M.Sc. CHEMISTRY

SEM	COURSE CODE	COURSE	COURSE TITLE	HRS / WEEK	CREDIT	CIA MARKS	SE MARKS	TOTAL MARKS
I	14PCH1C1	CORE-I	Structure bonding, Acid-base and Nuclear reactions	6	5	40	60	100
	14PCH1C2	CORE-II	Reaction Mechanism, Stereochemistry and Natural product	6	5	40	60	100
	14PCH1C3P	CORE-III	Inorganic Estimations and Complex Preparations- Practical	6	5	40	60	100
	14PCH1C4P	CORE-IV	Organic Estimations and Chromatography- Practical	6	5	40	60	100
	14PCH1CE1	CORE BASED ELECTIVE-I #		6	5	40	60	100
TOTAL				**30**	**25**	**200**	**300**	**500**
II	14PCH2C5	CORE-V	Organic Reactions and Mechanisms	6	5	40	60	100
	14PCH2C6	CORE-VI	Group Theory and Spectroscopy	6	5	40	60	100
	14PCH2C7P	CORE-VII	Inorganic Qualitative Analysis and Colorimetric Estimations- Practical	6	5	40	60	100
	14PCH2C8P	CORE-VIII	Organic Preparations and Mixture Analysis- Practical	6	5	40	60	100
	14PCH2CE2	CORE BASED ELECTIVE -II #		6	5	40	60	100
TOTAL				**30**	**25**	**200**	**300**	**500**
III	14PCH3C9	CORE-IX	Inorganic Spectroscopy, Solid State and Bio-Inorganic Chemistry	6	5	40	60	100
	14PCH3C10	CORE-X	Organic Spectroscopy	6	5	40	60	100
	14PCH3C11	CORE-XI	Industrial Chemistry	6	5	40	60	100
	14PCH3C12P	CORE-XII	Physical Chemistry Non-Electrical Practical	6	5	40	60	100
	14PCH3CE3	CORE BASED ELECTIVE -III #		6	5	40	60	100
	14PCH3EC1	EXTRA CREDIT-I	Analytical Techniques	-	5*	-	100*	100*
TOTAL				**30**	**25**	**200**	**300**	**500**
IV	14PCH4C13	CORE-XIII	Statistical Thermodynamics and Surface Chemistry	6	5	40	60	100
	14PCH4C14P	CORE X1V	Physical Chemistry Electrical- Practical	6	5	40	60	100
	14PCH4EC2	EXTRA CREDIT-II	Instrumentation and Separation Techniques	-	5*	-	100*	100*
	14PCH4PW	PROJECT WORK		18	5	40	60	100
TOTAL				**30**	**15**	**120**	**180**	**300**
GRAND TOTAL				**120**	**90**	**720**	**1080**	**1800**

Core Based Electives

SEMESTER	CORE BASED ELECTIVE
I	Quantum Chemistry, Electrochemistry and Chemical Kinetics
	Theory of spectroscopy and Quantum chemistry
II	Organometallics, Electronic spectra and Metallurgy
	Applications of Spectroscopy to Inorganic Complex and Organometallics
III	Nano and Green Chemistry
	Special Topics in Chemistry

* Not considered for Grand Total and CGPA

SEMESTER-I: CORE-I
STRUCTURE BONDING, ACID-BASE AND NUCLEAR REACTIONS

Course Code : 14PCH1C1 | **Max. Marks : 100**
Hours/Week : 6 | **InternalMarks : 40**
Credit : 5 | **External Marks : 60**

Objectives:

- *To study the nature of various types of bonds using MO theory and CFT of coordination compounds, carbon π - acceptor and donor complexes*
- *To study the detection of radioactivity and nuclear reactions*
- *To understand modern concepts of acids and bases*

UNIT– I **18 hours**

1.1 **Ionic Bond and Crystal Structure:** Packing of ions in crystals - Radius ratio rules – Calculation of limiting ratios for coordination number 3 to 6. Classification of ionic structures - AX type (ZnS, NaCl, NiAs, CsCl) and AX_2 type (CaF_2, TiO_2, CdI_2) - structures only.

1.2 **Defects in crystals:** Schottky and Frankel defects- stoichiometric and non-stoichiometric - Metal excess defects - F-Centre. Metal deficiency defects – Positive ion deficiency – extra interstitial negative ions. # Semiconductors, transistors and rectifiers, photovoltaic cells, superconductors#.

1.3 Lattice energy - Born - Lande equation – significance, Kapustinski equation.

UNIT – II **18 hours**

2.1 **Covalent and Coordinate Bonds:** M.O. theory – Symmetry and overlap – construction of molecular orbitals in homo and hetero nuclear diatomic molecules. Linnet's double quartet theory.

2.2 Crystal field theory – Splitting of d-orbitals in O_h Symmetry – Strong and weak fields – CFSE – Calculation. Splitting in T_d symmetry and tetragonal symmetry - Jahn Teller distortion - splitting pattern in square planar. # Factors affecting the magnitude of 10 Dq value# - Nature of the ligands - Spectrochemical series, Jorgensen's relation. π bonding and M.O. theory - Ligands with filled and empty π orbitals – Nephelauxetic effect.

UNIT – III **18 hours**

3.1 **Complexes of π acceptor ligands:** Carbonyls - 18 e^- rule - Structural study of poly nuclear carbonyls. carbonylate anions, carbonyl hydrides, isolobal fragments - Nitrosyl Complexes - Preparation. Bridging and terminal nitrosyls, bent and linear nitrosyls. Dinitrogen and dioxygen complexes.

3.2 **Carbon π -donor Complexes:** Synthesis, Structure and bonding of alkene, alkyne and allyl complexes. Metallocenes – Stability and Reactivity. # Molecular orbital concept of metallocenes – derivatives.#

UNIT-IV **18 hours**

4.1 **Acids and Bases:** Protonic acids - Proton affinities - Differentiating and leveling solvents – non-protonic concepts of acid base reactions – Lux-Flood concept - Usanowich concept. Hard and soft acids and bases - Classification of acids and bases as hard and soft - acid and base strength of hardness and softness – electro negativity of hardness and softness – applications of HSAB, symbiosis.

4.2 # **Non-aqueous solvents**: liq.SO_2, CH_3COOH, and HF# .

UNIT– V **18 hours**

5.1 **Nuclear Chemistry:** Radioactivity - orbital electron capture, nuclear isomerism, internal conversion.

5.2 **Detection and determination of radioactivity:** Nuclear radiation - Scintillation and Cherenkov Counter. Particle accelerators: Linear, Cyclotron, Synchrotron, Betatron and Bevatron - # Nuclear reactors#

5.3 **Nuclear Reactions:** Transmutation, Stripping and pick-up, Spallation, fragmentation and Scattering reactions – Sources of neutrons – Neutron activation and isotopic dilution analysis – applications.

_____ # Self study

TEXT BOOKS:

1. J.D. Lee – "A New Concise Inorganic Chemistry", 5th Edn., Oxford University Press, 2011.
2. Wahid Malik, G.D.Tuli and R.D.Madan, "Selected Topic in Inorganic Chemistry", S.Chand & Co., Ltd (2011).
3. H.J. Arnikar – "Essential of Nuclear Chemistry", 4th Edn., New Age International Publishers, 2011.

UNIT I : Text Book 1
UNIT II : Text Book 1, 2
UNIT III : Text Book 1
UNIT IV : Text Book 2
UNIT V : Text Book 3

REFERENCES:

1. G.Friedlander, J.W.Kennedy and J.M. Miller -"Nuclear and Radio Chemistry (2000).
2. Cotton and Wilkinson – "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons, New York- 2004.
3. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – "Inorganic Chemistry Principles of Structure and Reactivity", 4th Edn., Pearson Education, 11th Impression, 2011.
4. Bodie E. Douglas and D. McDaniel, " Concepts and Models of Inorganic Chemistry", 3rd Wiley India Pvt. Ltd., New Delhi, 2006.
5. Maheswar Sharon and Madhuri Sharon – "Nuclear Chemistry" Ane books Pvt. Ltd, New Delhi -2009.

SEMESTER-I: CORE-II

REACTION MECHANISM, STEREOCHEMISTRY AND NATURAL PRODUCT

Course Code : 14PCH1C2	**Max. Marks : 100**
Hours/Week : 6	**InternalMarks : 40**
Credit : 5	**External Marks : 60**

Objectives:

- *To make the students to know about the nomenclature of organic compounds.*
- *To learn the concepts of aromaticity and stereochemistry, conformational analysis and their application in the determination of reaction mechanism.*
- *To learn the nature and synthesis of natural products*

UNIT – I **18 hours**

1.1 **Nomenclature of organic compounds:** #IUPAC nomenclature of linear and branched alkanes, alkenes, polyenes and alkynes with and without functional groups#. Nomenclature of alicyclic, bicyclic and tricyclic compounds with and without single functional groups.

1.2 **Reaction intermediates**: Singlet oxygen, nitrenes and benzyne – generation, statibility, structure and reactivity – Non-classical carbocations – definition, generation and stability.

1.3 **Heterocyclic compounds**: Nomenclature of heterocycles having not more than two hetero atoms such as oxygen, nitrogen and sulphur. Synthesis and reactions of azoles – Imidazole, Oxazole and Thiazole. Synthesis and reactions of Azepine, Oxazine, Thiazine and Pyrazine.

UNIT – II **18 hours**

2.1 **Methods of determining reaction mechanism:**

Energy profile diagrams - Thermodynamic and kinetic control of organic reactions – intermediate versus transition state - isotopic effects – kinetic and non – kinetic methods of determination of reaction mechanisms – product analysis and its importance – cross over experiment – isotopic labelling studies –stereo chemical studies.

2.2 **Correlation analysis**: Linear free energy relations – Hammett equation – significance of sigma and rho – applications, deviations and limitations –Taft equation and applications.

UNIT – III **18 hours**

Stereochemistry – I

3.1 # Newman, Sawhorse and Fisher projection formulae and interconversion #. Concept of Chirality - R, S nomenclature; Enantiotropic and diastereotopic atoms and groups - Enantio and Diastereo selective synthesis. Newer methods of asymmetric synthesis including enzymatic and catalytic nexus. E – Z isomerism. Determination of configuration of geometrical isomers.

3.2 D, L and R, S notations of acyclic and cyclic chiral compounds – Stereo chemical features and configurational descriptors (R, S) for the following classes of compounds allenes, spiranes and biaryls. Stereogenic centre. Definition of Prochirality – Asymmetric synthesis – Crams rule – enantiomeric excess (optical purity).

3.3 **Conformational Analysis:** Conformation of some simple 1, 2-disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexane and their stereo chemical features (geometric and optical isomerism by these derivatives). Conformation of cyclic compounds (3, 4 & 5 membered), cyclohexanone and conformation and stereochemistry of cis and trans decalin.

UNIT – IV **18 hours**

4. **Stereochemistry – II**

Dynamic stereochemistry: Quantitative correlations between conformation and reactivity. Weinstein-Eliel equation – Curtin-Hammett principle – Conformation and reactivity of mono and di substituted cyclic systems – Saponification of ester – Esterification of an alcohol – Chromic acid oxidation of cyclohexanol – Neighbouring group participation – De-amination of 2-amino cyclohexanol – Sharpless asymmetric epoxidation – stereospecific and stereoselective reactions.

UNIT – V **18 hours**

5.1 **Aromaticity of Compounds:**

[#]Definition of aromaticity – Huckel's[#] and Craig's Rules – ring currents – Non-benzenoid aromatic compounds – Aromatic character in 3,5 and 7 membered ring compound – Anti-aromatictity – systems with 2, 4, 6, 8, 10, 14 and 18 electrons - Azulene - Annulenes – Sydnones and fullerenes – Alternant and non alternant hydrocarbons. Homoaromaticity.

5.2 **Terpenoids:** Structural elucidation and medicinal uses of α - Pinene, Zingiberene, and Squalene

5.3 **Alkaloids:** Structural elucidation and medicinal values of quinine, reserpine and morphine.

5.4 **Flavones:** Structural elucidation of flavones and isoflavones.

[#] [#] Self study

TEXT BOOKS:

1. Raj. K. Bansal – "A Text Book of Organic Chemistry" Revised 4th Ed.,(2005), New Age International Publishers Ltd., New Delhi.
2. Raj. K. Bansal – "Heterocyclic Chemistry", 4th Ed.,(2005), New Age International Publishers Ltd., New Delhi.
3. P.S. Kalsi – "Stereochemistry conformation and Mechanism", 6th Ed., (2005), New Age International Publishers Ltd., New Delhi.
4. T. Nasi Puri – "Stereochemistry of Organic Compounds", Revised Ed., (2005), Wiley Eastern Ltd.
5. Peter Sykes – "A Guide Book of Reaction Mechanism", 5th Ed., (2005).

UNIT I : Text Book 2,
UNIT II : Text Book 5
UNIT III : Text Book 3,4
UNIT IV : Text Book 3,4
UNIT V : Text Book 1

REFERENCES:

1. R. Panico, W.H. Powell, L. Jean, C.Richer, "A guide of IUPAC nomenclature of organic compounds", (1993).
2. Jerry March – "Advanced organic chemistry", Reactions, Mechanism and Structure",4th Ed., (2006), Wiley India Pvt. Ltd.
3. F.A. Carey and R.J. Sund berg – "Advanced organic chemistry" Vol. I and II– 3rd Ed., (1984), Plenum Publications.
4. Ernest. Eliel and Samuel H. Wilen – "Stereochemistry of Organic Compounds" – Wiley Student Ed., (2006). John Wiley and Sons Pvt. Ltd., Singapore.
5. T. Nasi Puri – "Stereochemistry of Organic Compounds", Revised Ed., (2005), Wiley Eastern Ltd.
6. I.L. Finar – "Stereochemistry and the Chemistry of Natural Products", Vol-2, 5th Ed., (2006), Dorling Kindersley (India) Pvt. Ltd.

SEMESTER-I : CORE BASED ELECTIVE - I
QUANTUM CHEMISTRY, ELECTROCHEMISTRY AND CHEMICAL KINETICS

Course Code : 14PCH1CE1 | **Max. Marks : 100**
Hours/Week : 6 | **Internal Marks : 40**
Credit : 5 | **External Marks : 60**

Objectives:

- *To study the fundamentals and applications of classical mechanics and quantum chemistry.*
- *To learn the applications of ARRT to solution kinetics, free energy change in solutions and kinetics and importance of different catalytic processes.*
- *To understand the kinetics of fast reactions.*
- *To study the concepts and applications of electrochemistry.*

UNIT - I **18 hours**

Introduction to Classical and Quantum Mechanics

1.1. Classical mechanics – General principles, basic assumptions, postulates of classical mechanics, conservation laws, #D'Alembert's principle, Lagrange's and Hamilton's equations of motion (no derivation)#.

1.2. Operators- algebra of operators, commutation relations, commutators, linear, angular momentum, Laplacian, Hermitian, Hamiltonian and Ladder operators, eigen values and eigen functions, Hermitian property of operators, orthogonality and normalization.

1.3. Postulates of quantum mechanics – Solving the Schrodinger wave equation to simple systems viz., particle in a box – one and three dimensional, Bohr's Correspondence principle.

UNIT - II **18 hours**

Applications of Quantum Mechanics- I

2.1. Setting up Schrödinger wave equation and solving for harmonic oscillator, rigid-rotator, Hydrogen and hydrogen like atoms (He^+ and Li^{2+}), significance of n, l and m, shapes of atomic orbitals – radial and angular probability distribution functions.

2.2. Approximation methods - linear variation principle, application to hydrogen and helium atoms, perturbation method for non degenerate systems, #application of perturbation theory to helium atom#.

UNIT - III **18 hours**

Applications of Quantum Mechanics-II

3.1 Two electron systems – symmetric and anti-symmetric wave functions, spin of electrons and Pauli's principles and Slater determinant, self consistent field theory - Hartree-Fock Self Consistent field theory, Slater type orbitals – Slater rules, orbital energies.

3.2 Theory of chemical bonding (diatomic molecules) – Born-Oppenheimer approximation, LCAO – MO and VB treatments of the hydrogen molecule, Huckel molecular orbital (HMO) theory and its applications to conjugated systems – ethylene, allyl radical and butadiene(linear), #principle of hybridization – sp, sp^2 and sp^{3}#.

UNIT- IV **18 hours**

Electro Kinetic Phenomena and Electrode Kinetics:

4.1 Debye -Huckel -Onsager theory of strong electrolytes, Debye Huckel limiting law, activity coefficient at higher concentration - Bjerrum model. Electrical double layer potential – Theory of multiple layers at electrode - Helmholtz, Goy-Chapmann, Stern, Devanathan models, electro kinetic phenomena – electrophoresis, electrosmosis, streaming potential and sedimentation potential - electro capillary phenomena .

4.2 Process at Electrode – Rate of Charge Transfer- Current Density – Butler-Volmer equation – Tafel equation.

4.3. Principles of Electro deposition of Metals, Electro chemical corrosion of Metals – Construction and use of Pourbaiux and #Evans diagrams and Prevention of Corrosion – Electro Chemical oxidation and Reduction#.

UNIT-V **18 hours**

Kinetics of Solution, Catalysis and Fast reactions

5.1 Factors influencing reaction rates in solution - application of ARRT to solution kinetics, effects of solvents, double sphere and single sphere model and effect of ionic strength - influence of pressure on rates in solution - significance of volume of activation.

5.2 Homogeneous catalysis: Acid-Base catalysis - Hammett-Deyrup acidity function - Bronsted relation - Enzyme catalysis - mechanism of single substrate reactions - Michaelis - Menten law - influence of pH and temperature.

5.3 Fast reactions: Study of kinetics by stopped flow technique, relaxation methods T and P Jump methods, #flash photolysis and magnetic resonance methods (NMR & ESR)#.

#_____# Self study

TEXT BOOKS:

1. A.K.Chandra, "Introductory Quantum Chemistry" 4th edition, Tata – McGraw Hill, 2010.
2. R. K. Prasad, "Quantum Chemistry", New Delhi, Wiley-Eastern Ltd, 1992.
3. J. M. Anderson, "Mathematics of Quantum Chemistry", I Edition, Massachusetts, W. A. Benjamine Inc. 1966.
4. John O'M Bockris and Amulya K.N Reddy, "Modern Electrochemistry" Anne Book India, 2008.
5. Laidler, "Chemical Kinetics," 3rd edition, New Delhi TATA McGraw Hill Co., 1984.
6. Kuriacose and Rajaram, "Kinetics and Mechanism of Chemical transformation", Macmillan &Co., 1993.

UNIT I : Text Book 1,2,3,
UNIT II : Text Book 1,2,3
UNIT III : Text Book 1,2,3
UNIT IV : Text Book 4
UNIT V : Text Book 5,6

REFERENCES:

1. F. L. Pillar, "Elementary Quantum Chemistry", Tata-McGraw Hill, 1970
2. I. N. Levine, "Quantum Chemistry", 4th edition, Prentice Hall OfInia, Pvt. Ltd, 1994.
3.D. A. McQuarrie, "Quantum Chemistry", University Science Books, 1988.
4. P. W. Atkins, "Molecular Quantum Mechanics", Clarendon 1973.
5. Anatharaman "Fundamentals of Quantum Chemistry", McMillan, New Delhi, 2001.
6. D.R. Crow, "Principles and Applications of Electrochemistry", 3rd edition Chapman and Hall, London, 1985.
7. P. H. Rieger, "Electro Chemistry", Chapman Hall, U.S.A., 2010.
8. John Albery, "Electrode Kinetics", Clarendon press, oxford, 1975.

SEMESTER-I: CORE BASED ELECTIVE - I
THEORY OF SPECTROSCOPY AND QUANTUM CHEMISTRY

Course Code : 14PCH1CE1 | **Max. Marks : 100**
Hours/Week : 6 | **InternalMarks : 40**
Credit : 5 | **External Marks : 60**

Objectives:

- *To study the theoretical background of molecular and magnetic resonance spectroscopy.*
- *To study the fundamentals and applications of classical mechanics and quantum chemistry.*

UNIT-I **18 hours**

Theory of spectroscopy:

IR spectra:

1.1 Einstein coefficient of absorption and transition probabilities – basics selection rules – representation of spectra – the width and intensity spectral transitions – oscillator strength.

1.2 Vibration spectra – selection rules – harmonic and anharmonic oscillators – hot band, overtones – Fermi resonance, combination bands, rotation – vibration spectra of diatomic molecules – transition for the rigid rotor – coupling of rotation and vibration – linear and perpendicular bonds – FT-IR spectroscopy. #PQR – branches#.

1.3 **Raman Spectra:**

Raman Effect – elastic and inelastic scattering – selection rules – pure rotational and rotational-vibrational Raman spectra – polarization of light and Raman Effect – mutual exclusion principle – #Fermi resonance – laser Raman spectroscopy#.

UNIT – II **18 hours**

THEORY OF NMR-I

2.1 Behavior of a bar magnet in a magnetic field – Magnetization vectors – resonance condition – relaxation process – Bloch equation – chemical shift and its measurement.

2.2 Scalar Spin-Spin Coupling Mechanism – Nature of the Coupling, Direct Dipolar Coupling – NMR in Solids – magic angle spinning – #nuclear magnetic resonance imaging (NMRI) – principles and applications#.

2.3 FT-NMR – Principle, Measurements of T_1 by FTS, Use of T_1 for peak assignment.

UNIT – III **18 hours**

THEORY OF NMR-II

3.1 Second Order Spectra – Introduction, More Complicated Second Order System , Double Resonance and Spin Tickling Experiments - elementary idea, Spectral Simplification.

3.2 Evaluation of thermodynamic data with NMR – Rate constants and activation energies from NMR – Determination of reaction orders by NMR – #some application of NMR kinetic studies#.

3.3 Two dimensional NMR –Theory of 2D NMR (preliminary)

UNIT – IV **18 hours**

Introduction to Classical Mechanics and Exact Quantum Mechanical Result

4.1 Classical mechanics – General principles, basic assumptions, postulates of classical mechanics, conservation laws, D'Alembert's principle, Lagrange's and Hamilton's equations of motion (no derivation).

4.2. Operators- algebra of operators, commutation relations, commutators, linear, angular momentum, Laplacian, Hermitian, Hamiltonian and Ladder operators, eigen values and eigen functions, Hermitian property of operators, #orthogonality and normalization#.

4.3. Postulates of quantum mechanics – discussion of the Schrödinger wave equation to simple systems viz., particle in a box – one and three dimensional, quantum numbers, harmonic oscillator – zero-point energy, Bohr's Correspondence principle, rigid-rotator-rotational and vibrational quantum numbers, Hydrogen and hydrogen like atoms (He^+ and Li^{2+}), #significance of n, l and m, shapes of atomic orbitals – radial and angular probability distribution functions#.

UNIT-V **18 hours**

Application of Quantum Mechanics to Multiectronic Systems

5.1. Approximation methods - linear variation principle, application to hydrogen and helium atoms, perturbation method for non degenerate systems, application of perturbation theory to helium atom.

5.2 Two electron systems – symmetric and antisymmetric wave functions, spin of electrons and Pauli's principles and Slater determinant, self consistent field theory - Hartrees theory, Hartree-Fock-Self-Consistent field theory, # Slater type orbitals – slater rules, orbital energies#.

5.3. Theory of chemical bonding (diatomic molecules)-Born-Oppenheimer approximation, LCAO- MO and VB treatments of the hydrogen molecule, Huckel molecular orbital (HMO) theory and its applications to conjugated systems - ethylene, allyl radical and butadiene(linear) principle of hybridization-sp, sp^2 and sp^3

#_____# Self study

TEXT BOOKS:

1. K. Veera Reddy, "Symmetry and Spectroscopy of Molecules", New Age International Publishers, 2010.
2. C. N. Banwell and E. M. Mccash, "Fundamentals of Molecular Spectroscopy", Tata McGraw-Hill Publishing Company Limited, New Delhi, 2009.
3. A. K. Chandra, "Introductory Quantum Chemistry" 4th edition, Tata – McGraw Hill, 2010.
4. R. K. Prasad, "Quantum Chemistry", New Delhi, Wiley-Eastern Ltd, 1992.
5. J. M. Anderson, "Mathematics of Quantum Chemistry", I Edition, Massachusetts, W. A. Benjamine Inc. 1966.

UNIT I : Text Book 1,2
UNIT II : Text Book 1,2
UNIT III : Text Book 1,2
UNIT IV : Text Book 3,4,5
UNIT V : Text Book 3,4,5

REFERENCES :

1.Manas Chanda, Structure and Chemical bonding including molecular spectra, Tata McGraw-Hill Publishing company Ltd., New Delhi-2.
2.G.Aruldhas, Molecular structure and spectroscopy, second edition, PHI learning Pvt. Ltd., New Delhi, 2008.
3.S.C.Rakshit, Physical chemistry, seventh edition – Sarat book distributors, Kolkata, 2004.
4. Rusell S.Drago, Physical Methods in Chemistry, W.B.Saunders Company.
5. F.L.Pillar, "Elementary Quantum Chemistry", McGraw Hill, 1970.
6. David.W.Ball, Physical Chemistry, Cengage Learning India Pvt. Ltd., New Delhi, 2009.

SEMESTER-II: CORE-V
ORGANIC REACTIONS AND MECHANISMS

Course Code : 14PCH2C5 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks : 60**

Objectives:

- *To learn the various types of reactions, rearrangements, their synthetic utility and to study about structure and bonding.*
- *To know modern synthetic methods and synthetic strategies. This help in planning the synthesis of any types of organic compounds.*
- *To develop the knowledge for new synthetic methods.*

UNIT – I **18 hours**

1.1 **Aliphatic Nucleophilic Substitution Reaction**

$^{\#}S_N1$, S_N2 and S_Ni mechanisms$^{\#}$ - Effect of substrate structure, leaving group, attacking nucleophiles and solvent. Neighbouring group participation - Substitution in norbornyl and bridgehead systems - substitution at allylic and vinylic carbons - substitution by ambident nucleophiles.

1.2 **Aliphatic Electrophilic substitution:**

S_E1, S_E2 and S_Ei mechanism - Reactivity. Effect of substrate, leaving group, attacking electrophiles and solvent. Keto-enol interconversion, Stark-Enamine reaction, halogenation of aldehydes and ketones and decarboxylation of aliphatic acids.

1.3 **Aromatic nucleophilic substitution:**

Unimolecular, bimolecular and benzyne mechanisms. Zeigler alkylation, Sandmayer, and Chichibabin reactions.

UNIT – II **18 hours**

2.1 **Reduction Reactions:**

Reduction of CO to CH_2 in aldehydes and ketones - Wolff-Kishner reduction and Huang-Minlon modification. Ra-Ni, desulfurization of thioketal - Metal hydride reduction- Boron reagents ($NaBH_4$, $NaCNBH_3$, $Na(OAc)_3BH$), Aluminium reagents- $LiAlH_4$, Red Al.

2.2 **Oxidation Reactions:**

Dehydrogenation/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), hypervalent iodine reagents (IBX, Dess-Martin periodinane). DMSO based reagents (Swern oxidation). Oxidation involving C-C bond cleavage using HIO_4, cycloalkanones using CrO_3, Oxidation of C=C using $NaIO_4$ and OsO_4, aromatic rings using RuO_4. Oxidation of aldehydes and ketones with H_2O_2 (Dakin reaction), with peracid (Baeyer-Villiger oxidation). Dess-Martin reagent.

2.3 Applications: Phase transfer catalysis (PTC), Crown ethers, Merrifield resin and Baker's yeast.

UNIT- III **18 hours**

3.1 **Addition Reactions:**

Addition to carbon – carbon multiple bonds – Electrophilic addition, nucleophilic and free radical additions, orientation and reactivity, Hydroxylation, Hydroboration, Epoxidation, Diels – Alder reaction. Michael addition, Ozonolysis, 1,3 – dipolar addition reaction - Stereo chemical studies in addition reactions.

3.2 **Elimination Reaction:**

$^{\#}\alpha$-Elimination, β-elimination, E_1, $E_2^{\#}$ and E1CB mechanism – stereochemistry of elimination – orientation of the double bond – effect of changes in the substrate, base, leaving group and medium on E1, E2, E1CB reactions – elimination vs substitution – pyrolytic cis elimination – Bredt's rule- Chugaev reaction – dehydration of alcohols – dehydrohalogenation.

UNIT – IV **18 hours**

4.1 **Name reactions:** Dieckmanns, Stobbe, Darzen's Glycidic ester condensation, Wittig. Houben –Houshch. Vilmesmier-Haack and Knoevenagal

4.1 **Concerted rearrangements:** Cope (including Oxy-Cope) and Claisen.

4.2 **Cationic rearrangements**: Demjanov, Pummerer, Schmidt and Dienone - phenol.

4.4 **Anionic rearrangements:** Brook, Favorski, Neber, Von Richter, Sommelet – Hauser and Wittig.

UNIT–V **18 hours**

5.1 **Steroids:** Classification – Structural elucidation and medicinal values of cholesterol (synthesis not required), Oestrone, progesterone, ergosterol, stigmasterol and equilenin. Stereochemistry of steroids

5.2 **Carotenoids:** Introduction – Classification, structural elucidation of α-carotene, β- carotene and xanthophylls.

5.3 **Lipids**: Classification and biological importance of fatty acids and lipids.

$^{\#}$_____$^{\#}$ Self study

TEXT BOOKS:

1. S.P. Shukla and G.L.Trivedi – "Modern Organic Chemistry", Millinium Ed., Rajendran Ravidra Printers Pvt. Ltd., New Delhi. 2000.
2. Raj. K. Bansal – "A Text Book of Organic Chemistry", Revised 4th Ed., New Age International Publishers Ltd., New Delhi. 2005.
3. I.L. Finar – "Stereochemistry and the Chemistry of Natural Products", Vol-2, 5th Ed., Dorling Kindersley (India) Pvt. Ltd. 2006.
4. Jerry March – "Advanced organic chemistry", 4th Ed., (2006), Wiley India Pvt. Ltd.

UNIT I : Text Book 1
UNIT II : Text Book 2,4
UNIT III : Text Book 1,4
UNIT IV : Text Book 4,
UNIT V : Text Book 3

REFERENCES:

1. F.A. carey and R.J. Sund berg – "Advanced organic chemistry" Vol. I and II– 3rd Ed., (1984), Plenum Publications.
2. S.P. Shukla and G.L.Trivedi – "Modern Organic Chemistry", Millinium Ed., (2000) Rajendran Ravidra Printers Pvt. Ltd., New Delhi.
3. R.O.C. Norman – "Principles of Organic Synthesis" – 2nd Ed., (1986), Chapman and Hall Publications, New York.
4. O.P. Agarwal – "Reactions and Reagents in Organic Chemistry", 5th Ed., (2005), Goel Publishing House, Meerut.
5. J.N. Gurtu and R.Kapoor – "Organic Reactions and Reagents", 1st Ed., (1988), Sultan Chand Company Pvt. Ltd.
6. Gurdeep Chatwal – "Organic Chemistry of Natural Products", Vol. I & II, Revised 5th Ed., (2005), Himalaya Publishing House.

SEMESTER-II: CORE-VI
GROUP THEORY AND SPECTROSCOPY

Course Code : 14PCH2C6 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks : 60**

Objectives:

- *To study the theoretical background of molecular and magnetic resonance spectroscopy.*
- *To understand the symmetry of molecules*
- *To learn the applications of group theory to structure and properties of the molecules.*

UNIT – I **18 hours**

Elements of Group Theory

1.1 Introduction – Symmetry elements, Symmetry operations , n-fold Proper axis of symmetry, Centre of Symmetry, Plane of Symmetry, n-fold Improper axis of Symmetry, Group, Rules for forming a Group, Finite Group, Infinite Group, Abelian Group, Cyclic Group, Sub Groups, Group Multiplication Table- Class and Similarity transformation.

1.2 Point Group – Method of Assigning Point Group- Schoenflies symbols, Matrix Representation Theory – Matrix Representation of Symmetry operation, Reducible and Irreducible Representation.

1.3 The Great Orthogonality Theorem – Properties of Irreducible Representation Construction of Character Table for $C_{2V,}$ C_{2h} and C_{3V} point Groups – Explanation of Character Table- Correlation table (basic idea only).

UNIT – II **18 hours**

Applications of Group Theory -I

2.1 The direct product and its applications, applications of group theory to spectroscopy – vanishing of integrals, symmetry selection rules for vibrational, Raman and electronic spectroscopy.

2.2 Reduction Formula and its applications, determination of symmetries of vibrational modes and their IR and Raman activities in non-linear molecules (H_2O, NH_3 and BF_3) and linear molecules (CO_2 and C_2H_2 - Integration method), mutual exclusion rule, symmetries of electronic transitions in formaldehyde and ethylene.

UNIT – III **18 hours**

Applications of Group Theory -II

3.1 Applications of Group theory - Hybridization schemes for atoms in molecules of different geometry - tetrahedral(CH_4), triangular(BF_3) planar linear(C_2H_2) and non linear (C_2H_4)molecules.

3.2 Symmetry in crystals - Hermann - Mauguin symbols. Space groups of crystals - Translational elements of symmetry - Comparison of crystal symmetry with molecular symmetry.

3.3 Projection Operator – Symmetry Adapted Linear Combination (SALC) proced8ure. symmetry factors of secular determinant and its applications to butadiene.

UNIT – IV **18 hours**

Theory of IR and Raman Spectroscopy

4.1 **IR Spectra**- Theory of Rotational-Vibrational spectra – harmonic and anharmonic oscillators – hot band, overtones – Fermi resonance, combination bands, rotation – vibration spectra of diatomic and polyatomic molecules, calculation of force constant, effect of isotopic substitution on vibrational frequencies – transition for the rigid rotor – coupling of rotation and vibration – linear and perpendicular bands – PQR branches – FT-IR spectroscopy.

4.2 **Raman Spectra-**[#] Polarization of light and Raman Effect– elastic and inelastic scattering[#]– pure rotational and rotational-vibrational Raman spectra- Lasers-special properties of laser, types of lasers-Laser Raman spectroscopy- theory and advantages-Resonance Raman Spectroscopy-theory and advantages.

UNIT – V **18 hours**

Theory of NMR Spectroscopy

5.1 Behavior of a bar magnet in a magnetic field – Magnetization vectors – resonance condition – relaxation process – Bloch equation – [#]chemical shift and its measurement[#].

5.2 Scalar Spin - Spin Coupling Mechanism – Nature of the Coupling, Direct Dipolar Coupling – NMR in Solids – magic angle spinning – nuclear magnetic resonance imaging (NMRI) – principles and applications.

5.3 FT-NMR – Principle, measurements of T_1 by FTS, Use of T_1 for peak assignment, Theory and advantages of 2D NMR

[#] [#] Self study

TEXT BOOKS:

1. K.V. Raman, "Group theory and its Application to Chemistry", Tata-McGraw –Hill Publishing Company Limited, New Delhi, 2000.
2. K. Veera Reddy, "Symmetry and Spectroscopy of Molecules", New Age International Publishers, 2010.
3. C. N. Banwell and E. M. Mccash, "Fundamentals of Molecular Spectroscopy", Tata McGraw-Hill Publishing Company Limited, New Delhi, 2009.

UNIT I : Text Book 1,2
UNIT II : Text Book 1,2
UNIT III : Text Book 1,2
UNIT IV : Text Book 2,3
UNIT V : Text Book 2,3

REFERENCES:

1. F. A. Cotton, "Chemical Application of Group Theory", 2nd edition, Wiley – Eastern Press, 1995.
2. G. M. Barrow, "Introduction to Molecular Spectroscopy", Tata-McGraw- Hill Edition, 1993.
3. G. Aruldhas, "Molecular Structure and Spectroscopy", Second edition, PHI learning Pvt. Ltd., New Delhi, 2008.
4. Manas Chanda, "Structure and Chemical Bonding including Molecular Spectra", Tata-McGrawHill Publishing company Ltd., New Delhi-2.
5. R. S. Drago, "Physical Methods in Chemistry", New Delhi, East West Press Ltd., 1971.

SEMESTER-II: CORE BASED ELECTIVE - II
ORGANOMETALLICS, ELECTRONIC SPECTRA AND METALLURGY

Course Code : 14PCH2CE2 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks: 60**

Objectives:

- *To understand reactivity and stability of complexes and organometallic chemistry*
- *To understand the identification of structure of complexes by various spectroscopic technique.*
- *To study lanthanides, actinides, metallurgy, inorganic polymers and rings*

UNIT – I **18 hours**

1.1. **Reactivity of Complexes in solutions** – Ligand displacement Reactions – hydrolysis – acid and base, aquation in O_h complexes. Electron Transfer Reactions, complementary and non-complementary, types – inner and outer sphere processes – Isomerism in square planar complexes – Trans effect – Theories and Applications. Template effect, synthesis of macrocyclic ligands and unique properties.

1.2. **Stability of coordination compounds:** Detection of complex formation in solution, stability constants, stepwise and overall formation constants pH metric, #polarographic and photometric methods of determining formation constants# - factors affecting stability - statistical and chelate effects.

UNIT – II **18 hours**

2.1**. Organometallic Chemistry:** 16 and 18 electron rules - Ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions – reactions of coordinated ligands in organometallics – Catalysis by Organometallics - Hydrogenation, hydroformylation, polymerisation of alkenes, olefin oxidation (Wacker Process), Fischer – Tropsch synthesis, epoxidation, metathesis.

2.2 **Oxygen Transport and energy transfer of metals proteins:** #Hemoglobin and myoglobin – Oxygen transport and storage#. Electron transfer and Oxygen activation. Ferredoxins and rubredoxines – Copper proteins – Oxidases and reductases – cytochrome oxidase – superoxide dismutase. (Cu, Zn), Urease and hydrogenases – Functions.

UNIT-III **18 hours**

3.1 **Electronic spectroscopy:** Electronic configuration - Terms, states and microstates of atoms and ions – Derivation of term symbols (p^2 and d^n) and arranging the various term according to their energies - spectroscopic terms – L-S coupling and jj coupling – #effect of interelectronic repulsion and spin-orbit coupling# – Racah parameters B and C – selection rules and the breakdown of selection rules – mixing of orbitals.

3.2 Orgel diagram – characteristics – prediction and assignment of transitions for d^n weak field systems. Tanabe – Sugano diagrams – prediction and assignment of transitions for weak field and strong field – d^n systems - band intensity, band width - band shape-calculation of β and 10 Dq for simple octahedral complexes of Co and Ni- charge transfer spectra.

UNIT-IV **18 hours**

4.1. **IR and Raman spectroscopy:** Combined uses of IR and Raman spectroscopy in the structural elucidation of N_2O, H_2O, ClF_3, NO_3^-, ClO_3^{2-} - Effect of coordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, cyanide, nitrate and sulphate - # Effect of isotopic substitution on vibrational spectra of metal carbonyls#.

4.2. **Mossbauer Spectroscopy:** Mossbauer transition and Doppler Effect - isomer Shift, quadrupole effect – simple application to iron and tin compounds.

4.3. **Lanthanides:** co-ordination compounds of lanthanides - spectral and magnetic properties.

4.4. **Actinides:** synthesis of elements - # magnetic and spectral characteristics of actinides#.

UNIT – V **18 hours**

5.1. **Extraction and Uses of Metals:** Metallurgy of Zr, Ge, Th and U – Preparation and # uses of their important compounds.#

5.2. **Inorganic Polymers:** Phosphorus based network polymers, Coordination Polymers – Synthetic and nature.

5 . 3 **Rings:** Preparation and Structure of Borazines & Phosphazenes – Craigg and Paddock model - Dewar model – Preparation and Structure of sulphur-nitrogen ring system (S_4N_4, $N_4S_4F_4$)

Self study

TEXT BOOKS:

1. R.Gopalan, V.Ramalingam – "Concise Coordination Chemistry", Vikas Publishing House Pvt. Ltd., Newdelhi, 2001.
2. B.D.Gupta, A.J.Elias - "Basic Organometallic Chemistry-Concepts, Syntheses and Applications", University Press, Hyderabad, 2011.
3. R.C.Mehrotra, A.Singh, "Organometallic Chemistry-A Unified Approach", revised 2nd Edn., New Age International Publishers, 2011.
4. Satya Prakash, G.D.Tuli, S.K.Basu, R.D.Madan, "Advanced Inorganic Chemistry Vol-I", S.Chand & Co., Ltd., New Delhi.
5. W. Kaim and B. Schewederski – Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: John Wiley & Sons, New York, USA, 2001.
6. E.A.V. Ebsworth, W.H. Rankin, Cradock – "Structural Methods in Inorganic Chemistry", ELBS, 1987.

UNIT I : Text Book 1
UNIT II : Text Book 2,3,5
UNIT III : Text Book 6
UNIT IV : Text Book 6
UNIT V : Text Book 4

REFERENCES:

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – "Inorganic Chemistry Principles of Structure and Reactivity"4th Ed., pearson Education –2009.
2. W. Kaim and B. Schewederski – Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: John Wiley & Sons, New York, USA, 2001.
3. Cotton and Wilkinson – "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons, New York- 2004.
4. R.H. Crabtree – The Organometallic Chemistry of the Transition Metals: John Wiley & Sons, New York (2000).
5. S.E. Kegley and A.R. Pinhas – Problems and Solutions in Organometallic Chemistry: University Science Books, Oxford University Press,2002.
6. P. Powell -Principles of Organometallic Chemistry, 2nd Ed.Chapman and Hall,London,2003.

SEMESTER-II: CORE BASED ELECTIVE - II
APPLICATIONS OF SPECTROSCOPY TO INORGANIC COMPLEX AND ORGANOMETALLICS

Course Code : 14PCH2CE2 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks: 60**

Objectives:

- *To understand reactivity and stability of complexes and organometallic chemistry*
- *To understand the identification of structure of complexes by various spectroscopic technique.*
- *To study lanthanides, actinides, metallurgy, inorganic polymers and rings*

UNIT-I **18 hours**

1.1 **Electronic spectroscopy:** Electronic configuration - Terms, states and microstates of atoms and ions – Derivation term symbols (p^2 and d^2) and arranging the various term according to their energies spectroscopic terms – L-S coupling and JJ coupling – #effect of interelectronic repulsion and spin-orbit coupling #– Racah parameters B and C – selection rules and the breakdown of selection rules – mixing of orbitals.

1.2 Orgel diagram – characteristics – prediction and assignment of transitions for dn weak field systems. Tanabe – Sugano diagrams – prediction and assignment of transitions for weak field and strong field – dn systems band intensity, band widths- band shapes- calculation of β and 10 Dq for simple octahedral complexes of Co and Ni- charge transfer spectra.

UNIT-II **18 hours**

2.1 **IR and Raman spectroscopy:** Combined use of IR and Raman spectroscopy in the structural elucidation of N_2O, H_2O, ClF_3, NO_3^-, ClO_3^- - Effect of coordination on ligand vibrations – uses of group vibrations in the structural elucidation of metal complexes of urea, cyanide, nitrate and sulphate – #Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal complexes#.

2.2 **Mossbauer Spectroscopy:** Mossbauer transition and Doppler Effect – isomer shift quadrupole effect – magnetic effect on spectra – simple application to iron and tin compounds.

2.3 **Lanthanides:** co-ordination compounds of lanthanides- spectral and magnetic properties.

2.4 **Actinides:** synthesis of elements – #magnetic and spectral characteristics of actinides#.

UNIT – III **18 hours**

3.1 **Extraction and Uses of Metals:** Metallurgy of Zr, Ge, Be, Th –Preparation and uses of their important compound.

3.2 **Inorganic chains:** Catenation, heterocatenation – silicate minerals (names and structure only) Intercalation chemistry – talc, muscovite (structure only)

3.3 **Rings:** Preparation and Structure of Borazines & Phosphazenes – Craigg and Paddock model - Dewar model – Preparation and Structure of sulphur-#nitrogen ring system (S_4N_4, $N_4S_4F_4$)#

UNIT – IV **18 hours**

4.1 **Reactivity of Complexes** – Kinetics and Mechanisms of reactions in solutions: Labile and inert complexes – Ligand displacement Reactions – hydrolysis – acid & base, aquation in O_h complexes. Electron Transfer Reactions, complementary and non-complementary types – inner and outer sphere processes – Isomerism in square planar complexes – Trans effect – Theories and Applications. Template effect and synthesis of macrocyclic ligands.

4.2 **Stability of coordination compounds:** Detection of complex formation in solution, stability constants, stepwise and overall formation constants pH metric, # polarographic and photometric methods of determining formation constants#- factors affecting stability – statistical and chelate effects.

UNIT – V **18 hours**

5.1 **Organometallic Chemistry:** 16 and 18 electron rule - Catalysis by Organometallics- Ligand association and dissociation – oxidative addition and reductive elimination – insertion reactions – reactions of coordinated ligands in organometallics – Hydrogenation, hydroformylation, polymerisation of alkenes, olefin oxidation (Wacker Process), Fischer – Tropsch synthesis, epoxidation, metathesis.

5.2 **Oxygen Transport and energy transfer of metals proteins:** # Hemoglobin and myoglobin – Oxygen transport and storage#. Electron transfer and Oxygen activation. Ferredoxins and rubredoxines – Copper proteins – classification – Electron transfer, oxygen transport. Oxidases and reductases – cytochrome oxidase – superoxide dismutase. (Cu, Zn), Urease and hydrogenases.

_____ # Self study

TEXT BOOKS:

1. R.Gopalan, V.Ramalingam – "Concise Coordination Chemistry", Vikas Publishing House Pvt. Ltd., Newdelhi, 2001.
2. B.D.Gupta, A.J.Elias - "Basic Organometallic Chemistry-Concepts, Syntheses and Applications", University Press, Hyderabad, 2011.
3. R.C.Mehrotra, A.Singh, "Organometallic Chemistry-A Unified Approach", revised 2nd Edn., New Age International Publishers, 2011.
4. Satya Prakash, G.D.Tuli, S.K.Basu, R.D.Madan, "Advanced Inorganic Chemistry Vol-I", S.Chand & Co., Ltd., New Delhi.
5. W. Kaim and B. Schewederski – Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: John Wiley & Sons, New York, USA, 2001.
6. E.A.V. Ebsworth, W.H. Rankin, Cradock – "Structural Methods in Inorganic Chemistry", ELBS, 1987.

UNIT I : Text Book 6
UNIT II : Text Book 6
UNIT III : Text Book 1,4
UNIT IV : Text Book 4
UNIT V : Text Book 2,3,5

REFERENCES:

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter – "Inorganic Chemistry Principles of Structure and Reactivity", 4th Ed., pearson Education –sixth impression - 2009.
2. W. Kaim and B. Schewederski – Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life: John Wiley & Sons, New York, USA, 2001.
3. Cotton and Wilkinson – "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons, New York- 2004.
4. R.H. Crabtree – The Organometallic Chemistry of the Transition Metals: John Wiley & Sons, New York (2000).
5. S.E. Kegley and A.R. Pinhas – Problems and Solutions in Organometallic Chemistry: University Science Books, Oxford University Press,2002.
6. P. Powell – Principles of Organometallic Chemistry, 2nd Edn.: Chapman and Hall,London,2003.

SEMESTER-III: CORE-IX
INORGANIC SPECTROSCOPY, SOLID STATE AND BIO-INORGANIC CHEMISTRY

Course Code : 14PCH3C9 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks: 60**

Objectives:

- *To study the theoretical concepts and applications of NMR, ESR and photo electron spectroscopy*
- *To learn photochemistry of coordination compounds and magnetic properties*
- *To know about medicinal bio inorganic chemistry, metal clusters and solid state*

UNIT-I **18 hours**

1.1. **NMR Spectroscopy:** Chemical shift and coupling constant (spin - spin coupling) involving different nuclei (H^1, C^{13}, F^{19} and P^{31}) interpretation and applications to inorganic compounds. Effect of quadrupolar nuclei (H^2 and N^{14}) on the H^1 NMR spectrum. NMR of paramagnetic molecules - isotopic shifts, contact and pseudocontact interactions - Lanthanide shift reagents - stereochemistry of non - rigid molecules

1.2. **ESR Spectroscopy:** Basic principles – presentation of spectra – hyperfine splitting – isotropic and anisotropic hyperfine coupling constants – Mc Connell relation – g value – factors affecting the magnitude of g values – # calculation of unpaired electron density on an atom in delocalized system#.

1.3. Factors affecting the g values of transition metal ions – dependence of spin-orbit coupling and crystal field effects – zero field splitting and Kramer's degeneracy – EPR spectra of transition metal complexes – spectrum of bis(salicylaldiminecopper(II)) – peroxo complex of cobalt – spin dilution.

UNIT-II **18 hours**

2.1 **Photoelectron spectroscopy:** Basic principles - UPES, XPES and AES - valence and core binding analysis - Koopmans theorem - ESCA and Auger spectroscopy - applications.

2.2 **Photochemistry of coordination compounds:** Photochemical reactions - Organo-metallic compounds - photo oxidation - reduction, substitution and photoisomerisation reactions.

2.3 **Magnetic properties:** #Types of magnetism - dia, para, ferro# and antiferro magnetism - magnetic properties of free ions - first and second order Zeeman effects.

UNIT – III **18 hours**

3.1 **Solid state:** Difference between point group and space group – screw axis – glide plane - #symmetry elements – crystal systems – unit cell - Bravais lattices# – equivalent positions - relationship between molecular symmetry and crystallographic symmetry – The Concept of reciprocal lattice – X-ray diffraction by single crystal – rotating crystal – powdered diffraction.

3.2 **Crystal Growth methods:** From melt and solution (hydrothermal, Gel methods)
Neutron diffraction: Elementary treatment – comparison with X-ray diffraction
Electron diffraction: Basic principles.

UNIT – IV **18 hours**

4.1 **Metals at the centre of photosynthesis:** # Primary processes - PS-I and II - Charge separation and electron transport# - Manganese catalysed oxidation of water to O_2.

4.2 Complexes of alkali and alkaline earth metal ions with macrocycles – Poly ethers, spherands, cryptands - ion channels - ion pumps (K^+, Na^+, Ca^{2+}).

4.3 **Metal Clusters:** Dinuclear clusters – Structure of Re_2Cl_8 – quantitative MO diagrams - quadruple bond – polynuclear clusters, polyacids – iso and heteropolyacids of V, Mo and W – Structure – Keggin's theory.

UNIT-V **18 hours**

5.1 **Medicinal Bioinorganic Chemistry:** Bioinorganic Chemistry of toxic metals - Lead, Cadmium, Mercury, Chromium. Detoxification by metal chelation.

5.2 **Chemotherapy:** Cisplatin – # Cancer therapy – cytotoxic compounds of other metals# – Gold containing drugs as antirheumatic agents – Lithium in psychopharmacological drugs.

5.3 **Radiotherapy:** Radioisotopes of Th, Co, Ra, I2, and Na.

_____ # **Self study**

TEXT BOOKS

1. H. Kaur – "Spectroscopy", 3rd Ed., Pragati Prakasan Publications, Meerut, 2006.
2. A. Abdul Jameel – "Application of Physical Methods to Inorganic Compounds", Jan Publications, (2007).
3. P.S.Kalsi, J.P.Kalsi, "Bioorganic, Bioinorganic and Supramolecular Chemistry", 2nd revised Edn., New Age International Publishers. 2010.

UNIT I : Text Book 1,2
UNIT II : Text Book 1,2
UNIT III : Text Book 1,2
UNIT IV : Text Book 3
UNIT V : Text Book 3

REFERENCES:

1. A.D.P. Lever, Inorganic Electronic Spectroscopy, 2nd Edition, Elsevier, London, 1984.
2. E.A.V. Ebsworth, W.H. Rankin, Cradock – "Structural Methods in Inorganic Chemistry", ELBS, 1987.
3. Anthony P. West, solid state Chemistry and its applications, John Wiley, New York, 2000.
4. W.Kaim, B.Schwederski, " Bioinorganic Chemistry: Inorganic Elements in the chemistry of life-An Introduction and Guide", Wiley India Pvt. Ltd., 2012.

SEMESTER-III: CORE-X

ORGANIC SPECTROSCOPY

Course Code : 14PCH3C10 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks : 60**

Objectives:

- *To study the different types of spectroscopic methods and it's applications in structural identification.*
- *To understand the photochemical and pericyclic reactions.*

UNIT – I **18 hours**

1.1 **Ultraviolet and Visible Spectroscopy:** #Basic principles of electronic transitions - correlation of energy change with electronic transitions. Applications of UV - Visible spectroscopy # - Woodward - Fieser - Scott rules -applications to conjugated dienes, trienes, polyenes, unsaturated carbonyl compounds, conjugated cyclic ketones and acetophenones - benzene and its substituted derivatives, Stereochemical factors affecting electronic spectra of biphenyl and binaphthyl, cis and trans isomers - angular distortion and cross conjugation, charge transfer spectra.

1.2 **Infrared Spectroscopy:** Types of stretching and bending vibrations - characteristics group frequencies – Fermi resonance - organic structure determination. Finger print region, factors affecting IR frequency -identification of functional groups - hydrogen bonding (intermolecular and intramolecular) - conformational aspects in cyclic 1,2-diols and 1,3-diols, trans annular interaction in UV and IR - Determination of reaction rates and mechanisms of reactions employing IR and UV spectroscopy (basic aspects).

UNIT – II **18 hours**

Proton NMR Spectroscopy

2.1 Chemical and magnetic non-equivalence - chemical shift – factors influencing δ values - coupling constant - first and second order proton, spin-spin splitting, dependence of J on dihedral angle, vicinal and geminal coupling constants-Karplus equation, Long-range coupling constant.

2.2 Influences of streochemical factors on chemical shift of protons - simplification of complex spectra - double resonance techniques, shift reagents. Chemical spin decoupling of rapid exchangeable protons (DH, SH, COOH, NH_2.)

UNIT – III **18 hours**

^{13}C NMR Spectroscopy

3.1 Basic principles - FT-NMR- relaxation - broad band decoupling, off-resonance decoupling. α, β and γ-effects of substituents. Calculation of chemical shifts for simple aliphatic and aromatic compounds.

3.2 Conformation and chemical shift correlations - peak assignments. NOE phenomenon and importance of NOE phenomenon in ^{13}C NMR spectroscopy.

3.3 Techniques of 2D NMR - COSY, NOSEY and #ROSY#.

UNIT – IV **18 hours**

4.1 **Mass Spectroscopy:** #Basic principle, base peak, isotopic peak, metastable peak, parent peak#, modes of ionization – EI, CI, FAB and ESI, recognition of molecular ion peak and isotopic peak - determination of molecular formula, nitrogen rule, fragmentation pattern for compounds containing CH_3, OH, CHO, COOH and NH_2 , McLafferty rearrangement, importance of metastable peaks.

4.2 **Electron spin resonance spectroscopy:** Basic principles - comparison between ESR and NMR spectra, hyperfine splitting - factors affecting the magnitude of g values. Applications to simple organic free radicals.

4.3 Combined spectral problem of organic compounds (UV, IR, ^{1}H, ^{13}C NMR and Mass).

UNIT – V **18 hours**

5.1 **Optical rotatory dispersion and circular dichroism:** Introduction to theory and terminology. Cotton effects and ORD curves. Axial haloketone rule, octant rule and its application.

5.2 **Organic Photochemistry:** Fundamental concepts - Jablonski diagram - energy transfer characteristics of photoreaction, photo reduction and photo oxidation - Norrish type I & II reactions - Photochemistry of alkenes and dienes - Photosensitisation- Photo additions - Barton reaction, Paterno - Buchi reaction.

5.3 **Pericyclic Reactions:** Concerted reactions - stereochemistry - orbital symmetry and correlation diagram - Frontier molecular orbital approach - Woodward Hoffman rules - electrocyclic reactions - cycloadditions selection rules, - sigmatropic rearrangements - selection rules with simple examples - 1,3 and 1,5 - hydrogen shifts.

#_____# Self study

TEXT BOOKS:

1. Y.R. Sharma, Elementary Organic Chemistry spectroscopy, Principle and chemical applications, S.Chand, 1992.
2. Willam Kemp, organic spectroscopy; ELBS, Macmillan, 1991
3. I.L. Finar, organic chemistry, Vol. II, 5th Edition ELBS 1975
4. P.S. Kalsi, spectroscopy of organic compounds, Niley, 1993.
5. R.B. Woodward and R.Hoffman, The conservation of orbital symmetry, Verlag Chemil, 1970.
6. C.H. Depuy and O.S. Chapman Molecular Reactions and Photo-Chemistry, Prentice Hall, 1975.

UNIT I : Text Book 1
UNIT II : Text Book 2
UNIT III : Text Book 3
UNIT IV : Text Book 4
UNIT V : Text Book 5,6

REFERENCES:

1. Willam Kemp, organic spectroscopy; ELBS, Macmillan, 1991.
2. P.M. Silvertein, G.C. Bassler and T.C. Morrill, spectroscopic Identification of organic compounds, 3rd Edition, 1974.
3. M.G. Arora, Organic Photochemistry and Pericyclic reactions.
4. B.B. Grill, MR. Willis. Pericyclic reactions, Chapman & Hall, 1974.
5. J.R. Dyer, Application of Absorption spectroscopy of organic compounds, Prentice Hall, 1965.
6. I.L. Finar, organic chemistry, Vol. II, 5th Edition ELBS, 1975
7. L.A. Pacesetter, Principles of modern heterocyclic chemistry W.A. Benzamin, 1968.
8. Raj, K. Bansal, Heterocyclic Chemistry, Synthesis Reactions, and Mechanisms, Wiley, 1990.

SEMESTER-III : CORE-XI

INDUSTRIAL CHEMISTRY

Course Code : 14PCH3C11 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks: 60**

Objectives:

- *To impart knowledge on fermentation, pigments, oils and fats.*
- *To understand the industrial applications of chemistry.*
- *To give an idea for the student about drugs and explosives.*

UNIT – I **18 hours**

Fermentation: Introduction - Historical - Conditions favourable for fermentation- Characteristics for enzymes - short accounts of some fermentation processes – Manufacture of beer – sprits- wines and vinegar. Ethyl alcohol from molasses- Preparation of wash-distillation-# Alcohol from waste sulphite liquor#.

UNIT – II **18 hours**

Pigments: Definition – composition, characteristics and uses of white pigments - white lead, Zinc oxide Lithopone and TiO_2 – Blue pigments – Ultra marine blue, cobalt blue and iron blue – characteristics – uses. Red pigments – red lead –characteristics and uses. Green pigments – chrome green, Guigwet's green and chromium oxide – characteristics and their uses-# Black pigments- Yellow pigments#.

UNIT – III **18 hours**

Drugs: Definition sources of drugs – some important drugs – aspirin – phenacetin – paracetamol – penicillin – chlormycetin – structure – properties – uses.

Organic diagnostic reagents – definition – uses – sodium diatrizoate, phenol red Evans blue, indigo carmine, methylene blue, xylose, Histamine and sodium benzoate - properties – uses.

Organic pharmaceutic aids – Definition – preservatives – antioxidants – flavouring agents – colouring agents – sweetening agents - Emulsifying agents and stabilising agents – examples for each class – uses (structure and preparation not necessary)

UNIT – IV **18 hours**

Adhesives: definition – classification of adhesives – animal glue – preparation- uses –protein adhesives - starch adhesives – preparation – uses.

Enamels: Introduction - Raw Materials – Manufacture and Applications

Explosives: Introduction- Classification- preparation and uses of explosives- Nitro cellulose, TNT, Picric acid, Gun Powder, Cordite and #Dynamite#.

UNIT – V **18 hours**

Oils and Fats: Introduction – distinction, properties- classification- vegetable oils- Manufacture of cotton seed oil and soybean oil- Refining of crude vegetable oils- coconut oil- palm oil- peanut oil- olive oil- #castor oil- safflower oil#.

Analysis of oils and fats : Definition and determination of Saponification value, Iodine value and RM value.

#_____# Self study

TEXT BOOKS:

1. B.N. Charabarthy – "Industrial Chemistry", 1st Ed., Oxford and IBh Publishing, New Delhi.
2. B.K. Sharma – "Industrial Chemistry", 1st Ed., (1983), Goel Publication, Meerut.
3. Arun Bahl and B.S. Bahl – "Text Book of Organic Chemistry", 11th and 18th Ed., S. Chand, New Delhi, 2006.
4. Ghosh, Jayashree – "Text Book of Pharmaceutical Chemistry", 3rd Ed., S.Chand & Co. Ltd., New Delhi, 1999.

UNIT I : Text Book 3,4
UNIT II : Text Book 1,2
UNIT III : Text Book 4
UNIT IV : Text Book 1,2
UNIT V : Text Book 1,2

REFERENCES:

1. V.P. Gowariker and N.V. Viswanathan – "Polymer Science", 1st Ed., Wiley Easter Pvt. Ltd., New Delhi.
2. Lakshmi. S – "Pharmaceutical Chemistry", 3rd Ed., (1995), Sultan Chand & Sons, New Delhi.
3. Rajasekaran, VN. – "Pharmaceutical Chemistry", 1st Ed., (2003), Sun Publications – Chennai.
4. Krishnamoorthy, P. Vallinayagan & K. Jaya Subramanian – "Applied Chemistry", 2nd Ed., (1999, 2001), Tata MaGraw-HillPublishing Co. Ltd., New Delhi.

SEMESTER-III: CORE BASED ELECTIVE - III

NANO AND GREEN CHEMISTRY

Course Code : 14PCH3CE3 **Max. Marks : 100**
Hours/Week : 6 **InternalMarks : 40**
Credit : 5 **External Marks: 60**

Objectives:

- *To give a basic idea for the student about special topics of chemistry nano and green chemistry*
- *To bring the knowledge for student about solvent free reaction*
- *To study about the sono chemistry*

UNIT-I **18 hours**

Nano Materials:

Introduction - Nanomaterials - classification – properties – Optical, electrical, mechanical and magnetic properties – Applications. Nanoparticles - Synthesis – Sol- gel method – Solvothermal methods – Bottom – up- Top – down – Methodology. Principles and applications of SEM, TEM and #AFM methods#.

UNIT-II **18 hours**

Carbon nanotubes:

CNT – Classification – Preparation - arc method – laser ablation method – Chemical vapour deposition method – Ball milling method. Properties of CNT – applications – fullerenes – properties – uses. Nanocomposites – Classification – Properties - uses.

UNIT-III **18 hours**

Green Chemistry:

Definition- Need for green chemistry- Twelve principles of green chemistry- concept of atom economy – efficiency of reaction – percentage yield – Theoretical yield – Atom economy in substitution reaction- elimination reaction – addition reaction and rearrangement reaction - #Atom economy synthesis of ethylene oxide and Ibuprofen#.

UNIT-IV **18 hours**

Green reactions: Green solvents –definition- super critical carbon dioxide - role of Ionic liquids – applications of zeolites in green chemistry – uses of microwave and sonication – Designing a green synthesis – choice of starting material - choice of reagents – choice of catalysts – #PTC catalyzed reaction#.

UNIT-V **18 hours**

Green Synthesis: adipic acid – methyl methacrylate, acetaldehyde, Ibuprofen, Paracetamol Microwave assisted reaction: Introduction – Esterification – Fries rearrangement – #Diels – Alder reaction#. **Ultrasound assisted reaction:** Introduction- Cannizaro reaction – Strecker synthesis – Reformatsky reaction.

#_____# Self study

TEXT BOOKS:

1.R.Sanghi and M.M srivastva, Green chemistry, Narosa 2003.

2. P.S. Kalsi & J.P Kalsi – Bioinorganic, Bioorganic and supra molecular chemistry – New Age International Publishers – 2010.

3. Nanotechnology: Principles and practices Sulabha K. Kulkarni (capital Pvt. Co.)-2002.

UNIT I : Text Book 3
UNIT II : Text Book 3
UNIT III : Text Book 1
UNIT IV : Text Book 1,2
UNIT V : Text Book 1

REFERENCES:

1. Nanoscale materials in chemistry, Wiley interscience, Kenneth, J.Klaburde, 2002.

2. M. M. Srivastva and R.Sanghi, Chemistry for green environment, Narosa, 2005.

3. S,Delvin Green chemistry, IVY publication house, 2006.

4 F.J.Ownes Introduction to Nano technology John Wiley and New Jersey, 2003.

SEMESTER-III: CORE BASED ELECTIVE - III

SPECIAL TOPICS IN CHEMISTRY

Course Code : 14PCH3CE3 | **Max. Marks : 100**
Hours/Week : 6 | **Internal Marks : 40**
Credit : 5 | **External Marks : 60**

Objectives:

- *To study about the sono chemistry and retrosynthesis*
- *To give a basic idea for the student about special topics of chemistry nano and green chemistry*
- *To bring the knowledge for student about solvent free reaction*

UNIT-I **18 hours**

Retrosynthesis: Synthons – Synthetic equivalents – Convergent and Linear synthesis – Retrosynthetic tree - Guidelines to a good disconnection – Functional Group Interconversions – One group and two group C-X disconnections – One group C-C disconnections – 1,1 C-C and 1,2 C-C disconnections to synthesise alcohols and carbonyl compounds – Regioselectivity – Michael and Wittig reactions – Use of acetylenes and aliphatic nitro compounds in organic synthesis – Two group C-C disconnections – Diels-Alder reaction – its stereochemical aspects – Robinson annelation.
Guidelines for solving the problem of chemoselectivity – #Umpolung reagents – Protecting groups for alcohols, amines and carbonyl compounds – Deprotection #.

UNIT-II **18 hours**

Sono Chemistry: Instrumentation – Physical aspects – Types - Homogeneous liquid phase – Heterogeneous solid-liquid reactions. Synthetic applications – Esterification – Saponification – Hydrolysis/Solvolysis – alkylation – oxidation and reduction reactions – Bouveault reaction.
Supramolecular Chemistry: Introduction – molecular forces, molecular recognition - basic concepts of host - guest complexation with examples from ionophore chemistry – non-covalent interactions - molecular receptors for different types of molecules, design and synthesis of co-receptor molecules, triangular, square, #rectangular supramolecules #.

UNIT-III **18 hours**

Nano Scale Materials:Introduction – classification – Preparation and properties of nano particles – metals, semiconductors, ceramics(oxides, carbides, sulphides) physical methods - vapour deposition methods – chemical methods – sol-gel methods – condensation reactions – controlling particle size and morphology - structure and bonding – chemical properties – size dependent properties – melting point – magnetism – colour – conductivity – arrangements – applications – colour – catalysis – nanoelectronics.

UNIT-IV **18 hours**

Carbon Nano Structures: Introduction – fullerenes C60 and C80 nanostructures – properties and applications. Carbon clusters – carbon nano tubes – fabrication – single and multiwalled nanotubes – preparation of carbon nanotubes by pyrolysis and thermal treatment – growth mechanism of carbon nanotubes – characterization of nano particles using SEM and XRD - electrical properties – mechanical properties – #application of carbon nano tubes #– field emission and shielding, computers, fuel cells, chemical sensors catalysis – mechanical reinforcement.

Nano Composites: Synthesis procedures - various systems (metal-polymer, metal- ceramics and polymer-ceramics). Characterization – procedures – Applications.

UNIT-V **18 hours**

Green Chemistry: Need for green chemistry – planning of green synthesis – solvent free reactions – microwave assisted synthesis – role of ionic liquids in green chemistry – cleaner technology with super critical fluids, catalytic approach to green chemistry. (Use of zeolites, clays, mesoporous materials) waste water treatment by exploitation and technology at ambient conductors. # Remediations method for textile effluents – green chemistry – bio-catalytic reactions #.

Green reactions: Aldol condensation, Cannizaro reaction and Grignard reaction-comparison of the above with classical reactions.

#_____# Self study

TEXT BOOKS:

1.R.Sanghi and M.M srivastva, Green chemistry, Narosa 2003.
2. P.S. Kalsi & J.P Kalsi – Bioinorganic, Bioorganic and supra molecular chemistry – New Age International Publishers – 2010.
3. Nanotechnology: Principles and practices Sulabha K. Kulkarni (capital Pvt. Co.),2002.
4. Jagadamba Singh and L.D.S.Yadav, Organic synthesis, 4th edn., Pragathi Prakashan, 2009.
5. V.K.Ahluwalia and Renu Aggarwal, Organic synthesis, 2nd edition, Narosa, 2006.

UNIT I : Text Book 4,5
UNIT II : Text Book 2
UNIT III : Text Book 3
UNIT IV : Text Book 3
UNIT V : Text Book 1

REFERENCES:

1. Kenneth, J.Klaburde. Nanoscale materials in chemistry, Wiley interscience 2002.
2. Stuart Warren organic synthesis, methods and starting materials, the disconnections approach John, Wiley & sons-1992.
3. Futhrhop, Penzlin, organic synthesis concepts, methods and starting materials, Verlag chemie 1983.
4. R.Sanghi & MM srivastva Green chemistry, Narosa 2003.
5. M.M.srivastva & R.Sanghi chemistry for green environment, Narosa 2005.
6. S,Delvin Green chemistry, IVY publication house 2006.
7. C.P.Jr. and F.J.Ownes Introduction to Nano technology John wiley &New jersey 2003.
8. P.S. Kalsi & J.P Kalsi – Bioinorganic, Bioorganic & supra molecular chemistry – New Age International Publishers – 2010.
9. Sulabha K. Kulkarni, Nanotechnology: Principles and practices (capital Pvt. Co.) 2002.

SEMESTER-III: EXTRA CREDIT - I

ANALYTICAL TECHNIQUES

Course Code : 14PCH3EC1	**Max. Marks : 100***
Hours/Week : --	**Internal Marks : --**
Credit : 5*	**External Marks : 100***

Objectives:

- *To understand the concepts of Analytical chemistry*
- *To gain an idea about solvent extraction and recrystallisation*
- *To learn the theories and importance of electrical instrumentation in chemistry*

UNIT-I

1.1 **Analytical chemistry** - chemical analysis – Advantages and limitations of chemical methods- types of chemical analysis- Instrumental methods- Advantages and Limitations of Instrumental methods- Analytical methods on the basis of Sample size – Sampling- sampling methods- sampling in different physical states- Sampling statistics- source of error in sampling- dangers during sampling.

1.2 **Techniques of Analysis** – Introduction- Classification of analytical techniques- classification of instrumental methods of analysis - factors affecting the choice of analytical methods- interferences- typical separation procedures- sensitivity and detection limits.

1.3 **Statistical Analysis of Data:**
Various types of errors – Precision and Accuracy – significant figures, mean value, variance and standard deviation.

UNIT-II

2.1 **Solvent extraction**: Principle, types of extractant systems- Extraction of liquids – Batch extraction process, continuous extraction process – Extraction by chemically active solvents- Extraction of solids – Drying agents- $MgSO_4$, anhydrous $CaCl_2$, anhydrous K_2CO_3, anhydrous $CaSO_4$ - Distillation theory – Steam distillation- fractional at atmospheric pressure- Vacuum/reduced pressure distillation.

2.2 **Recrystallisation** – solvent selection – Handling of flammable solvents – Use of decolourising Carbon – Difficulties in recrystallisation – recrystallisation at very low temperature – semi micro and micro recrystallisation – Drying of recrystallised materials.

UNIT-III

3.1 **Fluorimetry**: Fluorescence – mechanism – Fluorimetry – theory – Instrumentation and application - comparison of absorption and fluorescence methods, spectrofluorimeters – principle – Instrumentation and applications.

3.2 **Turbidimetry and Nephelometry**: Theory - Instrumentation and applications.

3.3 **Flame photometry and Phosphorimetry** – Principle - instrumentation - working - applications.

UNIT-IV

4.1 **Colorimetry**: principles, laws of colorimetry, instrumentation for visual and photocolorimetry, types of photo colorimeters – single beam and double beam-working – advantages - colorimetric estimation of Ni, Cu and Fe.

4.2 **Polarography**: Introduction – principle – Ilkovic equation – Instrumentation – working and advantages of DME – evaluation of polarographic curves – applications of polarography – pulse polarography.

4.3. **Thermo analytical methods:** thermo gravimetric analysis – principle – instrumentation – TG curve – factors affecting TGA - applications – Differential thermal analysis –DTA curves – applications – Differential Scanning Calorimetry – Thermometric titrations – principle – applications.

UNIT-V

5.1 **Voltammetry:** Instrumentation, capacitive current, linear potential sweep (dc) voltammetry – cyclic voltammetry, potential step methods – normal pulse, differential pulse and square wave voltammetry, stripping voltammetry – principles, electrodes used for stripping analysis, anodic and cathodic stripping voltammetry, voltammetry applications.

5.2 **Amperometry:** Amperometric titrations, principles, titrations with dropping mercury electrode (DME), apparatus, biamperometric titrations, advantages and applications of amperometric titrations.

5.3 **Coulometry:** Introduction – coulometric titrations – detection of end points – applications in titrimetric analysis – potentiostatic coulometry – advantages.

TEXTBOOKS:

1. H. Kaur - "Instrumental methods of Chemical Analysis", 6th edition, (2010), Pragati prakasan Publications, Meerut.
2. Willard, Meeritt, Dean and Settle – "Instrumental Methods of Analysis", 7th Ed., (1983), CBS Publishers.
3. B.K. Sharma – "Instrumental methods of Analysis", (2000), Goel Publications.
4. S.M. Khopkar, "Basic Concepts of Analytical Chemistry", Revised edition (2006) Wiley Eastern Ltd.,

UNIT I : Text Book 1,3,4
UNIT II : Text Book 2,3
UNIT III : Text Book 1,2,34
UNIT IV : Text Book 2,3,4
UNIT V : Text Book 2,3

REFERENCES:

1. R.A. Day and A.L. Underwood – "Quantitative Analysis", (1999), Prentice - Hall of India Pvt., Ltd., New Delhi.
2. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell – "Vogel's Text book of Practical Organic Chemistry", first Indian reprint, (2004), Pearson Education Publisher.
3 L.Pavia – "Spectroscopy" cengage learning India Pvt. Ltd, (2010).
4. Harald Guther, "NMR Spectroscopy", Wiley india (p) Ltd, 2nd Edn, (2010).

SEMESTER-IV: CORE-XIII
STATISTICAL THERMODYNAMICS AND SURFACE CHEMISTRY

Course Code : 14PCH4C13 | **Max. Marks : 100**
Hours/Week : 6 | **Internal Marks : 40**
Credit : 5 | **External Marks : 60**

Objectives:

- *To understand the thermodynamics of equilibrium and non-equilibrium systems.*
- *To inculcate interest in solving thermodynamic quantities by statistical and quantum mechanical approach.*
- *To learn the theories and importance of surface chemistry*

UNIT – I **18 hours**

Classical Thermodynamics:

1.1 Thermodynamics of systems of variable composition - partial molar property – partial molar quantities of E, V, H, A, G and S, chemical potential, physical significance of chemical potential, variation of chemical potential with respect to T and P, chemical potential in terms of U and H, partial molar quantities from experimental data – direct method, apparent molar properties, intercepts method and general methods.

1.2. Calculation of thermodynamic properties of real gases - fugacity concept, variation of fugacity with T and P – calculation of fugacity of real gases, determination of fugacity – graphical method, equation of state method, determination of fugacity in gas mixtures –Lewis-Randall rule.

1.3. Activity of non-electrolytes – definition, activity coefficient, standard states of sol vent and solute for liquids and solids, dependence of activity on T and P, experimental determination of activity (solvent and solute) – vapour pressure method, #cryoscopic method and EMF method#.

UNIT - II **18 hours**

Statistical Mechanics

2.1. Basic Concepts and Classical Statistics – introduction of statistical mechanics, mathematical probability, thermodynamic probability, relation between mathematical probability and thermodynamic probability of a system, Boltzmann-Planck's equation, Phase space, Ensembles – types of ensembles, definition of micro and macro states, different methods of counting macro states, postulates, Ergodic hypothesis, distinguishable and indistinguishable particles, Stirling's approximation

2.2. Classical statistics – derivation of Maxwell–Boltzmann statistics and distribution law, partition functions – definition, derivation of translational, rotational, vibrational and electronic partition functions, principle of equi-partition of energy.

2.3 Molar partition function and molecular partition function, partition functions and thermodynamic quantities - Internal energy (E), heat capacity (Cv), work function (A), pressure (P), #heat content (H), Gibb's free energy(G) and entropy(S), entropy of mono atomic gases (Sackur–Tetrode equation)#.

UNIT –III **18 hours**

Quantum Statistics

3.1. Quantum statistics – Bose–Einstein and Fermi–Dirac statistics and distribution function, comparison of them with Maxwell-Boltzmann statistics,

3.2. Application of B.E.statistics - photon gas and super fluidity of liquid helium, concept of negative Kelvin temperature, application of F.D.statistics - electron gas and thermionic emission.

3.3. Heat capacities of solids – Dulong and Petit's law, classical theory and its limitations, Einstein's theory and its limitations, Debye's theory and its limitations.

UNIT-IV **18 hours**

4.1. **Irreversible Thermodynamics:**

Non-equilibrium thermodynamics – definition, types of irreversibility of a process, postulates, entropy production - entropy production and rate in a chemical reaction, Onsagar relations - linear law, reciprocal relation and applications, stationary–state.

4.2 **Phase rule-Three component system:**

Maximum number of phases, maximum number of F, Roozeboom triangle- Types- formation of one pair partially miscible liquids, formation of two pairs of partially liquids, Formation of three pairs of partially miscible liquids.

4.3. **Solid liquid systems**:

Ammonium chloride - Ammonium nitrate - Water system, $^{\#}H_2O$ - Na_2SO_4 - NaCl system, $MgCl_2$, $CaCl_2.H_2O$ system$^{\#}$.

UNIT-V **18 hours**

Surface Phenomena

5.1 B.E.T. isotherms - Surface area determination - Heat of adsorption and its determination Adsorption from solution, Gibbs adsorption isotherm - solid - liquid interfaces - wetting and contact angle - solid gas interfaces - soluble and insoluble film.

5.2 Surface tension - methods of measuring surface tension - electrical phenomenon at Interfaces, including electro kinetic, micelles and reverse micelles, Solubilisation, Micro - emulsions.

5.3 Role of surface in catalysis - $^{\#}$semiconductor catalysis, n and p type surfaces - kinetics of surface reactions involving adsorbed species - Langmuir -Hinshelwood mechanism$^{\#}$.

$^{\#}$_____$^{\#}$ **Self study**

TEXTBOOKS:

1. K. Kuriacose and J. C. Rajaram, "Thermodynamics for Students of Chemistry", Shoban Lalnagin Chand and Co.Delhi, 2002.
2. Gurdeep Raj, "Thermodynamics Statistical Thermodynamics & Irreversible Thermodyanics", Goel Publishing House, Meerut, 1998.
3. M. C. Gupta, "Statistical Thermodynamics", New Delhi, East-West Affiliated Pvt.Ltd., 1969.
4. Laidler, "Chemical Kinetics," 3rd edition, New Delhi Tata-McGraw Hill Co., 1984.

UNIT I : Text Book 1
UNIT II : Text Book 2,3
UNIT III : Text Book 2,3
UNIT IV : Text Book 1
UNIT V : Text Book 4

REFERENCES:

1. F. W. Sears, "Statistical Mechanics", 2nd Edition, Addison Wesley, 1972.
2. H. W. Zemansky, "Heat and Thermodynamics", Tata- McGraw Hill, 1975.
3. P. W. Atkins, Physical Chemistry E.L.B.S. 6th Ed.1998.
4. Samuel Glasstone, "Textbook of Physical Chemistry" 2nd Edition, MacMillan India, 1981.
5. K. L. Kapoor, "A Text Book of Physical Chemistry", Volume-4 S. M.Yogan at Macmillan India Press, Chennai, 2009.

SEMESTER-IV: EXTRA CREDIT - II
INSTRUMENTATION AND SEPARATION TECHNIQUES

Course Code : 14PCH4EC2 | **Max. Marks : 100***
Hours/Week : -- | **InternalMarks : --**
Credit : 5* | **External Marks : 100***

Objectives:

- *To understand the concepts of Spectroscopy.*
- *To gain an idea about separation techniques*
- *To learn the theories and importance of conductometry and potentiomentry*

UNIT-I **18 hours**

1.1 **UV- Visible spectroscopy**- Instrumentation- sources, filters and monochromators, slits, grating, cuvete, radiation detectors and indicators, photoelectric spectrophotomer - types, sources of errors during recording, calibration- presentation of spectral data

1.2 **Infrared Spectroscopy:** Dispersive infrared spectrometer- source (Nernst, Globar) monochromater, detector, double-beam spectrophotometer - presentation of spectra- sample preparation techniques for IR, FT-IR- simple diagram of a Fourier transform infrared spectrometer- working mode – advantages.

1.3 **Raman spectroscopy**: Instrumentation- source of light, filters, sample holders, spectrograph, detectors, Sample preparation.

UNIT-II **18 hours**

2.1. **Nuclear Magnetic Resonance (NMR)**: Instrumentation - magnet, magnetic field sweep, radio frequency source, signal detector and recording system, sample holder, sample probe.

2.2 **Electron Spin Resonance (ESR):** Instrumentation - electromagnet, source of micro wave radiation, sample cavity, choice of solvent, crystal detectors and recorder-double resonance spectrometers.

2.3 **Mass Spectrometry:** Instrumentation - sample preparation, generation of ions, analyzer, ion collector and measuring system, resolution- representation of mass spectrum – double focusing mass spectrometer.

UNIT-III **18 hours**

3.1 **Conductometry:** Introduction, laws and definitions of conductance, effects of dilution, conductance measurements, conductometric titrations - apparatus, types and advantages.

3.2 **Potentiometry:** electrochemical series, reference electrodes – hydrogen electrode, calomel and silver-silver chloride electrode, measurement of pH – glass indicating electrode, potentiometric titrations, variations in potentiometric titrations, its advantages.

3.3 **Atomic Absorption Spectroscopy**: Introduction, principle of AAS, classification of atomic spectroscopic methods, measurement of atomic absorption, instrumentation – application. Atomic Emission spectroscopy – Introduction, origin of spectra, principle of emission spectroscopy, Instrumentation, measurement of light intensity and applications.

UNIT-IV **18 hours**

4.1 **Column Chromatography:** Definition, Types, Principles of column chromatography. Experimental techniques – Adsorption column – Packing of column – Adsorbents – Characteristics of good adsorbent – developers – Techniques of separation – Detectors, applications of column chromatography.

4.2 **Thin Layer Chromatography:** Principle, types, experimental techniques of TLC, applications of TLC.

4.3 **Paper Chromatography:** Principle, types, experimental techniques of Paper chromatography, applications.

4.4 **Ion Exchange Chromatography:** Principle, Ion exchanger and its types, experimental techniques of IEC, applications.

UNIT-V **18 hours**

5.1 **Gas Chromatography:** Principle, types (GSC, GLC), Instrumentation of GC, applications of GC. **GC-MS:** Principle, instrumentations, applications of GC-MS.

5.2 **High Performance Liquid Chromatography (HPLC):** Introduction, principle, characteristic features of HPLC, instrumentation, applications of HPLC.

5.3 **Exclusion Chromatography:** Principle, Types, Gel chromatography, Experimental techniques of GPC.

5.4 **Electrophoresis:** Introduction, Types of Paper electrophoresis, Techniques of Paper electrophoresis, thin layer electrophoresis, Zone electrophoresis, Electro dialysis, applications of Electrophoresis.

TEXT BOOKS:

1. H. Kaur - "Instrumental methods of Chemical Analysis", 6th edition, (2010), Pragati prakasan Publications, Meerut.
2. G.Aruldhas –"Molecular structure & Spectroscopy", PHI learning Pvt.Ltd.2nd Edition, -2008.
3. B.K. Sharma-"Instrumental Methods of Analysis", (2000), Goel Publications, Meerut.
4. S.M. Khopkar, "Basic Concepts of Analytical Chemistry", Revised edition (2006) Wiley Eastern Ltd.

UNIT I : Text Book 2
UNIT II : Text Book 2
UNIT III : Text Book 1,3,4
UNIT IV : Text Book 1,3,4
UNIT V : Text Book 1,3,4

REFERENCES:

1. Willard, Meeritt, Dean and Settle – "Instrumental Methods of Analysis", 7th Edn.,(2006), CBS Publishers.
2. R.A. Day and A.L. Underwood – "Quantitative Analysis", (1999), Prentice-Hall of India Pvt., Ltd., New Delhi.
3. B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatchell – "Vogel's Text book of Practical Organic Chemistry", 5th edition, 2009, Pearson Education Publisher.
4. L.Pavia – "Spectroscopy" cengage learning India Pvt. Ltd - 2010.
5. Harald Guther, "NMR Spectroscopy", Wiley india (p) Ltd, 2nd Edn,2010.
6. Colin N.Banwell – "Fundamentals of Molecular structure Spectroscopy" Mc.Graw – Hill publishing company Ltd. 4th edition, 1995.

SEMESTER- I: CORE – III

INORGANIC ESTIMATION AND COMPLEX PREPARATIONS-PRACTICAL

Course Code : 14PCH1C3P	**Max. Marks : 100**
Hours/Week : 6	**InternalMarks : 40**
Credit : 5	**External Marks : 60**

Objectives:

- *To learn quantitative separation of metal ions in binary mixtures.*
- *To learn simple single stage preparations of some inorganic complex.*

Volumetry, Gravimetry / Complexometric and complex preparations:

Estimation of the following elements by volumetric and gravimetric / complexometric methods:

1. Cu (V) Ni (G/C)
2. Cu (V) Zn (G/C)
3. Cu (V) Mg (G/C)
4. Zn (V) Cu (G/C)
5. Fe (V) Zn (G/C)
6.

Note: V - Volumetric
G - Gravimetric
C - Complexometric

Preparations:

1. Tetramminecopper(II)sulphate
2. Potassiumtrioxalatochromate(III)
3. Hexathiourealead(II)nitrate
4. Potassiumtrioxalatoaluminate(III)
5. Tristhioureacopper(I)chloride
6. Tristhioureacopper(II)sulphate
7.

Scheme of valuation

Procedure writing	-	10 marks
Results:		
1-2%	-	50 marks
2-3%	-	40 marks
3-4%	-	30 marks
>4%	-	20 marks

REFERENCES:

1. Vogel A I, A Text Book of Quantitative Inorganic Analysis, 3rd Edn., London, Longman Group.

SEMESTER- I: CORE – IV
ORGANIC ESTIMATIONS AND CHROMATOGRAPHY-PRACTICAL

Course Code : 14PCH1C4P	**Max. Marks : 100**
Hours/Week : 6	**InternalMarks : 40**
Credit : 5	**External Marks : 60**

Objectives:

- *To understand the organic qualitative separation and identification*
- *To know the concept of Thin Layer Chromatography*

1. Estimation of the following: **40 hours**

Phenol, Aniline, Ethyl methyl ketone, Glucose, Ascorbic acid (Vit-C).

2. Chromatographic Technique **10 hours**

1. Thin Layer Chromatography

3. Identification of chromophore / functional groups using UV / IR spectra. **10 hours**

Scheme of valuation

Procedure writing - 10 marks

Results:

1-2%	-	50 marks
2-3%	-	40 marks
3-4%	-	30 marks
>4%	-	20 marks

REFERENCES:

1. Vogel s text book of practical Organic Chemistry., 5th Edition, 1989.

SEMESTER- II: CORE –VII
INORGANIC QUALITATIVE ANALYSIS AND
COLORIMETRIC ESTIMATIONS - PRACTICAL

Course Code	**: 14PCH2C7 P**	**Max. Marks**	**: 100**
Hours/Week	**: 6**	**Internal Marks**	**: 40**
Credit	**: 5**	**External Marks**	**: 60**

Objectives:

- *To learn the technique of inorganic qualitative analysis.*
- *To understand the concept of common ion effect and solubility product.*
- *To learn colorimetric analysis.*
-

Semi-micro Qualitative Analysis:

Analysis of two common and two rare earth elements in a given inorganic mixture
Common**:** Pb, Cu, Bi, Cd, Zn, Co, Ni, Ca, Ba, Sr
Rare**:** W, Se, Te, Mo, Ce, Zr, Th, V, Li

Colorimetric Estimations:

Cu, Fe, Mn, Ni, Cr, Co

Scheme of valuation

Analysis:

4 radicals correct with suitable tests:	40 marks
3 radicals correct with suitable tests:	30 marks
2 radicals correct with suitable tests:	20 marks
1 radical correct with suitable tests:	10 marks

Colorimetric Estimations:

1-2%	-	20 marks
2-3%	-	15 marks
3-4%	-	10 marks
>4%	-	05 marks

REFERENCES:

1. Vogel A I, A Text Book of Quantitative Inorganic Analysis, 3rd Edn., London, Longman Group.

SEMESTER-II :CORE –VIII
ORGANIC PREPARATIONS AND MIXTURE ANALYSIS-PRACTICAL

Course Code : 14PCH2C8 P	**Max. Marks : 100**
Hours/Week : 6	**Internal Marks : 40**
Credit : 5	**External Marks : 60**

Objectives:

- *To learn technique of organic qualitative analysis.*
- *To learn some double stage organic preparations.*

Separate the following types of mixture and analyse only one of the components present as desired by the Teacher / Examiner.

1. Mixture Analysis:

1. Soluble and insoluble
2. Acidic and Neutral
3. less acidic and neutral
4. Basic and neutral

2. Two Stage Preparations:

1. Acetylsalicylicacid from methylsalicylate
2. 1,3,5 – Tribromobenzene from Aniline
3. *p*-Nitroaniline from acetanilide
4. *p*-Bromoaniline from acetanilide
5. Benzilic acid from benzoin
6. Benzaldehyde to chalcone epoxide via chalcone
7. Cyclohexanone to caprolactone via cyclohexanone oxime

Scheme of valuation

Organic analysis : 40
Organic preparation : 20

Pilot separation	-	5 marks
Special elements present / absent	-	5 marks
Aromatic/ aliphatic	-	5 marks
Saturated/ unsaturated	-	5 marks
Functional group present	-	10 marks
Derivative	-	10 marks

REFERENCES:

1. Vogels text book of practical Organic Chemistry., 5th Edition, 1989.

SEMESTER- III: CORE-XII

PHYSICAL CHEMISTRY NON-ELECTRICAL - PRACTICAL

Course Code	**: 14PCH3C12P**	**Max. Marks**	**: 100**
Hours/Week	**: 6**	**Internal Marks**	**: 40**
Credit	**: 5**	**External Marks**	**: 60**

Objectives:

- *To understand Phase diagram and kinetics*
- *To learn the instrumental techniques*

Non- Electrical

1. Phase diagram of a binary system (Eutectic formation)
2. Phase diagram of a two-component system forming compound (with congruent melting point).
3. Phase diagram of a three component liquid system (with one partially miscible pair) (Toluene-Water-Acetic acid).
4. Heat of solution of benzoic acid in water.
5. Comparison of strengths of three acids from kinetic study (Iodination of acetone)
6. Rast micro method of determining k_f and molecular weight.
7. Determination of E_a and A (for the hydrolysis of ethyl acetate at different temperatures)
8. Primary salt effect (on the kinetics of reaction between $S_2O_8^{2-}$ and I^-).
9. Verification of Freundlich adsorption isotherm (Adsorption of oxalic acid on Charcoal).
10. Estimation of KI by partition method.

Scheme of valuation

Procedure with formula-		10 Marks
Up to 5%	-	50 marks
05-10%	-	40 marks
10-15%	-	30 marks
>15%	-	20 marks

REFERENCES:

1. Daniels., Experimental Physical Chemistry, (7th edition), NewYork, McGraw Hill, (1970).
2. Findlay, A., Practical Physical Chemistry, (7th edition), London, Longman (1959).

SEMESTER- IV: CORE-XIV
PHYSICAL CHEMISTRY ELECTRICAL-PRACTICAL

Course Code : 14PCH4C14P	**Max. Marks : 100**
Hours/Week : 6	**Internal Marks : 40**
Credit : 5	**External Marks : 60**

Objectives:

- *To understand the principles of conductometry and potentiometry*
- *To learn the instrumental techniques*

CONDUCTOMETRY:

1. Estimation of mixture of acids.
2. i. Determination pK_a – Ostwald's dilution law.
   ii.Determination of solubility product-Kohlrausch's law.
3. Estimation of mixture of halides.
4. Determination of hydrolysis constant (for aniline hydrochloride)
5. i. Saponification of ethyl acetate (Kinetics study).
   ii. Determination of critical micelle concentration by conductometric method.

POTENTIOMETRY:

1. Estimation of mixture of acids.
2. Determination of solubility product
   a. Galvanic cell method.
   b. Concentration cell method.
3. Estimation of mixture of halides.
4. Determination of $E^o_{Zn^{2+}/Zn}$ and estimation of Zn^{2+}.
5. Determination of hydrolysis constant (for aniline hydrochloride).

Scheme of valuation

Procedure with formula : 10 marks
Practical : 50 marks

<1%	-	50 marks
1-2%	-	40 marks
2-3%	-	30 marks
3-4%	-	20 marks
>4%	-	10 marks

REFERENCES:

1. Daniels, Experimental Physical Chemistry, (7th edition), New York, Mc Graw Hill, (1970).
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