DOMBIVLI SHIKSHAN PRASARAK MANDAL'S,

K.V. PENDHARKAR COLLEGE OF ARTS, SCIENCE AND COMMERCE, AUTONOMOUS.

DOMBIVLI (EAST), MAHARASHTRA, 421 203, INDIA.

Faculty of Sciences

DEPARTMENT OF CHEMISTRY

Programme: Masters of Science (M.Sc.)

SYLLABUS FOR:

M. Sc. Part I (Semesters I & II)

Choice Based Credit System (CBCS) with effect from the Academic Year

2021-22

CONTENT

Semester-I

PAPER I (PHYSICAL CHEMISTRY)
Course Code: PPSCHI21-101

Learning objectives:
The learner to be imparted with:
1. Knowledge of Thermodynamics, the terms involved, Third Law of Thermodynamics.
2. Quantum Chemistry, Particle waves and Schrödinger wave equation.
3. Chemical Dynamics, Electrochemistry, various equations.
4. Surface active agents and micelle, Hydrogen storage by Adsorption.

Learning Outcomes:
On successful completion of this course students will be able to:
1. Explain the concept of Thermodynamics, explain Third Law of Thermodynamics.
2. explain quantum Chemistry, various wave equations, etc.
3. Understand chemical dynamics, concept of electrochemistry and other equations.
4. Understand surface active agents and micelle, gain knowledge of hydrogen energy and storage of hydrogen.

Unit - 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 changes 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]

Unit 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.

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]

Unit III

Chapter 1 Chemical Dynamics-I [7L]

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.

[Ref. 2 and 15, 17, 18]

Chapter 2 Electrochemistry [8L]

Recapitulation – basics of electrochemistry.

3.2. Debye-Hückel theory of activity coefficient, Debye-Hückel limiting law and it's extension to higher concentration (derivations are expected).

3.3. Electrolytic conductance and ionic interaction, relaxation effect,. Debye-HückelOnsager 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.

[Ref: 14 and 16, 17, 18]

UNIT-IV Modern Applications of Surface Chemistry (15L)

4.1 Surface active agents and micelle: (08L)

4.1.1Surface active agents andt their classification, hydrophile-lipophile balance(02L)
4.1.2Micellization: shape and structure of micelles, hydrophobic interaction, critical Micelles concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, micelle catalysis,reverse micelles. (04L)
4.1.3 Emulsions: Solubilization, micro emulsions, characterization of microemulsions, (02L)

4.2 Hydrogen storage by Adsorption: (07L)

4.2.1 Hydrogen storage: fundamentals physisorption, temperature and pressure influence, chemisorption, adsorption energy, 'Electrochemical' adsorption. (03L)

4.2.2. Practical adsorption: Storage of hydrogen with carbon materials, activated carbon, graphite graphene, carbon nano structures, fullerene. Carbon nano fibres (CNF) and graphite nano fibers electrochemical storage of hydrogen in carbon materials. (04)

[**Note: Numerical and theoretical problems from each unit are expected**]

PRACTICAL PAPER I (PHYSICAL CHEMISTRY)
Course Code: PPSCHI21-P101

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. 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
19. 'Carbon nanoforms and applications' Sharon and Sharon, published by McGraw Hill, USA , 2009.

PAPER II (INORGANIC CHEMISTRY)
Course Code: PPSCHI21-102

Learning objectives:

The learner to be imparted with:

1. Knowledge of Chemical Bonding, MOT, Van der Waal's forces.
2. Molecular symmetry, Group theory, SALC.
3. Solid state Chemistry, Nanomaterials.
4. Characterization of Coordination compounds using various instrumental methods.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Explain different chemical bonding, molecular orbital theory and weak forces.
2. Understand molecular symmetry, intricacies of group theory and SALC.
3. Understand solid state chemistry and synthesis of CNMs, and their properties.
4. Understand the use of different instruments and their use in characterization of coordination compounds.

Unit I

Chemical Bonding: [15 L]

1.1 Recapitulation of hybridization Derivation of wave functions for sp, sp^2, sp^3 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 SF_6, CO_2, B_2H_6, I_3^- 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.

Unit II

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.
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 C_{2v}, C_{3v} and D_{2h}, structure of character tables.
2.4 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

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)], AB_2 [fluorite (CaF_2) and anti-fluorite structures, rutile (TiO_2) structure and layer structure [cadmium chloride and iodide ($CdCl_2$, CdI_2)].
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 Special nanomaterials - Carbon nanotubes
3.2.1. Discovery
3.2.2. Types and Properties
3.2.3 Methods of preparation
3.2.4 Applications

Unit - IV
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, B, C, Nephelauxetic ratio.
4.3 Determination of formation constants of metal complexes (Overall and Stepwise): Comparative studies of Potentiometric and spectral methods.

PRACTICAL PAPER II (INORGANIC CHEMISTRY)
Course Code: PPSCHI21-P102

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.

References:

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).

PAPER III (ORGANIC CHEMISTRY)
Course Code: PPSCHI21-103

Learning objectives:

The learner to be imparted with:

1. Physical aspects of organic chemistry like thermodynamics, kinetics etc.
2. Different nucleophilic substitution reactions like S_N1, S_N2, S_N^i etc. and aromaticity.
3. Stereochemistry, chirality, Prochirality
4. Oxidation and reduction reactions involving organic molecules and Neighbouring group participation.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Explain physical concepts of organic reactions.
2. Distinguish different nucleophilic reactions and explain the nuance of aromaticity.
3. Understand stereochemistry, chirality and prochirality.
4. Write the different oxidation and reduction reactions involving organic molecules. Explain the concept of neighbouring group participation.

Unit I

1.0 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]

Unit II

2.0 Nucleophilic substitution reactions and Aromaticity

2.1. Nucleophilic substitution reactions: (9 L)

2.1.1. 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, α- 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.

2.1.2. Aromatic nucleophilic substitution: S_NAr, S_N1, 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)

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 (C_{60}).
[Reference Books: 4-15]

Unit-III

3.0 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.

[Reference Books: 6-8]

Unit-IV

4.0 Oxidation and Reduction: (12 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:

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,

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: Wolff-Kishner reduction and Huang-Minlon modification.

4.2.2. Metal hydride reduction: Boron reagents ($NaCNBH_3$, diborane, 9-BBN, $Na(OAc)_3BH$, aluminium reagents (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 and Mg under neutral and acidic conditions, Li/Na-liquid NH_3 mediated reduction (Birch reduction) of aromatic compounds and acetylenes.

B. Neighbouring group participation: 3L

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)

[Reference Books: 17, 18, 14]

PRACTICAL PAPER III (ORGANIC CHEMISTRY)
Course Code: PPSCHI21-P103

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-diphenylqunooxaline.
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.

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.

PAPER IV (ANALYTICAL CHEMISTRY)
Course Code: PPSCHI21-104

Learning objectives:

The learner to be imparted with:

1. Information of language of analytical chemistry and concept of quality.
2. Calculations based on Chemical Principles and Sampling technique.
3. UV & visible spectroscopy and IR spectroscopy.
4. Different thermal methods like DTA and DSC and Automation in chemical analysis.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Interpret the way analytical chemistry is used. Also, understand the concept of quality.
2. Will be able to solve various numerical problems and calculations based on chemical principles including those of sampling techniques.
3. Analyze and Interpret UV-Visible and IR spectroscopy.
4. Understand thermal methods like DTA, DSC etc. and use automation in chemical analysis.

Unit - 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.

1.2 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), 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

2.1 Calculations based on Chemical Principles [10 L]

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).

2.2 Sampling technique [05]
For special solid industrial material ores, alloys, powders etc.

Unit III

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]

3.2.1 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.
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
3.3.4 Introduction and basic principles of diffuse reflectance spectroscopy.

Unit - IV

4.1 Thermal Methods: [9 L]

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: [6 L]

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.

PRACTICAL PAPER IV (ANALYTICAL CHEMISTRY)
Course Code: PPSCHI21-P104

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 $TiCl_3$.

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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.
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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.
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12. Z. M. Khoshhesab (2012). Infrared Spectroscopy- Materials Science, Engineering and Technology. Prof. Theophanides Theophile (Ed.). ISBN: 978-953- 51-0537- 4, InTech,(open access)

Unit IV

1. Introduction to instrumental methods of analysis by Robert D. Braun, Mc. Graw Hill (1987): Chapter 27
2.Thermal Analysis-theory and applications by R. T. Sane, Ghadge, Quest Publications

3. Instrumental methods of analysis, 7 th Edition, Willard, Merrit, Dean: Chapter 25
4. Instrumental Analysis, 5 th Edition, Skoog, Holler and Nieman: Chapter 31
5. Quantitative Chemical Analysis, 6 th Edition, Vogel: Chapter 12
6. Analytical Chemistry by Open Learning: Thermal Methods by James W. Dodd & Kenneth H. Tonge
7. Instrumental methods of analysis, 7 th 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, Mc. GrawHill (1987): Chapter 28

Practical

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.
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SEMESTER II

PAPER I (PHYSICAL CHEMISTRY)
Course Code: PPSCHII21-201

Learning objectives:

The learner to be imparted with:

1. Knowledge of Thermodynamics, fugacity of real gases, Gibbs Duhem Margules equation, bioenergetics.
2. Quantum Chemistry, Schrödinger equation, Hückel Molecular Orbitals theory.
3. Chemical Kinetics and Molecular Reaction Dynamics, Kinetics of reactions in the Solid State.
4. Various aspects of Polymer Chemistry.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Understand fugacity of real gases, equations like Gibbs Duhem Margules equaition, also bioenergetics like standard free energy change in biochemical reactions, ATP, ADP.
2. Use Schrödinger equation, Hückel Molecular Orbitals theory in the purview of Quantum Chemistry.
3. Explain Chemical kinetics like elementary reactions in solution, Kinetics of reactions catalyzed by enzymes, reactions in solid state.
4. Understand Polymer Chemistry, 2Thermodynamics of polymer solutions, Properties and applications of some commercially important polymers.

Unit 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.

Unit 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 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. (Derivation expected)

Unit 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. (Ref: 7 and 2)

Unit IV Polymer Chemistry (15L)

4.1Techniques of polymerization: Bulk polymerization, solution polymerization, suspension polymerization, emulsion polymerizations (03L)

4.2Thermodynamics of polymer solutions: Solubility parameter, thermodynamics of mixing, theta temperature. (02L)

4.3Polymer technology:

4.3.1 Polymer auxiliaries, plasticizers, heat Stabilizers, colorants, flame retardants. Fillers, reinforcements.

4.3.2 Elastomers: Introduction, Processing, Rubber Types, Vulcanization, Properties. Reclaiming.

4.3.3 Fibers: Introduction, production, Fiber spinning, Textile fibers, Industrial fibers, recycling.

4.3.4 Films sheets: Introduction and processing techniques (injection and blow moulding extrusion), Recycling of plastics. (05L)

4.4 Properties and applications of some commercially important polymers. Carbon chain polymers- Polyolefins, ABS group, elastomers, vinyl polymers, acrylic polymers, heterochain polymers- polyethers, polycarbonates, polysaccharides, polyamides fluoropolymers, Resins (epoxy, alkyd, phenol-formaldehyde and urea-formaldehyde), Silicones, polyphosphazenes, sulphur containing polymers. (05L)

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

PRACTICAL PAPER I (PHYSICAL CHEMISTRY)
Course Code: PPSCHII21-P201

Non – instrumental:

1. Polar plots of atomic orbitals such as 1s, 2 and 3 2orbitals 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:

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

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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.
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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.
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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
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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.
26. P. Bahadur and N. V. Sastry, Principles of Polymer Science, second edition, Narosa Publishing House, 2005.
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PAPER II (INORGANIC CHEMISTRY)
Course Code: PPSCHII21-202

Learning objectives:

The learner to be imparted with:

1. Inorganic Reaction Mechanism.
2. Organometallic Chemistry of Transition metals.
3. Environmental Chemistry.
4. Bioinorganic Chemistry.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Understand factors affecting rate of reactions, Ligand substitution reactions, Redox reactions, along with stereochemistry.
2. Explain Eighteen and sixteen electron rules, alkyl and aryl derivatives of metals, properties of sandwich compounds.
3. Explain the concept of heavy metals, metal toxicity, Interaction of radiation in context with the environment.
4. Understand biological oxygen carrier, Activation of oxygen in biological system, nitrogen fixation, Metal ion transport and storage etc.

Unit 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 noncomplimentary reactions.

1.4 Stereochemistry of substitution reactions of octahedral complexes. (Isomerization and racemization reactions and applications.)

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)

$[Pt(PPh_3)_2(HC{\equiv}CPh)_2]$, diallylnickel(II), ferrocene and bis(arene)chromium (0), tricarbonyl (η^2 -butadiene) iron (0).

Unit 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
1. Jaduguda uranium mine
2. Minamata mercury poisoning
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

Bioinorganic Chemistry: [15 L]
4.1 Biological oxygen carriers; haemoglobin, hemerythrene and hemocyanin- structure of metal active center and differences in mechanism of oxygen binding, Differences between haemoglobin and myoglobin: Cooperativity of oxygen binding in haemoglobin and Hill equation, pH dependence of oxygen affinity in haemoglobin 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

PRACTICAL PAPER II (INORGANIC CHEMISTRY)
Course Code: PPSCHII21-P202

Inorganic Preparations (Synthesis and Characterization)
1)Bis-(tetraethylammonium) tetrachloro Cuprate (II) $(Et_4N)_2[CuCl_4]$
2)Bis-(tetraethylammonium) tetrachloro Nickelate (II) $(Et_4N)_2[NiCl_4]$
3)Bis-(tetraethylammonium) tetrachloro Cobaltate (II) $(Et_4N)_2[CoCl_4]$ (Any two from 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.

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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,
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4. Environmental Science 13th edition, G. Tyler Miller Jr. and Scott E. Spoolman, ISBN10: 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
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Unit IV

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PAPER III ORGANIC CHEMISTRY
Course Code: PPSCHII21-203

Learning objectives:

The learner to be imparted with:

1. Alkylation of Nucleophilic Carbon Intermediates, Name reactions with mechanism and application.
2. Reactions and Rearrangements
3. Molecular Orbital Theory for Organic Chemistry, Applications of UV and IR spectroscopy.
4. NMR spectroscopy and Mass spectrometry.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Write different reactions leading to alkylation of nucleophilic carbon intermediates, explain different name reactions and their mechanism.
2. Explain various reactions and rearrangements.
3. Understand molecular orbitals, FMOs, their applications, interpret UV-visible and IR spectroscopy.
4. Understand and interpret NMR and Mass spectroscopy.

Unit I

1.1. Alkylation of Nucleophilic Carbon Intermediates: (7 L)

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 Name reactions with mechanism and application (8L)
1.2.1 Mukaiyama esterification, Mitsonobu reaction, Darzen's Glycidic Ester synthesis, Ritter reaction, Yamaguchi esterification, Peterson olefination. [5L]
1.2.2 Domino reactions: Characteristics; Nazerov cyclization [3L]

Unit II

2.0 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:, Von Richter, Wittig, Gabriel–Colman, Payne.
[Reference Books: 19-22]

2.5. Overman Rearrangement, Claisen-Johnson Rearrangement
[Reference Books: 19-22]

Unit-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, 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, € 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.

Unit-IV

4.0 NMR spectroscopy and Mass spectrometry (15 L)

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.

PRACTICAL PAPER III (ORGANIC CHEMISTRY)
Course Code: PPSCHII21-P203

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.

References:

1. 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 (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 & 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.

PAPER IV ANALYTICAL CHEMISTRY
Course Code: PPSCHII21-204

Learning objectives:

The learner to be imparted with:

1. Basic concepts in chromatography, GC, HPLC, Gel Chromatography.
2. X-Ray and Mass spectroscopy and radioanalytical methods.
3. Surface analytical techniques and atomic spectroscopy.
4. Electroanalytical Methods.

Learning Outcomes:

On successful completion of this course students will be able to:

1. Explain and use the concept of Chromatography, GC, HPLC, Gel Chromatography.
2. Explain the principle, instrumentation and applications of X-ray, Mass spectroscopy, and Radioanalytical methods.
3. Explain Introduction, Principle, Instrumentation and Applications of SEM, STM, TEM, ESCA etc. and Advantages and Limitations of AAS.
4. Use Ion selective potentiometry and Polarography, Electrogravimetry, Coulometry.

Unit I

Chromatography [15 L]

1.1 Recapitulation of basic concepts in chromatography: [4 L]

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.

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.

1.2 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. [4 L]

1.3 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. [4 L]

1.4 Gel Chromatography [3 L]

Principle, gel preparation, column packing, detector, applications.

Unit II

2.1 X-ray spectroscopy: principle, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy. [4 L]

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 analysers: Quadrupole, time of flight and ion trap. Applications. [6 L]

2.3 Radioanalytical Methods – recapitulation, isotope dilution method, introduction, principle, single dilution method, double dilution method and applications. [5 L]

Unit III

3.1 Surface Analytical Techniques – [9 L]

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 [6 L]

3.2.1 Advantages and Limitations of AAS

3.2.2 Atomic Spectroscopy based on plasma sources – Introduction, Principle, Instrumentation and Applications.

Unit IV

Electroanalytical Methods (Numericals 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. 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]

PRACTICAL PAPER IV (ANALYTICAL CHEMISTRY)
Course Code: PPSCHII21-P204

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 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.

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. 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. 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, ISBN-13: 978-8131505427

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.

Practical

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",PartII, 4th Ed.,A Wiley Interscience Publication, New York,1978