Total Contact Hours= 27 **Total Marks= 700** **Total Credits= 23**

1st Semester		Contact Hrs.			Marks			Credits
Code	**Name**	**L**	**T**	**P**	**Int.**	**Ext.**	**Total**	
MCHMS1-101	Electronic Spectra & Magnetic Properties of Transition Metal Complexes	4	0	0	40	60	100	4
MCHMS1-102	Organic Reactions & Mechanisms-I	4	0	0	40	60	100	4
MCHMS1-103	Thermodynamics& Solid State	4	0	0	40	60	100	4
Departmental Elective-I (Choose any one)		4	0	0	40	60	100	4
MCHMD1-111	Computational Skills & Simulations in Chemistry							
MCHMD1-112	Polymer Chemistry							
MCHMD1-113	Chemical Kinetics & Electrochemistry							
Open Elective		3	0	0	40	60	100	3
MCHMS1-104	Inorganic Chemistry Lab.-I	0	0	4	60	40	100	2
MCHMS1-105	Organic Chemistry Lab.-I	0	0	4	60	40	100	2
	Total	**19**	**0**	**08**	**320**	**380**	**700**	**23**

ELECTRONIC SPECTRA & MAGNETIC PROPERTIES OF TRANSITION METAL COMPLEXES

Subject Code: MCHMS1-101 **L T P C** **Duration: 60 Hrs.**
4 0 0 4

Course Objectives

1. To understand the concept of symmetry elements and symmetry operations.
2. To introduce the concept of inter electronic repulsion parameters and crystal field strength in various fields.
3. To familiarize with the Orgel and correlation diagrams.
4. To understand molecular orbital diagrams for octahedral and tetrahedral diagrams

Course Outcomes:
The completion of this course will make student to acquire the knowledge of:

1. Interpretation of electronic and magnetic properties.
2. Interpretation of molecular orbital diagrams of octahedral and tetrahedral diagrams for various electronic properties.
3. Concepts of symmetry and group theory in solving chemical structural problems.
4. Use of character tables and application of group theory in spectroscopy.

UNIT-I **(13 Hrs.)**

1. Symmetry
Symmetry elements, symmetry operations, point group determination, determination of reducible and irreducible representations, character tables, use of symmetry in obtaining symmetry of orbitals in molecules qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables.

UNIT-II **(7 Hrs.)**

2. Inter Electronic Repulsions
Spin-spin, orbital-orbital and spin orbital coupling, L.S. and jj coupling schemes, determination of all the spectroscopic terms of p^n , d^n ions, determination of the ground state terms for p^n , d^n , f^nions using L.S. scheme, determination of total degeneracy of terms, order of inter electronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, term wave functions, spin orbit coupling parameters (λ) energy separation between different j states

3. Free Ions in Crystal Field of various Strengths **(10 Hrs.)**
The effect of Voct on S, P, D and F terms (with help of the character table), Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d^2 cases in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d^2 configuration in octahedral and tetrahedral fields, study of energy level diagrams for higher configurations, derivation of selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams.

UNIT-III **(13 Hrs.)**

4. Covalent Character into the Metal Ligand Bond

Construction of Molecular orbital energy level diagrams for octahedral, tetrahedral and square planar complexes showing σ and π bonding. Transformation properties of atomic orbitals, molecular orbitals for sigma and pi bonding in tetrahedral and octahedral molecules.

UNIT-IV **(9 Hrs.)**

5. Electronic Spectra of Transition Metal Complexes

Spectrochemical series, band intensities, factors influencing band widths (variation of 10Dq, vibrational structure, spin orbit coupling, low symmetry components, Jahn-Teller effect), discussion of electronic spectra of octahedral and tetrahedral $d^1 - d^9$ metal ions, calculation of 10Dq and B with and without the use of Tanabe Sugano diagrams, low spin complexes of Mn^{3+}, Mn^{2+}, Fe^{3+}, Co^{3+}, Fe^{2+}, comment on the spectra of second and third transition series, Charge Transfer spectra, comparison of d – d band with f –f spectra.

6. Magnetic Properties **(8 Hrs.)**

General discussion about magnetism in metal complexes (magnetic susceptibility, para-, dia-, ferro-, antiferro- and ferri-magnetic behavior, Curie and Curie Weiss law, magnetic properties of *d* block transition metal ions for d^1 to d^9 configuration, quenching of orbital magnetic moment, spin only magnetic moment, first order orbital contribution to the magnetic moment, orbital contribution due to spin –orbit coupling.

1. B.N. Figgis, 'Introduction to Ligand Field', Wiley Eastern, **1966**.
2. A.B.P. Lever, 'Inorganic Electronic Spectroscopy', Elsevier, **1984.**
3. R. L. Dutta and A. Syamal, 'Elements of Magnetochemistry', East-West Press Pvt. Ltd. Bangalore, **1993**.
4. J.E. Huheey& Others, 'Inorganic Chemistry: Principles of Structure and Reactivity', Harper Inter-Science, **2006.**
5. Russell S. Drago, 'Physical Method for Chemistry', W.B. Saunders Company, **1992**.
6. F.A. Cotton and G. Wilkinson, 'Advanced Inorganic Chemistry', 6th Edn., Wiley Inter- Science, **2004.**
7. F.A. Cotton, 'Chemical Application of Group Theory', 3rd Edn., Wiley Eastern, **2004**.

ORGANIC REACTION AND MECHANISM –I

Subject Code: MCHMS1-102 | **L T P C** 4 0 0 4 | **Duration: 60 (Hrs.)**

Course Objectives:

1. To familiarize with the methods determining reaction mechanism and various reaction intermediates.
2. To understand the diversity of aliphatic & aromatic nucleophilic and electrophilic reactions.
3. To understand the effect of substrate, leaving group, reaction medium and attacking reagent on substitution and free radical reaction.
4. To acquaint with the named reaction following electrophilic, nucleophilic and free radical mechanism.

Course Outcomes:

The students will acquire knowledge of:

1. Various methods to determine the mechanisms of the reactions and different reaction intermediate involved.
2. Mechanistic aspects in nucleophilic and electrophilic substitution.
3. Reaction mechanism and various factors affecting rate of free radical reactions
4. Reaction conditions, products formation and mechanisms of some named reactions.

UNIT-I (15 Hrs.)

1. Reaction Mechanism: Structure and Reactivity

Type of mechanisms, types of reactions, kinetic and thermodynamic control of reactions, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining reaction mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants.

Stereochemistry: Conformational analysis of Cycloalkanes and Decalins, Effect of conformation on reactivity, Conformation of sugars, Steric-strain due to unavoidable crowding. Elements of symmetry, Chirality, R-S nomenclature, Diastereoisomerism in Acyclic and Cyclic systems, E-Z isomerisms, Interconversion of Fischer, Newman and Sawhorse projections, Molecules with more than one chiral center, Threo and erythro isomers, Methods of resolution, Optical purity,. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape.

UNIT-II **(15 Hrs.)**

2. Aliphatic Nucleophilic Substitution

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by π- and σ-bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN1 mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis

3. Aliphatic Electrophilic Substitution

Bimolecular mechanisms- SE2 and SE1. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction.

UNIT-III **(15 Hrs.)**

4. Aromatic Nucleophilic Substitution

The SNAr, SN1, benzyne and SRN1 mechanisms, Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser, and Smiles rearrangements.

5. Aromatic electrophilic substitution

The arenium ion mechanism, orientation and reactivity in mono substitution and di-substituted aromatics, energy profile diagram, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles. Diazo coupling, Vilsmeir reaction, Gatterman-Koch reaction, Bechmann reaction, Hoben-Hoesch reaction.

UNIT-IV **(15 Hrs.)**

6. Elimination Reactions

The E2, E1 and E1cB mechanisms and their spectra. Orientation of the double bond. Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

7. Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto- oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

Recommended Text Books / Reference Books:

1. Jerry March & Michael Smith, 'March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure', 6^{th} Edn., John Wiley & Sons, **2007.**
2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structure and Mechanisms, Vol, A', 5^{th} Edn., Springer, **2007**.
3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reaction and Synthesis, Vol. B', 4^{th} Edn., Springer, **2006.**

THERMODYNAMICS AND SOLID STATE

Subject Code: MCHMS1-103 | **L T P C** 4 0 0 4 | **Duration: 60 (Hrs.)**

Course Objectives:

1. To recall concepts involved in laws of thermodynamics.
2. To introduce various thermodynamic functions.
3. To recall concept of Thermodynamic equation of state.
4. To understand various thermodynamic properties and partition function.
5. To introduce microstates, macrostates and different types of statistics.

Course Outcomes:

The students will acquire knowledge of

1. Classical thermodynamics and understanding thermodynamic phenomenon in a chemical system
2. Statistical thermodynamics and understanding thermodynamic properties in terms of partition functions
3. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics.
4. Theories of specific heat for solids.

UNIT-I **(20 Hours)**

Recall:

First law: Concept of heat, q, work, w, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, calculations of q, w, U and H for reversible, irreversible and free expansion of gases under isothermal and adiabatic conditions, Heats of reactions: standard states; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations, Second Law: Concept of entropy; statement of the second law of thermodynamics. Calculation of entropy change for reversible and irreversible processes. Free energy and chemical equilibrium. Gibbs-Helmholtz equation; Thermodynamic equation of state. Maxwell relations.

UNIT-II **(15 Hours)**

Non-ideal Systems:

Excess functions for non-ideal systems. Activity and activity coefficients and their determination. Concept of fugacity and its experimental determination. Partial molar quantities, dependence of thermodynamic parameters on composition; Gibbs-Duhem equation, chemical potential of ideal mixtures, change in thermodynamic functions in mixing of ideal gases.

Third Law of the Thermodynamics:

Identification of statistical and thermodynamic entropy. Nernst postulate, Plank's contribution. Alternate formulation of third law. Evaluation of absolute entropy. Gibbs equations for non-equilibrium systems. Clausius-Clapeyron equation. Chemical potential of ideal gases. Ideal-gas reaction equilibrium-derivation of equilibrium constant. Temperature dependence of equilibrium constant-the van't Hoff equation.

UNIT-III **(15 Hours)**

Statistical Thermodynamics:

General introduction, microstates, macrostates, thermodynamic probability. Brief introduction to different types of statistics. Ensemble concept. Canonical, grand canonical and microcanocical ensembles. Maxwell Boltzmann distribution law.

Partition Function and Thermodynamic Properties: Partition function and its factorization. Translational, rotational, vibrational; electronic and nuclear partition functions. Expressions for internal energy, entropy, Helmholtz function, Gibb's function, pressure, work and heat in terms of partition function. Thermodynamic properties of ideal gases. Vibrational, rotational, electronic and nuclear contributions to the thermodynamic properties.

UNIT-IV **(10 Hours)**

Crystal structures: Crystalline and amorphous solids, Crystal size and shapes, Space lattice and unit cell. Bravais lattices, reciprocal lattices, unit cells, Miller indices, Bragg's law, Limiting radius ratio and radius ratio rule, defects in crystals, stoichiometric defects: Shottky defect, Frenkel defect, non-stoichiometric defects: metal excess defect, metal deficiency defect, thermal defects. Line defects: edge dislocation and screw dislocation. Liquid crystals: mesomorphic state, thermotropic mesomorphism, thermography.

Recommended Text Books / Reference Books:

1. Aston and Fritz, 'Thermodynamic and Statistical Thermodynamics', John Wiley & Sons, Inc., 1959.
2. Lee, Sears and Turcotte,'Statistical Thermodynamics', Addison-Wesley Publishing Company 1963.
3. Dickerson, 'Molecular Thermodynamics', Benjamin-Cummings Publishing Company, 1969.
4. Glasstone, 'Thermodynamics for Chemists', EWP,2008.
5. R. C. Srivastva, S. K. Saha, A. K. Jain, 'Thermodynamics: A Core Course', PHI, 2007.
6. P. Atkins, J. D. Paula, 'Physical Chemistry', 7thIndian Edn.,Oxford University Press, 2007.
7. R. P. Rastogi& R. R. Mishra, 'An Introduction to Chemical Thermodynamics',6thEdn., Vikas Publishing House, 2007.

COMPUTATIONAL SKILLS AND SIMULATIONS IN CHEMISTRY

Subject code: MCHMD1-111 **L T P C** **Duration: 60 Hrs.**
4 0 0 4

Course Objectives

1. To learn principles of computational chemistry and computer-based molecular design.
2. 2. To understand the basic concepts of molecular mechanics, semi-empirical method and density-functional theory.
3. To familiarize with different software packages, including MOLDEN for general model building.
4. To understand GAMESS Gaussian for quantum chemical calculations, and BOSS for liquid simulations.

Course Outcomes

The students will acquire knowledge of

1. Advantages and principle of computer based calculation methods in chemistry
2. Fundamentals of various calculation methods viz: molecular mechanics, semi-empirical method and density-functional theory.
3. Running calculation and model building using different algorithms in software packages, like Hyperchem, Gaussian
4. Quantum mechanical calculations in gaseous phase with GAMESS and Liquid simulations in BOSS

UNIT – I **(15 Hrs.)**

1. **OVERVIEW OF THE COURSE**
   Promises of computational chemistry, molecular mechanics of bond vibrations. Minimization methods, forces in polyatomic molecules, intermolecular forces, parameterization and testing of force fields, docking.

2. **MONTE CARLO METHOD (4 Hrs.)**
   Principles, chemical & biochemical applications.

UNIT – II **(15 Hrs.)**

3. **MO THEORY**
   Foundations, semi-empirical MO theory, Ab Initio MO Theory: Basis Sets; Hartree–Fock theory: Principles and applications.

UNIT – III **(15 Hrs.)**

4. **TREATMENT OF ELECTRON CORRELATION**
   MCSCF, CI methods, Treatment of electron correlation: MP and CC methods.

UNIT – IV **(15 Hrs.)**

5. **SPECTROSCOPY**
   Vibrational spectroscopy and gas phase thermodynamics, description of electronically excited states. Description of solvent effects.

6. **DENSITY FUNCTIONAL THEORY (DFT)**
   Principles, applications in materials. Transition states in gas phase reactions.

Recommended Books

1. Peter Comba, Trevor W. Hambley, 'Molecular Modelling of Inorganic Compounds', John Wiley & Sons, **2009**.
2. F. Jensen, 'Introduction to Computational Chemistry', John Wiley & Sons, **1998**.
3. Warren J. Hehre, 'A Guide to Molecular Mechanics and Quantum Chemical Calculations', **2003.**
4. H.D. Holtje, W. Sippl, D. Rognan, G. Folkers, 'Molecular Modeling: Basic Principles and Applications', Wiley, **2008**.
5. Christopher Cramer, 'Essentials of Computational Chemistry, Theories & Models', 2nd Edn., Wiley, **2002**.

6. Note: Freely available packages like GAMESS, MOLDEN, AVOGADOOS, MOPAC may be used for computational Lab.

POLYMER CHEMISTRY

Subject Code: MCHMD1-112 **L T P C 4 0 0 4** **Duration: 60 Hrs.**

Course Objectives

1. To impart knowledge about polymers and polymerization mechanism.
2. To understand the difference between crystalline and amorphous polymers.
3. To familiarize polymer characterization with various spectroscopic techniques.
4. To learn molecular weight measurement by osmometry, mass spectrometry and Viscometry.

Course Outcomes:

The students will acquire knowledge of

1. Properties of polymers and polymerization mechanism.
2. Polymer morphology and characterization of polymers with spectroscopic techniques.
3. Advantages and disadvantages of polymer composites.

UNIT-I (15 Hrs)

1. INTRODUCTION TO POLYMERS

IUPAC nomenclature of vinyl, non-vinyl polymers, copolymers and end groups. Abbreviations for polymers. Introduction to industrial polymers-plastic thermoplastic- & thermosetting plastics), fibres (commonly used natural & synthetic fibre).

2. POLYMERIZATION MECHANISMS

Mechanism of free radical chain polymerization & ionic chain polymerization-initiators, inhibitors & stereochemistry. Mechanism of coordination chain polymerization (Ziegler-Natta, Cossee), polycondensation step polymerization, polyaddition step polymerization & ring opening step polymerization.

UNIT-II (15 Hrs)

1. KINETICS OF POLYMERIZATION MECHANISMS

Kinetics of free radical chain polymerization, ionic chain polymerization, catalyzed and non-catalyzed polycondensation polymerization including kinetic chain length, chain transfer reactions.

2. AVERAGE MOLECULAR WEIGHT OF POLYMERS

Number average molecular weight – its measurement by osmometry (membrane & vapour phase), end group analysis, mass spectrometry. Weight average molecular weight – its measurement by light scattering method (dissymmetry method & Zimm plot method).

Viscosity average molecular weight – its measurement by viscometry. Determination of molecular weight distribution by gel permeation chromatography (size exclusion chromatography).

UNIT-III (15 Hrs.)

1. CHEMICAL STRUCTURE & POLYMER MORPHOLOGY

Macrostructure of polymers. Geometrical isomerism & optical isomerism, Tacticity, degree of crystallinity, liquid crystallinity, crystallizability, crystallites (bundles),spherulites, polymer single (ideal) crystals. Glass transition temperature-concept of glassy state, viscoelastic state, viscofluid state for amorphous and crystalline substances including polymers. Specific volume change vs temperature curves.

a. POLYMER PROPERTIES

Mechanical properties - tensile strength, compressive strength, flexural strength, impact strength, toughness, fatigue, yield point, elongation at break, tensile modulus, relaxation & retardation (creep) phenomena. Thermal stability, flammability & flame resistance, chemical resistance, degradability, electrical conductivity, nonlinear optical properties.

Polymer additives to modify mechanical, surface, chemical, aesthetic & processing properties.

UNIT-IV (15 Hrs.)

1. FIBRES REINFORCED POLYMER COMPOSITES

Introduction to composites. Polymer matrix materials & fibres reinforcement. Types of fibres- glass, aramid & silica fibres. Advantages & disadvantages of polymer composites.

2. CHARACTERIZATION TECHNIQUES OF POLYMERS

Infrared, Raman, NMR, ESR, UV-Vis, fluorescence studies. X-ray scattering, SEM, thermal- DSC, DTA, TMA, TGA studies.

Recommended Books

1. D. Campbell and J.R. White, 'Polymer Characterization: Physical Techniques'**,** Chapman and Hall, New York, **1989**.
2. Malcolm P. Stevens, 'Polymer Chemistry: An Introduction'**,** 3rd Edn., Oxford University Press, Indian Edn,, Reprint, **2011**.
3. A.H. Fawcett, 'Polymer Spectroscopy'**,** Wiley, New York, **1996**.
4. R.J. Young, 'Spectroscopy of Polymers'**,** Wiley, New York, **1996**.
5. M. Lewin, S.M. Atlas, E.M. Pearce, 'Flame Retardant Polymeric Materials'**,** Plenum Press, New York, **1975**.
6. E.M. Pearce, Y.P. Khanna, D. Raucher, 'Thermal Characterization of Polymeric Materials'**,** Academic Press, New York,**1981.**
7. I.M. Ward, 'Mechanical Properties of Polymers'**,** Wiley Interscience, New York, **1971**.
8. Jan M. Gooch, 'Encyclopedic Dictionary of Polymers'**,** Springer, **2007**.
9. Anita J. Brandolini, Deborah D. Hills, 'NMR Spectra of Polymers & Polymer Additives'**,** Marcel Dekker, New York, **2000**.
10. Fred W. Wilmeyer, 'Text Book of Polymer Science'**,** A. Wiley Intersciense Publication, 1994.
11. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar; 'Polymer Science'**,** New Age International, **1986**.

CHEMICAL KINETICS AND ELECTROCHEMISTRY

Subject Code: MCHMD1-113 | **L T P C** 4 0 0 4 | **Duration: 60 (Hrs.)**

Course Objectives:

1. To introduce the concept of activation energy.
2. To introduce various theories of reaction rates.
3. To familiarise with the methods of determining rate laws.
4. To understand kinetics of various complex reactions.
5. To introduce various theories of electrolytic solutions and electrolytic conductance.

Course Outcomes:

The students will acquire knowledge of

1. Kinetics of various complex reactions and their rate laws.
2. Activation energy and kinetics of reaction.
3. Electrolytic solution and conductance.
4. Interfacial electrochemistry

UNIT-I (18 Hrs.)

Recall of basic concepts of chemical kinetics, methods of determining rate laws, Arrhenius equation, the concept of activation energy, theoretical calculation of energy of activation, collision and transition state theories of rate constants.

Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type). Kinetics of chain reactions, steady state approximation; determination of reaction mechanisms; detections of radical and kinetics of HBr, H_2O_2 reactions, explosion limits, The Eyring equation. Unimolecular reactions and Lindemann's theory, application of following to the reaction kinetics: solvent effect, kinetic isotope effect and salt effect, kinetics of acid, base and enzyme catalysis, Hinshelwood mechanism of catalysis.

UNIT-II (12 Hrs)

Electron transfer in homogeneous systems, theory of electron transfer processes, electron tunneling, electron transfer in heterogeneous systems, electrode-solution interface, rate of charge transfer in electrode reactions, study of kinetics of electrode processes.

UNIT-III (15 Hrs)

Concept of activity and activity coefficients in electrolytic solutions. The mean ionic activity coefficient. Debye-Huckel theory of electrolytic solutions. Debye-Huckel limiting law (derivation not required). Calculation of mean ionic activity coefficient. Limitations of Debye-Huckel theory. Extended Debye-Huckel law.

Theory of electrolytic conductance. Derivation of Debye-Huckel-Onsager equation – its validity and limitations.

Concept of ion association – Bjerrum theory of ion association (elementary treatment)-ion association constant – Kohlrausch's law and its applications

UNIT-IV (15 Hrs)

Electrochemistry: Nernst equation, redox systems, Chemical and concentration cells (with and without transference). Liquid junction potential (LJP) – derivation of the expression for LJP – its determination and elimination**.** Methods of determining structures of electrified interfaces, Guoy-Chapman, Stern. Types of electrodes. Applications of EMF measurements:

Solubility product, potentiometric titrations.
Decomposition potential and its significance. Electrode polarization – its causes and elimination. Concentration over-potential.

Recommended Text Books / Reference Books:

1. P. Atkins, J. D. Paula, 'Physical Chemistry', 7thIndian Edn.,Oxford University Press, 2007.
2. Ira N. Levine, 'Physical Chemistry', McGraw Hill, 2008.
3. D.A. McQuarrie and J.D. Simon, 'Physical Chemistry-A Molecular approach', University Science Books, 1997.
4. J. Rajaraman and J. Kuriacose, 'Kinetics and Mechanism of Chemical Transformations', McMillan, 2011.
5. S. Glasstone, 'Introduction to Electrochemistry', Litton Educational Publishing, 2011.
6. J. O. M. Bockris& A. K. N. Reddy, 'Modern Electrochemistry', Plenum, 1973.
7. E.S. Amis, 'Solvent Effect of Reaction Rates and Mechanism', Academic Press, 1966.
8. K.J. Laidler, 'Chemical Kinetics', McGraw Hill, 1965.

INORGANIC CHEMISTRY LAB-I

Subject Code: MCHMS1-104 **L T P C** **Duration: 60 (Hrs.)**
0 0 4 2

Course Objectives

1. To develop basic understanding of various lab practices including safety measures.
2. To synthesize inorganic complexes and their characterization.

Course Outcomes:

The students will acquire knowledge of:

1. Volumetric and gravimetric analysis of cations and anions.
2. Understand complexometric and redox titrations.
3. Syntheses of various complexes and their structural analysis

Note:

1. Students will have to perform atleast 10-12 experiments from the given syllabus.

2. Any other subject related experiment can also be included.

EXPERIMENTS

1. Preparation of coordination compounds, their purification by chromatography and elucidation of structures by physical methods (UV, IR, NMR, magnetic susceptibility etc.)

a. Synthesis of Tris(acetylacetonato)manganese(III), $Mn(acac)_3$ and their characterization.
b. Synthesis and Characterization of Hexamminechromium(III) nitrate $[Cr(NH_3)_6](NO_3)_3$ using magnetic susceptibility balance (MSB) and IR spectroscopy (Green Preparation).
c. Synthesis of Iron(III) dithiocarbamate and its characterization using magnetic succeptibility balance (MSB) and IR spectroscopy.
d. Synthesis and characterization of nitro- and nitritopentamminecobalt(III) chlorides using IR spectroscopy.
e. Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride.
f. Synthesis of cis- and trans- potassiumdioxalatodiaquochromate(III).

2. Complexometric Titrations

a. Determination of calcium in the presence of magnesium using EDTA as titrant
b. Determination of the total hardness (permanent and temporary) of water
c. Determination of calcium in the presence of barium using EDTA as titrant.

3. Redox Titrations:

a. Determination of chlorate, preparation of 0.1M cerium(IV) sulphate.
b. Determination of copper, determination of dissolved oxygen.

Recommended Books

1. H. Denny, W. Roesky, 'Chemical Curiosites', Wiley VCH,1996.
2. G. Marr and B.W. Rocket, 'Practical Inorganic Chemistry', University Science Books, **1999.**
3. G. Pass and H. Sutcliffe, 'Practical Inorganic Chemistry', 2nd Edn., Chapman and Hall, London, **1974.**
4. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Textbook of Quantitative Analysis', 5th Edn., Pearson Education, **2006.**
5. G. Svehla, 'Vogel's Textbook of Quantitative Analysis', Pearson Education, **2006.**

6. Anil J. Elias, 'A Collection of Interesting General Chemistry Experiments', Orient Longman Ltd., Universities Press (India) Pvt. Ltd., **2008**.
7. http://dst.gov.in/green-chem.pdf

ORGANIC CHEMISTRY LAB-I

Subject Code: MCHMS1-105 **L T P C** **Duration: 60 (Hrs.)**
0 0 4 2

Course Objectives

1. To learn the skills of distillation and separation
2. To impart knowledge of synthesis of organic compounds
3. To develop experimental skills of various purification techniques.

Course Outcomes:
The students will acquire knowledge of:

1. Distillation and separation methods
2. Chromatographic methods
3. Synthesis of various organic compounds and their structural analysis

Note:

1. Students will have to perform atleast 10-12 experiments from the given syllabus.

2. Any other subject related experiment can also be included.

1. Distillation & Separation
   a. To purify common organic solvents
   b. Extract rose oil from rose petals by steam distillation.

2.. Thin Layer Chromatography (TLC):
   a. Identification of phytoconstituents
   b. To check TLC purity of Acetaminophen, Aspirin, Caffeine, Phenacetin and Salicylamide after completion of reactions.

3. Organic Analysis:

Detection of common functional groups in the given organic compounds and identification of compounds through derivatives.

4. Organic Preparations:
   a. Benzoylation: Hippuric acid
   b. Oxidation: Adipic acid/p-Nitrobenzoic acid
   c. Aldol condensation: Dibenzalacetone/Cinnamic acid
   d. Sandmeyer's reaction:p-Chlorotoluene
   e. Benzfused Heterocycles:Benzimidazole
   f. Cannizzaro's reaction: p-Chlorobenzaldehyde as substrate
   g. Friedel Crafts reaction: S-Benzoylpropionic acid
   h. Aromatic electrophilic Substitution:p-Nitroaniline/p-Iodoaniline

Recommended Books

1. David T. Plummer, 'An Introduction to Practical Biochemistry', 3rdEdn., TataMcGraw Hills, **1998**.
2. A.I. Vogel, 'Text Book of Practical Organic Chemistry', 5thEdn., PearsonEducation, **2005**.
3. P.R. Singh, D.S. Gupta and K.S. Bajpai, 'Experimental Organic Chemistry', Vol. 2, Tata McGraw Hill, **1981**.
4. G. Mann, B.C. Saunders, 'Practical Organic Chemistry' ELBS Edn,,**1989**.

N.K. Vishnoi, 'Advanced Practical Organic Chemistry', 2nd Edn.,Vikas PublishingHouse Pvt. Ltd.,**1994.**

Total Credits= 23

2nd Semester		Contact Hrs.			Marks			Credits
Code	**Name**	**L**	**T**	**P**	**Int.**	**Ext.**	**Total**	
MCHMS1-201	Molecular Spectroscopy-I	4	0	0	40	60	100	4
MCHMS1-202	Organometallics	4	0	0	40	60	100	4
MCHMS1-203	Organic Reactions & Mechanisms-II	4	0	0	40	60	100	4
MCHMS1-204	Seminar - I	0	0	2	100	--	100	1
Departmental Elective-II (Choose any one)		4	0	0	40	60	100	4
MCHMD1-211	Nano Chemistry							
MCHMD1-212	Bio-organic Chemistry							
MCHMD1-213	Analytical Chemistry							
Departmental Elective-III (Choose any one)		4	0	0	40	60	100	4
MCHMD1-221	Natural Products							
MCHMD1-222	Bio-physical Chemistry							
MCHMD1-223	Asymmetric Synthesis							
MCHMS1-205	Inorganic Chemistry Lab.-II	0	0	4	60	40	100	2
Total		**20**	**0**	**06**	**360**	**340**	**700**	**23**

MOLECULAR SPECTROSCOPY-I

Subject Code: MCHMS1-201	L T P C	Duration: 60 (Hrs.)
	4 0 0 4	

Course Objectives:
1. To introduce the concept of spectroscopy, selection rules, line width and broadening.
2. To familiarize with concepts of Microwave and Raman Spectroscopy
3. To provide the knowledge of concepts of Infrared and UV-visible Spectroscopy
4. To familiarize with concepts of NQR, Mossbauer and photoelectron Spectroscopy

Course Outcomes:
The students will acquire knowledge of

1. Selection rules, line width and broadening.
2. Various spectroscopic techniques.
3. Importance of spectroscopy for structural elucidation.

UNIT-I (15 Hours)

General Features of Spectroscopy
Introduction to spectroscopy, Nature of electromagnetic radiation, Regions of the electromagnetic spectrum Units and conversion factors, Intensities line width and line width broadening of spectral lines, transition probability, transition moment and selection rules

Microwave Spectroscopy
Classification of molecules according to their moment of inertia, Rotational spectra of rigid diatomic molecules, Intensities of spectral lines, isotopic substitution effects. Non-rigid rotator, Polyatomic molecules – Linear and symmetric top molecules, Stark effect

Raman Spectroscopy

Introduction, Classical and Quantam theory of Raman effect, Stokes and antistokes lines, anisotropic polarizability, Pure rotational raman spectra of linear and symmetric top molecules, vibrational raman spectra of H_2O and CO_2 molecules, Polarisation of the light and raman effect, Rule of mutual exclusion

UNIT-II (15 Hours)

Infrared Spectroscopy

Energy of vibrating diatomic molecule, simple harmonic oscillator, force constants, Fundamental vibration frequencies, Anharmonicity of molecular vibrations and its effect on vibrational frequencies, Frequencies of the vibrational transitions of HCl. Vibrational rotation spectra of CO, P, Q and R branches, Vibrations of polyatomic molecules. Examples of CO_2, H_2O, Mechanics of measurement of infrared and Raman spectra, absorption of common functional groups, their dependence onchemical environment (bond order, conjugation, H – bonding), Use of group theory to determine the number of active infrared and Raman active lines. Fermi resonance, combination bands and overtones, Infrared spectrometer, Application of IR in structure elucidation of organic compounds – Various Carbonyl compounds, alkane, alkenes, alkynes, unsubstituted, mono and di-substituted aromatic compounds, alcohols, phenols, ethers, Far IR region, Metal ligand vibrations, – CN, Nitro-nitrito- and CO ligands and the effect of their co-ordination with metal ions and IR spectra.

UNIT-III (14 Hours)

UV and Visible Spectroscopy

Measurement technique, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra. Chromophores, auxochromes, electronic spectra of polyatomic molecules, Woodward rules for conjugated dienes and α, β- unsaturated carbonyl groups, extended conjugated and aromatic sterically hindered systems, red shift, blue shift, hypo- and hyperchromic effect.

UNIT-IV (16 Hours)

Mossbauer Spectroscopy

Mossbauer effect, Principles of Mossbauer spectroscopy, Formation of Mossbauer nuclides, Applications of Mossbauer spectroscopy

Photoelectron Spectroscopy

Introduction, Basic principles of electron spectroscopy, Photoelectric effect, Koopman's theorem, X-ray photoelectron spectroscopy (XPS) or ESCA, Instrumentation for XPS, chemical shifts in XPS, applications of XPS, ultraviolet photoelectron spectroscopy (UPS)

Nuclear Quadrupole Resonance

Introduction- quadrupole nuclei and quadrupole moment, experimental considerations, Electric Field Gradient (EFG), quadrupole coupling constant (QCC), Splitting in NQR spectra, Applications of NQR spectroscopy

Recommended Text Books / Reference Books:

1. Russell S. Drago, 'Physical Method for Chemistry', 2nd Edn., Surfside Scientific Publishers,**1992.**
2. R.M. Silverstein, G.C. Bassler, T.C. Morrill, 'Spectrometric Identification of Organic Compounds', 3rd Edn., Wiley,**1974**.
3. William Kemp, 'Organic Spectroscopy', 3rd Edn., W.H. Freeman,**1991**.
4. Dudley H. Williams & Ian Fleming, 'Spectroscopic Methods in Organic Chemistry', 6th Edn., McGraw Hill, Science,**2008.**
5. J.R. Dyer, 'Application of Absorption Spectroscopy of Organic Compounds', Prentice Hall, Englewood Cliffs, N.J.,**1965**.
6. Dudley H. Williams & Ian Fleming, 'Spectroscopic Problems in Organic Chemistry', 5th Edn., McGraw Hill, London,**1985**.
7. R.C. Banks, E.R. Matjeka, G. Mercer, 'Introductory Problems in Spectroscopy' Manlo Park, CA,**1980**.
8. G.M. Barrow, 'Introduction to Molecular Spectroscopy', McGraw Hill, New York,**1962**.
9. C.N. Banwell 'Fundamentals of Molecular Spectroscopy' 4th Edn., TataMcGrawHill Education,**1994**.
10. D.L. Pavia, G.M. Lampan and G.S. Kriz, 'Introduction to Spectroscopy', 4th Edn., Cengage Learning, **2008**.
11. Jag Mohan, 'Organic Spectroscopy-principles and applications', 2nd Edn., Narosa Publishing house Pvt. Ltd., **2007**
12. P S Sindhu, 'Fundamentals of Molecular spectroscopy' 2nd Edn., New age international Publishers. **2011**

ORGANOMETALLICS

Subject Code: MCHMS1-202 **L T P C** **Duration: 60Hrs.**
4 0 0 4

Course Objectives

1. To recall classification of ligands and nomenclature of organometallic compounds.
2. To understand structure, bonding and reactivity of organometallic compounds.
3. To familiarize with the role of organometallic compounds in organic syntheses.
4. To understand the applications of organometallic compounds ascatalysts.

Course Outcomes:

The students will acquire knowledge of

1. Organometallic compounds and their nomenclature.
2. Bonding and reactivity of metal complexes.
3. Role of organometallic complexes in organic syntheses.
4. Importance of catalyst in syntheses.

UNIT-1 (11 Hrs.)

Introduction- Stability & decomposition pathways, classification of ligands, nomenclature of Organometallic compounds.

18 valence electron rule- Introduction to the 18 valence electron rule, total electron counts and finding metal-metal bonds & related problems.

UNIT-II (17 Hrs.)

Synthesis, structure, bonding & reactivity of organo transition metal complexes.

a) Carbenes, Carbynes, Alkenes, Alkynes, Allylmoieties, Butadiene, Cyclobutadiene, Cyclopentadiene, Arenes, Cycloheptadienylmoieties & Cyclooctatetraenemoieties, Carbonyl.
b) Ferrocenes- Structure & bonding of ferrocenes, basic chemical reactions of ferrocenes, chirality in ferrocene derivatives, ferrocene based condensation polymers.

UNIT-III (16 Hrs.)

Organometallic compounds in organic Synthesis-Green rules, synthesis & use of Zinc dialkyls, Collaman's reagent, organ mercuric& chromium carbonyls in organic synthesis, Heck reaction, Hydrozirconation.

UNIT-IV (16 Hrs.)

Applications of organometallic complexes to Catalysis-Basic principles, Industrial requirements of catalysts, sequences involved in catalytic reaction, asymmetric synthesis using catalyst, Hydrogenation catalysts & their classification, hydrogenation by lanthanide organometallic compounds. Hydro formylation: Cobalt catalyst & phosphine modified cobalt catalysts, Rhodium-phosphine catalysts, factors affecting n/iso ratio of hydro formylation products. Monsato, Cativa & Wacker processes, polymerization & oligomerisation of olefins & dienes, catalyticconverters.

Recommended Books

1. 'Basic Organometallic Chemistry: Concepts, Synthesis & Application ofTransition Metals', CRC Press & Univ. Press, **2010**.
2. R.C. Mehrotra & A, Singh, 'Organometallic Chemistry, A Unified Approach', New Age International.
3. B.D. Gupta & A.J. Elias, 'Basic Organometallic Chemistry', UniversitiesPress.
4. F.A. Cotton & G. Wilkinson, 'Advanced Inorg, Chemistry', WileyInterssciences.

ORGANIC REACTION AND MECHANISM –II

Subject Code:MCHMS1-203 **L T P C** **Duration: 60 (Hrs.)**

4 0 0 4

Course Objectives:

1. To acquire the knowledge of addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds
2. To understand the chemistry behind elimination, oxidation and reduction reactions.
3. To know the concepts of rearrangement reactions.
4. To acquire the knowledge and use of various reagents and retro synthetic approach used in organicsyntheses.

Course Outcomes:

The students will acquire knowledge of

1. Chemistry behind oxidation, reduction and Carbon-Carbon multiple bond reactions
2. Chemistry behind rearrangement reactions.
3. Use of diverse reagents in organicsynthesis
4. Retro synthetic approach in organic synthesis

UNIT-I (15 Hrs.)

1. Addition to Carbon-Carbon and Carbon-Hetero Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gillman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction, Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis ofesters.

UNIT-II (15 Hrs.)

2. Oxidation :

Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups) activated and inactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides.

Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villeger reaction, Cannizarro oxidation-reduction reaction.

UNIT-III (15 Hrs.)

3. Reduction :

Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyano borohydride, LAH, disobutylaluminium hydride, tin hydride, trialkyl tin hydride, trialkylsilanes, alkoxy substituted LAH, DIBAL, diborane, diisoamyl borane, hexyl borane, 9-BBN, isopinocamphenyl and disiopinocamphenyl borane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemmensen reduction,

UNIT-IV (15 Hrs.)

4. **Rearrangements :**
General mechanistic consideration – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement

5. **Retrosynthesis:**
Synthons and synthetic equivalents, Definitions, Guidelines, Functional group interconversions, Use of acetylenes and aliphatic nitrocompounds in organic synthesis; Two-group C-C disconnections – Diels-Alder reaction, 1,3- and 1,5-difunctional compounds (Michael addition and Robinson annulation), Order of events in organic synthesis, Chemoselectivity, Reversal of polarity (umpolung), Cyclisation reactions, Amine synthesis

Recommended Text Books / Reference Books:

1. Jerry March & Michael Smith, 'March's Advanced Organic Chemistry:Reactions, Mechanisms, and Structure', 6th Edn., John Wiley &Sons,**2007**.
2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structureand Mechanisms, Vol, A', 5th Edn., Springer,**2007**.
3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reactionand Synthesis', Vol. B, 4th Edn., Springer,**2006.**
4. K.C. Nicolaou and E.J. Sorensen, 'Classics in Total Synthesis: Targets, Strategies, Methods', Wiley,**1996**.

SEMINAR – I

Subject Code: MCHMS1-204	L T P C 0 0 2 1	Duration: 30 Hrs.

1. In the beginning of the semester, a teacher will be allocated maximum 30 students. The latter will guide/teach them how to prepare/present 15 minutes Power Point Presentation for the Seminar.

2. If there are more than 30 students in the class, then class will be divided into two group shaving equal students. Each group may be allocated to a different teacher.

3. Each student will be allotted a topic by the teacher at least one week in advance for the presentation. The topic for presentation may be from the syllabus or relevant to the syllabus of the program.

4. During the presentation being given by a student, all the other students of his/her group will attend the seminar. The assessment/evaluation will be done by the teacher. However, Head of Department and other faculty members may also attend the seminar, ask questions and give their suggestions.

5. This is a turn wise continuous process during the semester and a student will give minimum two presentations in a semester.

6. For the evaluation, the following criteria will be adopted,
a) Attendance in seminar: 25 Marks
b) Knowledge of subject along with Questions handling during the seminar: 25 Marks
c) Presentation and communication Skills: 25 Marks
d) Contents of the presentation: 25 Marks.

NANOCHEMISTRY

Subject Code: MCHMD1-211 **L T PC** **Duration: 60 Hrs.**
4 0 0 4

Course Objectives

1. To understand the concept of self-assembly and its applications to various nanostructures.
2. To understand synthesis of nanomaterials.
3. To learn characterization of nanomaterials.
4. To understand the applications of nano materials in biologicalsystem.

Course Outcomes:

The students will acquire knowledge of

1. Introduction to the concept of nanochemistry and its classification andterminology.
2. Synthesis of nanomaterials by different routes and their characterization.Applications in biological and electronic systems.

UNIT-I(15Hrs)

1. Introduction:
Introduction to nanochemistry and nanotechnology, definition & classification of nanomaterials. Properties & applications of nanomaterials.

2. Self-Assembly and Nanostructures:
Types of self-assemblies, self-assembling materials. Use of self-assembly in nano rod devices, nano wires, nano tubes, molecular logic gates, molecular storage devices, DNA, fullerenes, nano gas sensors.

UNIT-1I(15Hrs.)

3. Nano Material Synthesis:
Top down and bottom up approach, synthesis: Vapour phase synthesis by chemical routes; Nucleation & growth from solutions, stabilization against agglomeration. Processing of nano materials; Nano structured sol gel materials. Consolidation of nano crystalline materials by compaction and sintering, nanolithography.

UNIT-1II(15Hrs.)

4. Characterization Techniques:
Characterization of nano structured materials – by scattering techniques, proximal microscopy (AFM & STM).

UNIT-1V(15Hrs.)

5. Applications:
Bionano composites, biometrics, nano technology enabled sensors, Microelectronics,

drug delivery, bionano information.

Recommended Books:

1. C.P. Poole & F.J. Owens, 'Introduction to Nanotechnology', Wiley,**2003**.
2. M. Ratner & D. Ratner, 'Nanotechnology'**,** Prentice Hall,**2003**.
3. M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse 'Nanotechnology'**,** CRC Press BocaRaton,**2002**.
4. A. Ozin Geoffery & C. Andre, 'Nanochemistry, A Chemical Approach to Nanomaterials'**,**Arsenault Royal Society of Chemists,**2005**.
5. E. Foster Lynn, 'Nanotechnology, Science Innovation & Opportunity', Pearsoneducation,2007.

BIO-ORGANICCHEMISTRY

Subject Code: MCHMD1-212 **L T PC** **Duration: 60 Hrs.**

4 0 0 4

Course Objectives

1. To illustrate the link between organic chemistry and biochemistry by discussing the organic chemistry of selected processes of living systems.
2. To integrate the chemical principles with biological applications with examples drawn from biochemistry, molecular and cellbiology.
3. To understand the mechanism of enzymecatalysis.
4. To understand the mechanism of combinatorial synthesis in medicinal chemistry.

Course Outcomes:

The students will acquire knowledge of

1. Relationship between organic chemistry and biochemistry.
2. Kinetics and mechanism of enzyme catalysis.
3. Determination of enantio- and diastereoselectivity using various analytical methods

UNIT-1 (15 Hrs.)

Amino Acids and Proteins:

Structure, classification, synthesis and properties of amino acids, isoelectric point, biosynthesis of amino acids. Peptides: oligo- and polypeptides, geometry of peptide linkage, N-terminal and C-terminal residue analysis, synthesis of peptides-amino and carboxyl protecting groups-solid phase peptide synthesis. Proteins: classification and properties (denaturation, isoelectric point and electrophoresis), primary, secondary, tertiary and quaternary structures of proteins, collagen and triple helix.

UNIT-1I (15 Hrs.)

Enzymes and Cofactors:

Mechanism of enzyme catalysis, Factors influencing enzyme action, Examples of typical enzyme mechanisms: chymotrypsin, ribonuclease and lysozyme, Enzyme-catalyzed addition, elimination, condensation, carboxylation and decarboxylation, isomerization, group transfer and rearrangement reactions-structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid and Vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

UNIT-III (15 Hrs.)

Nucleic Acids and Protein Synthesis:

Nucleotides and nucleosides, DNA: primary and secondary structure-replication of DNA. RNA and protein synthesis: Messenger RNA synthesis-transcription, Ribosomes-rRNA, Transfer RNA, genetic code translation.

Determination of base sequence of DNA. Polymerase Chain Reaction (PCR). Antisense technology in chemotherapy and other nucleic acid-targeted drugs-intercalates, sequence specific drugs. A brief account of ribozyme and iRNA.

UNIT-IV (15 Hrs.)

Lead and Analogue Synthesis-1:

Designing organic synthesis-disconnection approach- synthons and synthetic equivalents-one group disconnections: alcohol, olefin, ketone, acids- two group disconnections:1,2-, 1,3-, 1,4- and 1,5-difunctional compounds-convergent synthesis-functional group interconversions- functional group additions-carbon heteroatom bonds-methods for 3- to 6-membered rings.

Lead and Analogue Synthesis-2:

Combinatorial synthesis in medicinal chemistry: Solid phase techniques-methods of parallel synthesis-mix and split techniques-dynamic combinatorial chemistry-screening and deconvolution-limitations of combinatorial synthesis Asymmetric synthesis: basic principles-stereo selective and stereospecific reactions- methods for determining enantiomeric excess-chiral auxiliary, reagents and catalysts and their applications (wherever applicable) in alkylation, hydrogenation, hydroxylation, epoxidation and hydroboration of alkenes, reduction of ketones-Cram and Felkin-ahn models. Noyori’s BINAP – Jacobson catalyst – Evans catalyst.

Recommended Books:

1. Hermann Dugas and C. Penny, ‘Bioorganic Chemistry: A Chemical Approach to Enzyme action’,Springer-Verlag.
2. N.C. Price and L. Stevens, ‘Fundamentals of Enzymology’, Oxford UniversityPress.
3. C. Walsh, W.H. Freeman, ‘Enzymatic ReactionMechanisms’.
4. Stuart Warren, ‘Designing Organic Synthesis: The Disconnection Approach’, 2ndEdn., Wiley,**1984**.
5. H.B. Kagan, ‘Asymmetric Synthesi’, Thieme Medical Publishers,**2003**.
6. Francis A. Carey and Richard B. Sundberg, ‘Advanced Organic Chemistry: Part-A and Part-B’, 5th Edn., Springer,**2007**.

ANALYTICAL CHEMISTRY

Subject Code: MCHMD1-213	**L T P C**	**Duration: 60 (Hrs.)**
	4 0 0 4	

Course Objectives:

1. To learn the theory and importance of analyticalchemistry.
2. To acquire knowledge about various methods of quantitative estimations.
3. To know the methods of analyzing the chemicals applying the electroanalytical and thermogravimetric instruments.
4. To know the methods of separating the mixture of compounds by chromatographic techniques.
5. To get familiar with various microscopic and radiochemical methods of analysis.

Course Outcomes:

The students will acquire knowledge of:

1. Basic concepts and importance of analytical chemistry.
2. Significance of significant figures and data analysis.
3. Thermogravimetric, electroanalytical, chromatographic and radiochemical methods of analysis.
4. Electron microscopic techniques and their application

UNIT-I (18 Hrs.)

Introduction to Analytical Chemistry

Classification of Analytical Methods. Types of samples, Preparation of sample for analysis, effect of sampling uncertainties, sample treatment, procedure of sampling of solids, liquids and gases.

Errors and Evaluation

Accuracy, precision, sensitivity, detection limits, significant figures, rounding off noise and sources, Uncertainties, errors. Types of errors – determinate and indeterminate errors. Ways of expressing accuracy, absolute and relative errors. Significant figures and propagation of errors. Confidence limit, Test of significance – the F-test and T-test. The statistical Q-test for rejection of a result, calibrations, mean, standard deviations. Linear least squares method. The correlation coefficient. Calculation for the above parameters.

Thermo analytical Techniques

Principle of thermogravimetry, thermogravimetric analysis, differential thermal analysis, differential scanning calorimetry, instrumentation for TGA, DTA and DSC, Methodology of TG, DTA and DSC. Application of TG to study of oxalates and chromates, factors affecting TGA and DTA curves. Applications of thermal analysis.

UNIT-II (15 Hrs.)

Electrochemical Techniques

a) D.C Polarography: Instrumentation - Dropping mercury electrode- -polarogram. Types of Currents: Residual, Migration, Limiting. Two and Three electrode assemblies. Ilkovic equation (derivation not required). Applications of polarography in qualitative and quantitative analysis. Analysis of mixtures. Application to inorganic and organic compounds. Determination of stability constants of complexes.

b) Brief account of following techniques:

(i) Pulse technique (ii) Differential pulse technique (iii) Cyclic Voltammetry (iv) Square-wave technique

c) Amperometric titrations: Principle, Instrumentation. Types and applications amperometric titrations.

Chromatography

Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory HPLC: Principle, instrumentation, supports in HPLC. Applications of HPLC systems. Supercritical fluid chromatography (SFC). Recent developments in SFC and applications.

UNIT-III (12 Hrs.)

Microscopy Techniques

Basic principle, instrumentation and applications of electron microscopy - SEM, TEM, scanning probe microscopy – STM, AFM.

Cryo-electron microscopy

Principle, instrumentation and applications, advantages and challenges, cryo-SEM, cryo-TEM, vitrification, cryo-electron microscopy of vitreous sections, ice contamination, cryo-negative staining, brief account of cryo-fixation methods, 2-D crystallization of membrane protein and cryo-preparation of 2-D crystal samples, brief discussion on cryo- electron tomography.

UNIT-IV (15 Hrs.)

Nuclear Chemistry:

Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, Q-value. Natural and artificial radioactivity, radioactive decay and equilibrium, Nuclear fission-fission product and fission yields, Nuclear fusion.

Radiochemical methods of analysis:

Radioactive tracer techniques and its applications, isotope dilution analysis, neutron activation analysis, Counting techniques such as G.M. Ionization and proportional counters.

Separation methods:

Solvent extraction: Partition law and its limitations, distributionratio, separation factor, factor influencing extraction, multiple extractions.

Recommended Text Books / Reference Books:

1. A Douglas, Skoog and Donald M. West, F.J. Holler, 'Fundamentals of Analytical Chemistry', 8thEdn., Harcourt College Publishers, **2004**.
2. Skoog, Holder, Nieman, 'Principles of Instrumental Analysis', 5thEdn., Thomson Books, **1998**.
3. J. Mendham, R.C. Denney, J.D. Barnes, M. Thomas, 'Vogel's Text Book of Quantitative Chemical Analysis', 6thEdn., Pearson Education, **2006**.
4. R. Gopalan, P.S. Subramaniam and K. Rengarajan, 'Elements of Analytical Chemistry', 3rdEdn.,Sultan Chand and Sons,**2003**.
5. S. Usharani, 'Analytical Chemistry', Macmillan Publishers,**2000**.
6. A. Cavalier, D. Spehner, B.M. Humbel, 'Handbook of Cryo-Preparation Methods for Electron Microscopy', CRC Press, Taylor & Francis Group, **2009**.
7. B. C. Harvey, 'Introduction to Nuclear Chemistry',Prentice-Hall, **1969**.
8. G. Friedlander, J. W. Kennedy, E.S. Marcus, J.M. Miller, 'Nuclear & Radiochemistry', John Wiley & Sons, **1981**.

9. H.J. Arnikar, 'Nuclear Chemistry', Wiley Eastern Co., II Edition, **1987**.
10. A. Braithwaite and F.J. Smith, 'Chromatographic Methods',5th Ed., Blackie Academic and Professional, London, **1996**.

NATURAL PRODUCTS

Subject Code: MCHMD1-221 | **L T P C 4 0 0 4** | **Duration: 60Hrs.**

Course Objectives

1. To acquire basic knowledge of isolation, purification, identification and standardization of natural products.
2. To discuss structure elucidation of alkaloids and terpenoids.
3. To discuss isolation, purification and structure elucidation of sterols
4. To understand the importance of vitamins, xanthophyll and carotenes.

Course Outcomes:

The students will acquire knowledge of

1. Isolation, purification, identification and standardization of natural products.
2. Structure elucidation of alkaloids, sterols and terpenoids,
3. Importance of vitamins, xanthophyll and carotenes.

UNIT-I (15 Hrs.)

1. Introduction & General Methods

Isolation, purification, identification and standardization of natural products. Carbohydrates and metabolism: Introduction, stereoisomerism, mutarotation, configuration and ring structure of monosaccharides, disaccharides and polysaccharides. Glycolysis, alcoholic and lactic acid fermentation, citric acid cycle.

UNIT-II (15 Hrs.)

Introduction, classification, isolation and purification of alkaloids and terpenoids. Structure elucidation of alkaloids (atropine, quinine, morphine) and terpenoids (camphor and menthol). Biosynthesis of alkaloids and terpenoids.

UNIT-III (15Hrs.)

2. Steroids

General introduction, isolation, purification and structure elucidation stereochemistry of sterols with special reference to cholesterol. Vitamin D group and bile acids. Biosynthesis of sterols.

UNIT-IV (15Hrs.)

3. Carotenoids andVitamins

Introduction to carotenoids and vitamins, Carotenes. Vitamin A, xanthophyll, vitamin B complex, vitamin K and vitamin E group.

Recommended Books

1. I.L. Finar, 'Organic Chemistry: Stereochemistry and The Chemistry Natural Products', Vol. II, 5th Edn., Longman Scientific & Technical, **1988**.
2. O.P. Agarwal, 'Chemistry of Organic Natural Products', Vol. I, 40th Edn., Krishna Prakashan Media, **2010.**
3. O.P. Aggarwal, 'Organic Chemistry Natural Products', Vol. II, 38th Edn., Krishna Prakashan Media, **2010.**

BIO-PHYSICALCHEMISTRY

Subject Code: MCHMD1-222 **L T PC** **Duration: 60Hrs.**

4 0 0 4

Course Objectives:

1. To equip with basic knowledge of the physical principles that governs chemicalsystems.
2. To provide knowledge of various biological systems with emphasis onbiochemical reactions.
3. To recall enzymes, their role in chemical and biologicalcatalysis.
4. To understand various principles that govern cellularprocesses.

Course Outcomes:

The students will acquire knowledge of

1. Basic concepts and mechanism of enzyme catalyzedreactions.
2. Interactions between various biomolecules.
3. Thermodynamics of ADP and ATP syntheses

UNIT I (15Hrs)

Biological Cell and its Constituents:

Biological cell, DNA and RNA in living systems. Basic consideration. Proximity effects and molecular adaptation.

Enzymes:

Introduction and historical perspective, chemical and biological catalysis, Remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Line Weaver-Burk plots, reversible and irreversible inhibition.

UNIT II (15Hrs)

Kinds of Reactions Catalyzed by Enzymes:

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate, addition and elimination reaction, enolic intermediates in isomerization reactions, b-cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation.

Co-Enzyme Chemistry:

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, Pyridoxal phosphate, NAD+, NADP+, FMN, FAD, lipoic acid, vitamin B12. Mechanism of reaction catalyzed by the above cofactors.

UNIT III (15Hrs)

Biological Macromolecules:

The Nucleic Acids:

Nucleotide, torsion angles in poly nucleotide chains, the helical structure of polynucleic acids, high order structure in polynucleotides.

Interactions in Macromolecules:
Basic principles of interaction between molecules, water structure and its interaction with biomolecules, dipole interactions, side chain interactions, electrostatic interactions, base pairing in nucleic acids, base stacking, hydration and the hydrophobic effect.

Structural Transition in Bio-macromolecules:
Coil – helix transitions in proteins, statistical methods for predicting protein secondary structures; melting and annealing of polynucleotide duplexes, helical transitions in double stranded DNA, super coil dependent DNA transitions predicting helical structures in genomic DNA.

UNIT IV (15 Hrs)

Bioenergetics and ATP cycle

Standard free energy change in biochemical reaction, exergonic, endergonic reactions. Hydrolysis of ATP, synthesis of ATP from ADP, metal complexes and transition of energy, chlorophylls, photo system I and photo system II in cleavage of water.

Thermodynamics of Biopolymer Solutions
Thermodynamics of biopolymers solutions, osmotic pressure, membrane equilibrium, muscular contraction and Energy generations in mechano-chemical system.

Recommended Books:
1. A.L. Lehninger, 'Principles of Biochemistry', WorthPublishers.
2. Voet; 'VoetBiochemistry', John Wiley,**1995**.
3. E.E. Conn, P.K. Stumpt, 'Outlines of Biochemistry', JohnWiley.
4. Hermann Dugas, C. Penny, 'Bioorganic Chemistry: Chemical Approach toEnzyme Action', Springer Verlag,**1982**.
5. M.I. Page, A. Williams, 'Enzyme Mechanisms, 'Royal Society ofChemistry'.
6. Richard B. Silverman, 'Organic Chemistry of Enzyme CatalysedReaction'.
7. I. Bertini, H.B. Gray, S.J. Lippard, J.S. Valentine, 'Bioinorganic Chemistry', UniversityScience Books.
8. William Jolley, 'BioinorganicChemistry'.
9. K.E. VanHolde, W.C. Johnson, P.S. Ho, 'Principles of Physical Biochemistry',Prentice Hall,**1998**.
10. L.Stryer, 'Biochemistry', W.H.Freeman.
11. J. DavidRawn, 'Biochemistry', NeilPatterson.
12. F. Wold, 'Macromolecules: Structure and Function', PrenticeHall.
13. C.R. Cantor, P.R. Schimmel, 'Biophysical Chemistry', Vol. 1-3, Freeman, **1980**.

ASYMMETRIC SYNTHESIS

Subject Code: MCHMD1-223	L T P C	Duration: 60 (Hrs.)
	4 0 0 4	

Course Objectives:
1. To learn the theory and importance of asymmetric Synthesis.
2. To acquire knowledge of various concepts of inducing enantio- and diastereoselectivity.
3. To give an understanding of various methods of asymmetric Synthesis.
4. To understand various analytical methods used for purifications & separations.

Course Outcomes:

The students will acquire knowledge of:

1. Methods for inducing enantio- anddiastereoselectivity.
2. Determination of enantio- and diastereoselectivity using various analyticalmethods.
3. Chemistry behind a range of asymmetricreactions

UNIT-I (18 Hrs.)

Basic Principles of Chirality and Asymmetric Synthesis:

Phenomenon of chirality, Need for asymmetric synthesis, Selective synthesis of enantiomers, Enantiomeric purity of natural products, stereogenic unit and types of chiral compound , Centrally chiral compounds of carbon, Centrally chiral compounds of nitrogen and phosphorus, Centrally chiral compounds of sulphur, Axially chiral compounds, Chiral molecules with more than one stereo genic unit: diastereomers, The selective synthesis of diastereomers, Prochirality: enantotopic and diastereotopic groups. Definition: enantiotropic and diastereotropic groups and faces – Symmetry, substitution and addition criteria. Prochirality nomenclature: Pro – R, Pro – S, Re and Si. Selectivity in synthesis: Stereospecific reactions (substrate stereoselectivity), Stereoselective reaction (Product stereoselectivity), Enantioselectivity and diastereoselectivity. Chemoselectivity, Regioselectivity. Conditions of Stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods for inducing enantio- and diastereoselectivity.

UNIT-II (12 Hrs.)

Analytical Methods:

Determining % Enantiomeric excess, % Enantioselctivity, Optical Purity, % Diastereomeric excess and % diatereoselectivity. Resolving agents and resolution of recemic compounds having common functional groups e.g. alcohol, amine, acid. Techniques for determination of Enantioselectivity, Polarimetric methods, Gas chromatography methods, Liquid chromatographic methods. NMR spectroscopy-Chiral derivatising agents (CDAs), Chiral solvating agents (CSAs), Chiral lanthanide shift reagents (CLSRs).

UNIT-III (18 Hrs.)

Classification of Asymmetric Reactions:

i) Substrate controlled asymmetric synthesis: Nucleophilic addition to chiral carbonyl compounds, 1,2 –Asymmetric induction, Felkin-Anh model, Double stereo differentiation; matched pair and mismatched pair, Examples from aldol condensation and hydroborationreactions

ii) Chiral auxiliary controlled asymmetric synthesis: α-alkylation of chiral enolates, azaenolates, imines and hydrazones, chiral sulphoxides. 1,4-asymmetric induction and Prelog's rule, use of chiral auxiliary in Diels-Alder and Cope reactions

iii) Chiral reagent controlled asymmetric synthesis: Asymmetric reduction using BINAL-H. Asymmetric Michael addition to α, β-unsaturated carbonyl compounds, Chiral lithium amides- enantioselective deprotonation, applications of chiralorganoboranes.

UNIT-IV (12 Hrs.)

Classification of Asymmetric Reactions (Continued Unit III):

iv) Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobson and Shi asymmetric epoxidation, Sharpless asymmetric dihydroxylation and amino hydroxylation. Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalyst. Chiral catalyst controlled Diels-Alder and Michael reactions, Jacobson Catalysts-Evans Catalyst- Aziridination, Enzyme mediated enantioselective synthesis.

Recommended Text Books / Reference Books:

1. R. A. Aitken, S. N. Kilenyi, Asymmetric Synthesis, Originally published by Chapman &Hall, **1992**.
2. Guo-Qiang Lin, Yue-Ming Li, Albert S. C. Chan, Princilpes and applications of Asymmetric Synthesis, Wiley Interscience, **2001**
3. J.D. Morrison and H.S. Moscher, 'Asymmetric Organic Reactions', Vol 1-5, Academic Press,**1983.**
4. E.N. Jacobsen, A. Pfaltz, H. Yamamoto, 'Comprehensive Asymmetric Catalysis', Eds. Springer,**2000.**
5. R.S. Ward, 'Stereoselectivity in Organic Molecules', Wiley, New York,**1999**.
6. E.L. Eliel, 'Stereochemistry of Carbon Compounds', Wiley,**1992**.
7. W. Carruthers, 'Some Modern Methods of Organic Synthesis', Cambridge University Press, 4th Edn.,**2012.**
8. I. Ojima, 'Catalytic Asymmetric Synthesis', VCH-NY,Pergamon.**1998.**
9. R.E. Gawley, J. Aube, 'Principles of Asymmetric Synthesis' (Tetrahedron Series in Organic Chemistry),Pergamon,**1996.**
10. H.B. Kagan, 'Asymmetric Synthesis', Edn., I, Thieme Medical Publishers,**2003**.
11. G. Proctor, 'Asymmetric Synthesis', Oxford University Press, USA,**1997**.

INORGANIC CHEMISTRY LAB-II

Subject Code: MCHMS1-205 **L T P C** **Duration – 60 Hrs.**
0 0 4 2

Course Objectives

1. To extend knowledge of use of standard laboratory equipment, modern instrumentation and classical techniques to carry out experiments.
2. To synthesize various inorganic complexes and their qualitative determination by UV,IR, NMR and ESR techniques.

Course Outcomes:

The students will acquire knowledge of

1. Volumetric and gravimetric analysis of cations and anions.
2. Understand electro analytical techniques.
3. Syntheses of various complexes and their structural analysis.
4. Use of various spectroscopic techniques like UV, IR, NMR for structural determination.

Note:

1. Students will have to perform atleast 10-12 experiments from the given syllabus.

2. Any other subject related experiment can also be included.

1. **Gravimetric Analysis of Cations and Anions:** Iodide, thiocyanate, Sulphate, oxalate chloride, nickel, copper cobalt, zinc and their mixture.
2. **Determination of Metal Ions Using Solvent Extraction**:
   a) Determination of copper as the diethydithiocarbamatecomplex
   b) Determination of iron as the 8hydroxyquinolate
   c) Determination of nickel as the dimethylglyoxime complex,
3. **Electro Analytical Techniques**
   pHmetric, Conductometric Titration: Representative acid/base and redox titrations.
4. **Colorimetry and Spectrophotometry**
   a) Determination of λ_{max} the absorption curve and concentration of asubstance
   b) Determination of copper (II) with EDTA
   c) Determination of iron (III) with EDTA.

Recommended Books:

1. H. Denny, W. Roesky, 'Chemical Curiosites', WILEY VCH,**1996**.
2. G. Marr and B.W. Rocket, 'Practical Inorganic Chemistry', University ScienceBooks, **1999.**
3. G. Pass and H. Sutcliffe, 'Practical Inorganic Chemistry', Chapman and Hall,London, **1968**.
4. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, 'Vogel's Textbook of Quantitative Analysis', Pearson Education,**2006.**
5. G. Svehla, 'Vogel's Textbook of Quantitative Analysis', PearsonEducation,**2006**.
6. Anil J. Elias, 'A Collection of Interesting General Chemistry Experiments', University Press,**2002.**

Note: The students are required to perform atleast 2 experiments from each section.