derivation of Gibbs Duhem Margules equation , know the thermodynamics of surfaces, understand relation between surface tension and adsorption and derivation of Gibbs and BET adsorption equations, understand free energy changes accompanying biochemical reactions.
CO2	After studying this module of **Quantum Chemistry II** students shall be able to: write the Schrödinger equation for Rigid Rotator, solve the Schrödinger equation for Rigid Rotator, write the Schrödinger equation for Hydrogen atom ,solve the Schrödinger equation for Hydrogen atom,write the radial wave-function of electronic hydrogen atom Schrödinger equation, write the expressions for the total wave function for 1s,2s, 2p and 3d orbitals of hydrogen, study the application of the Schrödinger equation to two electron system
CO3	After studying this module **Chemical Kinetics and Molecular Reaction Dynamics**, student shall be able to- learn about Solution Kinetics, learn about ionic reactions, learn about effect of solvent on the rate of ionic reaction, know about ionic strength, learn about the effect of solvent on the rate of the reaction, derive the relationship between the rate constant of the reaction and dielectric constant of the solvent, learn about primary and secondary salt effects, study of free energy changes accompanying biochemical reactions, specificity of enzyme substrate reactions and their catalytic power, learn the derivation of the Michaelis-Menten equation in understanding enzyme kinetics and its applications, also learn the Lineweaver-Burk and Eadie Analyses , learn the importance and significance of Vo, Km, Vmax , understand the Inhibition of Enzyme action i.e. Competitive, Noncompetitive and Uncompetitive Inhibition , study the Kinetics of reactions in solid states such as rate laws .

CO4	After the course on **Solid State Chemistry** the student will be able to- understand the origin and nature of defects in crystals, learn types of crystal defects and Stoichiometry, learn thermodynamics of formation of defects and mathematical derivation to find concentration of defects.

Unit	Topics	No of Lectures
I	**Chemical Thermodynamics II [15 L]** 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. (Ref: 7 and 2)	**15**
II	**Quantum Chemistry II [15 L]** **2.1.** Rigid rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wavefunction, 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 □ * and the □ 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	**15**

	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. ***(Derivation expected)***	
III	**Chemical Kinetics and Molecular Reaction Dynamics [15 L]** 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 Analyses**.** 3.3. **Inhibition of Enzyme action**: Competitive, Noncompetitive and Uncompetitive Inhibition. Effect of pH, Enzyme activation by metal ions, Regulatory enzymes. 3.4. **Kinetics of reactions in the Solid State:-** Factors affecting reactions in solids **Rate laws for reactions in solid**: The parabolic rate law, The first order rate Law, the contracting sphere rate law,Contracting area rate law, some examples of kinetic studies.	**15**
IV	**Solid State Chemistry and Phase Equilibria [15 L]** **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) (Ref: 17, 18 and19) **4.2 Phase equilibria**	**15**

	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 (Ref: 4, 6, 11, 12 ,13,16, 24)	

References

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 & Elaine A. Moore, Taylor & 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	Major Course	Credits	Lectures/Week
K23PSCHEMJ212	**Paper-II Inorganic Chemistry**	**4**	**4**

About the Course:

CO1	In this unit students will study Inorganic reaction mechanism where rate of reaction, factor affecting it and techniques for its determination. Ligand substitution reactions and redox reaction along with stereochemistry of substitution reactions of octahedral complexes is studied.
CO2	In this unit Organometallic Chemistry of Transition metals is studied for some compounds with their preparation and properties, structure and bonding of some organometallic compounds is studied on the basis of VBT and MOT.
CO3	Learner will get knowledge of environmental chemistry with respect to heavy metals toxicity along with radioactive materials and their effect on living things.
CO4	In Bio-inorganic Chemistry unit students will get knowledge of biological oxygen carriers, copper containing enzymes, nitrogen fixation, metal ion transport and cis-platin related compounds with their applications.

Unit	Topics	No of Lectures
I	**Inorganic Reaction Mechanism: [15 L]** 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.)	
II	**Unit II** **Organometallic Chemistry of Transition metals: [15 L]** 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, 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(PPh3)2(HC≡CPh)2], diallylnickel(II), ferrocene and bis(arene)chromium(0), tricarbonyl (η2-butadiene) iron(0).	
III	**Environmental Chemistry:[15 L]** **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.	
IV	**Bioinorganic Chemistry:[15 L]**	

	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 it‟s 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	

References:

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 & 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 & 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 & Sons, Calcutta, 1988.
6. J.Chem. Educ. (Special issue), Nov, 1985.
7. E.Frienden, J.Chem. Educ., 1985, 62.
8. Robert R.Crechton, Biological Inorganic Chemistry – An Introduction, Elsevier
9. J. R. Frausto da Silva and R. J. P. Williams *The Biological Chemistry of the Elements*, Clarendon Press, Oxford, 1991.
10. JM. D. Yudkin and R. E. Offord *A Guidebook to Biochemistry*, Cambridge University Press, 1980.

Course Code	Major Course	Credits	Lectures /Week
K23PSCHEMJ213	**Paper-III Organic Chemistry**	**4**	**4**

CO1	In the topic **Alkylation of Nucleophilic Carbon Intermediates**, the students will learn about Carbanions, formation and alkylation of enolates,alkylation of aldehydes, ketones, esters, amides and nitriles; Reactions of Carbon nucleophiles with carbonyl groups, their mechanism, a few name reactions like Aldol condensation, Robinson annulation, Knoevengel reaction, Mannich reaction.
CO2	In the topic **Reactions and Rearrangements**, the students shall learn about mechanisms, stereochemistry and applications of reactions like Baylis-Hilman reaction, McMurry coupling, Corey-Fuchs reaction, etc.; rearrangements like Hoffman, Curtius, Lossen, Schmidt, Wolff, etc.
CO3	In the topic Introduction to **Molecular Orbital Theory for Organic Chemistry**, the students will learn about molecular orbitals of various alkene systems; concepts of FMO, HOMO-LUMO, Application of FMO concepts to organic reactions.
CO4	In the topic **Applications of UV and IR Spectroscopy**, the students will get clear ideas about fundamentals of UV and IR spectroscopy, factors affecting the position and intensity of uv bands, calculation of absorption maxima by using Woodward-Fischer rules; characteristics and factors affecting vibrational frequencies and study of vibrational frequencies of organic compounds.
CO5	From the topic **NMR Spectroscopy and Mass Spectrometry**, the students shall learn about the fundamentals, principles, theory,applications in structural elucidation, factors affecting the values of H1-NMR, 13C, and Mass spectrometry (m/z) and various terminologies involved in them.

About the Course:

Unit	Topics	No of Lectures
I	**1.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)**	**15**

	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: (8 L)** 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. [Reference Books: 1-11]	
II	**Reactions and Rearrangements: (15 L)** Mechanisms, stereochemistry (if applicable) and applications of the following: **2.1. 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. [Reference Books: 19-22]	**15**
III	**3.1. Introduction to Molecular Orbital Theory for Organic Chemistry: (7 L)** **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,	**15**

	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) SN2 reaction, (b) Lewis acid base adducts (BF3-NH3 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: (8 L)** **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.	
IV	**NMR spectroscopy and Mass spectrometry (15 L)**	**15**

	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. 13C 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. [Reference Books: 13-18]	

References:

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, page no. 713-769, 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 (7th 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 & 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 & Sons.

Course Code	Major Course	Credits	Lectures /Week
K23PSCHEMJP211	**Practical Inorganic + Organic Chemistry**	**2**	**4**

Course Objectives:

CO1	In Inorganic preparations students will prepare the metal complexes along with their characterization.
CO2	In Instrumentation conductance measurement is done for the determination of electrolytic nature of inorganic compounds.
CO3	Spectrophotometer is used to measure the optical density for different concentrations of metal and ligand for the determination of equilibrium constant by slope intercept method for Fe^{+3}/SCN^{-}.

CO 2	The students will also learn about the characterization of one of the separated components with the help of chemical analysis.
CO 3	The students will learn about the confirmation of the structure (of the characterized compound) by preparation of its derivative and physical constant of the derivative.
CO 4	The students shall learn about the purification of the second compound methods like crystallization and distillation, and the determination of its physical constant.
CO 5	At the end, the students will be good at **separation** of various types of bi mixtures, **characterization** of one of the components and its **confirmati** by the preparation of derivative and **determination** of physical constant.

	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
5	Estimation of Copper using Iodometric method Potentiometrically.
6	Estimation of Fe+3 solution using Ce(IV) ions Potentiometrically

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
4. 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.

Inorganic Reference:

1. Advanced experiments in Inorganic Chemistry., G. N. Mukherjee., 1st Edn., 2010., U.N.Dhur & Sons Pvt Ltd

2. The Synthesis and Characterization of Inorganic Compounds by William L. Jolly

3. Inorganic Chemistry Practical Under UGC Syllabus for M.Sc. in all India Universities By: Dr Deepak Pant

Organic 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	ELECTIVE Course	Credits	Lectures /Week
K23PSCHEEL221	**Analytical Chemistry**	**2**	**2**

About the Course:

CO1	Recapitulation of basic concepts in chromatography:outcome:The basic concepts of chromatography ,detectors used in GC andLC their comparison and applications are clarified is to the learner very well outlining to the learner the principles of a very versatile method of separation and analysis Outcome of the topic on gas chromatography is that it gives a overview of all the advanced and modern systems of injection.detectors such as mass spectrometric used in GC to the learner which will help them in handling the instrument easily HPLC:outcome:All the sophisticated and recent applications ,systems used commercially available columns are discussed which will update the learner about the industrial applications of HPLC
CO2	X RAY Spectroscopy:outcome: XRay Diffraction and absorption methods are discussed in detail which totally equips the learner for its use commercially Mass spectroscopy:outcome :since it the most widely used technique when accurate results are required .the topic gives a good overview to the learner about its instrumentation electron impact ,chemical and field ionisation mass analysers and its applications Radioanalytical methods :outcome:It prepares the learner to takeup further studies in Forensic sciences since it has vast applications in forensic studies the topic discusses in detail isotope,single and double dilution method applications to enhance the knowledge of the learner
CO3	Surface Analytical Techniques: the core purpose of coaching this course is to impart knowledge in students in the subject of Introduction, Principle, Instrumentation and Applications of Scanning Electron Microscopy (SEM), Scanning Tunneling Microscopy (STM), Transmission Electron Microscopy (TEM) Electron Spectroscopy (ESCA and Auger), Atomic Spectroscopy. AAS, Atomic Spectroscopy.
CO4	Electroanalytical Methods: the core purpose of coaching this course is to impart knowledge in students in the subject of Ion selective potentiometry and Polarography, Ion selective electrodes and their

	applications, ion selective field effect transistors, biocatalytic membrane electrodes and enzyme-based biosensors. In the subject of Polarography, Coulometry and Electrogravimetry students learn Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves. Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications.

Unit	Topics	No of Lectures
I	**Chromatography [15 L]** **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**.[2 L]** **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**.[5 L]** **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. **[3 L]** **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. **[5 L]**	15
II	**Electroanalytical Methods (Numerical are Expected)** **4.1 Ion selective potentiometry and Polarography: [10 L]** 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.	15

	Polarography: Ilkovic equation, derivation starting with Cottrell equation, effect of complex formation on the polarographic waves. **4.2 Electrogravimetry**: Introduction, principle, instrumentation, factors affecting the nature of the deposit, applications**.[3 L]** **4.3 Coulometry:** Introduction, principle, instrumentation, coulometry at controlled potential and controlled current **[2 L]**	

References:

Unit I

1. Instrumental Analysis, Skoog, Holler & Crouch
2 HPLC Practical and Industrial Applications, 2 nd Ed., Joel K. Swadesh, CRC Press

Unit II

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	ELECTIVE Course	Credits	Lectures /Week
K23PSCHEELP221	**Practical Physical + Analytical Chemistry**	**2**	**4**

Course Objectives:

CO 1	In the practical course of **Physical Chemistry** students will gain understanding of: the preparation for each experiment by studying handouts, safety requirements and lab skills to perform physico-chem experiments, keeping records of instruments, parameters and experim observations, key techniques including Uv-Vis spectroscopy, pHm potentiometry, conductometry etc.
CO 2	After performing this experiment the student will be able to- understand quantum mechanical concepts about atomic orbitals (Polar plots of atomic orbitals such as 1s, 2Pz and $3dz^2$orbitals by u angular part of hydrogen atom wave functions)
CO 3	After performing this experiment the student will be able to- learn effect of ionic strength on rate of the reaction (To study the influence of ionic strength on the base catalyzed hydrolys ethyl acetate)
CO 4	After performing this experiment the student will be able to- learn how to construct the phase diagram for ternary system (To study phase diagram of three component system water – chloro /toluene - acetic acid)
CO 5	After performing this experiment the student will be able to- learn dialtometric method-(To determine the rate constant of decompos reaction of diacetone alcohol by dialtometric method)
CO 6	After performing this experiment the student will be able to- .learn application of conductivity method in surfactants(To determine CM sodium Lauryl Sulphate from measurement of conductivities at diff concentrations.)
CO 7	After performing this experiment the student will be able to- understand the importance of Hammette equation-(To determine Hamm constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by measurement.)

CO 8	After performing this experiment the student will be able to- learn enzy catalysed reactions-(To determine the Michaelis – Menten's constant va (Km) of the enzyme Beta Amylase spectrophotometrically.

	Non – instrumental:
1	Polar plots of atomic orbitals such as 1*s*, and 3 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 dialtometric method.
	Instrumental:
5	To determine the formula of silver ammonia complex by potentiometric method.
6	To determine CMC of sodium Lauryl Sulphate from measurement of conductivities at different concentrations.
7	To determine Hammette constant of *m*- and *p*- amino benzoic acid/nitro benzoic acid by pH measurement.
8	To determine the Michaelis – Menten"s constant value (Km) of the enzyme Beta Amylase spectrophotometrically.
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 pectrophotometrically.
7	To determine the percentage composition of HCl and H2SO4 on weight basis in a mixture of two by conductometric titration with NaOH and BaCl2.
8	To determine amount of potassium in the given sample of fertilizers using flame photometer by standard addition method.

Physical 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.

Analytical References:

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels, 3rd Ed. ELBS (1964)
2. Vogel's textbook of quantitative chemical analysis, Sixth Ed. Mendham, Denny, Barnes, Thomas, Pearson education
3. Standard methods of chemical analysis, F. J. Welcher
4. Standard Instrumental methods of Chemical Analysis, F. J. Welcher
5. W.W.Scott."Standard methods of Chemical Analysis",Vol.I, Van Nostrand Company, Inc.,1939.
6. E.B.Sandell and H.Onishi,"Spectrophotometric Determination of Traces of Metals",Part-II, 4th Ed.,A Wiley Interscience Publication,New York,1978

Evaluation Scheme for First Year (PG) under NEP

(4 Credits)

I. Internal Evaluation for Theory Courses – 40 Marks

Continuous Internal Assessment 1 (Seminar Presentations) – 40 Marks

II. External Examination for Theory Courses – 60 Marks

Duration: 2.5 Hours

Theory question paper pattern:

All questions are compulsory.

Question	Based on	Marks
Q.1	Unit I	15
Q.2	Unit II	15
Q.3	Unit III	15
Q.4	Unit IV	15

- All questions shall be compulsory with internal choice within the questions.
- Each Question may be sub-divided into sub questions as a, b, c, d, etc. & the allocation of Marks depends on the weightage of the topic.

III. Practical Examination

- Each core subject carries 50 Marks
- Duration: 4Hours for each practical course
- Minimum 80% practical from each core subjects are required to be completed.
- Certified Journal is compulsory for appearing at the time of Practical Exam

Evaluation Scheme for First Year (PG) under NEP

(2 Credits)

I. Internal Evaluation for Theory Courses – 20 Marks

Continuous Internal Assessment 1 (Seminar Presentations) – 20 Marks

II. External Examination for Theory Courses – 30 Marks

Duration: 2 Hours

Theory question paper pattern:

All questions are compulsory.

Question	Based on	Marks
Q.1	Unit-I	15
Q.2	Unit-II	15

- All questions shall be compulsory with internal choice within the questions.
- Each Question may be sub-divided into sub questions as a, b, c, d, etc. & the allocation of Marks depends on the weightage of the topic.
- Each unit will have 25% objective questions.

III. Practical Examination

- Each core subject carries 50 Marks
- Duration: 4Hours for each practical course
- Minimum 80% practical from each core subjects are required to be completed.
- Certified Journal is compulsory for appearing at the time of Practical Exam