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 S_N2, S_N1, mixed S_N1 and S_N2 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 S_N1 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- S_E2 and S_E1. The S_E1 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 S_NAr, S_N1, benzyne and $S_{RN}1$ 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', 6th Edn., John Wiley & Sons, **2007.**
2. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Structure and Mechanisms, Vol, A', 5th Edn., Springer, **2007**.
3. Francis A. Carey & Richard J. Sundberg, 'Advanced Organic Chemistry: Reaction and Synthesis, Vol. B', 4th 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** **Duration: 60 Hrs.**
4 0 0 4

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**	**Duration: 60 (Hrs.)**
	4 0 0 4	

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.**