

DEVI AHILYA VISHWAKARMA UNIVERSITY, INDORE

Scheme of Marks

M. Sc. Chemistry

(w.e.f. 2016 and onwards)

SEMESTER - I

Paper	Compulsory/Optional	Paper Title	Code (MCH)	Max. Marks
I	Compulsory	INORGANIC CHEMISTRY	401	85+ 15(CCE) = 100
II	Compulsory	ORGANIC CHEMISTRY	402	85+ 15(CCE) = 100
III	Compulsory	PHYSICAL CHEMISTRY	403	85+ 15(CCE) = 100
IV	Compulsory	GROUP THEORY & SPECTROSCOPY I	404	85+ 15(CCE) = 100
V	For Students Without Mathematics in B.Sc.	MATHEMATICS FOR CHEMISTS	405(a)	85+ 15(CCE) = 100
	For Students Without Biology in B.Sc.	BIOLOGY FOR CHEMISTS	405(b)	85+ 15(CCE) = 100
		PRACTICAL - 1. Inorganic 2. Organic 3. Physical		33 33 34 =100
		Total		600

M. Sc. Chemistry

SEMESTER - II

Paper	Compulsory/Optional	Paper Title	Code (MCH)	Max. Marks
I	Compulsory	INORGANIC CHEMISTRY	406	85+ 15(CCE) = 100
II	Compulsory	ORGANIC CHEMISTRY	407	85+ 15(CCE) = 100
III	Compulsory	PHYSICAL CHEMISTRY	408	85+ 15(CCE) = 100
IV	Compulsory	SPECTROSCOPY II & DIFFRACTION METHODS	409	85+ 15(CCE) = 100
V	Compulsory	COMPUTER FOR CHEMISTS	410	85+ 15(CCE) = 100
		PRACTICAL - 1. Inorganic 2. Organic 3. Physical		33 33 34 =100
		Total		600

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M.Sc. CHEMISTRY (SEMESTER - I)

Paper No.

Compulsory / Optional

Max. Marks

: I (Code-MCH-401)

: Compulsory

100

Paper - I : Inorganic Chemistry

Unit - I	Stereochemistry and Bonding in Main Group Compounds : VSEPR, Walsh diagram (triatomic and penta-atomic molecules), $d\pi-p\pi$ bond, Bent rule and energetics hybridization, some simple reactions of covalently bonded molecules.
Unit - II	Metal-Ligand Equilibrium in Solution Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.
Unit - III	Reaction Mechanism of Transition Metal Complexes Energy profile of a reaction, reactivity of metal complex, inert and labile complex; kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, ar reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction. Reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere reactions.
Unit - IV	Metal-Ligand bonding Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π -bonding and molecular orbital theory.
Unit - V	HSAB Theory Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Suggested :

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.I. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

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M.Sc. CHEMISTRY (SEMESTER - I)

Paper No. : II (Code- MCH-402)
 Compulsory / Optional : Compulsory
 Max. Marks : 100

Paper - II : Organic Chemistry

Unit - I	Nature of Bonding in Organic Molecules Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy level of π -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compound, catenanes and rotaxanes.
Unit - II	Stereochemistry Strain due to unavoidable crowding, Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane) chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.
Unit - III	Conformational analysis and linear free energy relationship Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.
Unit - IV	Reaction Mechanism : Structure and Reactivity Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects.
Unit - V	Aliphatic Nucleophilic Substitution The SN^2 , SN^1 mixed SN^1 and SN^2 and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN^1 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.

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Books Suggested :

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wi
2. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
4. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University Press.
5. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.
6. Modern Organic Reactions, H.O. House, Benjamin.
7. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

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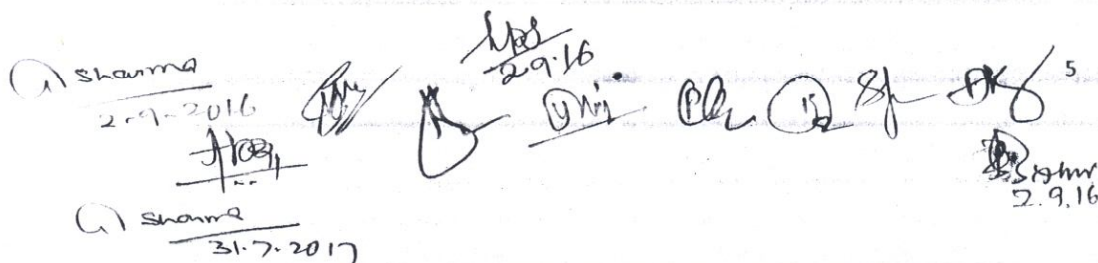
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M.Sc. CHEMISTRY (SEMESTER - I)

Paper No. : III (Code- MCH-403)
 Compulsory /Optional : Compulsory
 Max. Marks : 100

Paper - III : Physical Chemistry

Unit - I	Introduction to Exact Quantum Mechanical Results Schrödinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrödinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom and helium atom.
Unit - II	Approximate Methods The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom. Molecular Orbital Theory Huckel theory of conjugated systems bond and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Huckel theory.
Unit - III	Angular Momentum Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum operator using ladder operators addition of angular momenta, spin, anti-symmetry and Pauli exclusion principle.
Unit - IV	Classical Thermodynamics Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.
Unit - V	Statistical Thermodynamics Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

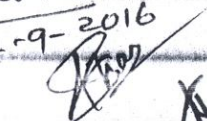

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Books Suggested :

1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata Mc Graw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. Mc Ween y, ELBS.
5. Chemical Kinetics. K. J. Laidler, McGraw-Hill.
6. Kinetics and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, Mc Millan.
7. Micelles, Theoretical and Applied Aspects, V. MOraoi, Plenum.
8. Modern Electrochemistry Vol. 1 and Vol. II J.O.M. Bockris and A.K.N. Reddy, Planum.
9. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.
10. Introduction to Quantum Chemistry-R.K. Prasad, New Age Publication.

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M.Sc. CHEMISTRY (SEMESTER - I)

Paper No. _____
 Compulsory / Optional _____
 Max. Marks _____

: IV (Code-MCH-404)
 : Compulsory
 : 100

Paper - IV : Group Theory & Spectroscopy I

Unit - I	<p>Symmetry and Group theory in Chemistry Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh} group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.</p>
Unit - II	<p>Microwave Spectroscopy Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.</p>
Unit - III	<p>Infrared Spectroscopy Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. P.Q.R. branches, Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal ligand vibrations, normal co-ordinate analysis.</p>
Unit - IV	<p>Raman Spectroscopy Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).</p>
Unit - V	<p>Electronic Spectroscopy Molecular Spectroscopy Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.</p> <p>Photoelectron Spectroscopy Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy-basic idea.</p>

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Books suggested:

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH- Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.

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DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER - I)

Paper No.
Compulsory / Optional
Max. Marks

: V [Code-405(a)]
: Compulsory
: 100

Paper - V : (a) Mathematics For Chemists

(For students without Mathematics in B.Sc.)

Unit - I	Vectors Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus. Matrix Algebra Addition and multiplication; inverse, adjoint and transpose of matrices.
Unit - II	Differential Calculus Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).
Unit - III	Integral Calculus Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).
Unit - IV	Elementary Differential equations First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.
Unit - V	Permutation and Probability Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit).

Books suggested

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suicific, Logman.
3. Mathematical for Physical Chemistry : F. Daniels, Mc. Gray Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.

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DEVI AHILYA VISHWAVIDYALAYA, INDORE

M.Sc. CHEMISTRY (SEMESTER - I)

Paper No.
Compulsory / Optional
Max. Marks

: V [Code-405(b)]
: Compulsory
: 100

Paper - V : (b) Biology For Chemists

(For students without Biology in B.Sc.)

Unit - I	<p>Cell Structure and Functions</p> <p>Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP - the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of bio-macromolecules.</p>
Unit - II	<p>Carbohydrates</p> <p>Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.</p>
Unit - III	<p>Lipid</p> <p>Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaic model of membrane structure. Lipid metabolism-β-oxidation of fatty acids.</p>
Unit - IV	<p>Amino-acids, Peptides and Proteins</p> <p>Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. Force responsible for holding of secondary structures. α-helix, β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure, Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination : chemical / enzymatic / mass spectral, racemization /detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).</p>
Unit - V	<p>Nucleic Acids</p> <p>Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of</p>

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nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

Books suggested :

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawan, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.

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DEVI AHILYA VISHWAVIDYALAYA, INDORE
M. Sc. CHEMISTRY PRACTICALS (SEMESTER - I)

Practical examination shall be conducted separately for each branch : (Duration : 6-8 hrs in each branch).

Inorganic Chemistry

Qualitative & Quantitative Analysis	12
Chromatography	06
Preparation	06
Record	04
Viva Voce	<u>05</u>
Total :	33

Qualitative Analysis :

- (a) Analysis of Less common metal ions : W, Mo, Se, Ti, Zr, Ce, V, etc. (Two metal ion in cationic / anionic forms).
(b) Analysis of Insoluble residue : Oxides, sulphates & halides.

Quantitative Analysis : Separation & estimation of two metal ions viz., Cu - Zn, Fe - Mg, Ni - Zn, etc. involving volumetric & gravimetric methods.

Chromatography: Separation, identification & determination of cations & anions by Paper Chromatography.

Preparations : Preparation of selected inorganic complexes, their analysis, test & characterization by spectral techniques (may be).

- (1) VO (acac)₂.
- (2) Ni (acac)₂.
- (3) [Co(NH₃)₆]Cl₃.
- (4) NH₄ [Cr (NH₃)₂(SCN)₄] ... Reinecke's salt.
- (5) Prussian Blue; Turnbull's Blue.
- (6) Oxalate complexes of Chromium (III) & Copper (II).

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Organic Chemistry

Qualitative Analysis	12
Organic Synthesis	12
Record	04
Viva-Voce	05
Total :	33

Qualitative Analysis : Separation, purification & identification of compounds of ternary mixture (solid or solid + liquid) using TLC & columns chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis :

Acetylation, Nitration, Halogenation, Oxidation, Reduction, Polymerization.

Physical Chemistry

Any one Experiment / Exercise from Section - A	12
Any one Experiment / Exercise from Section - B	13
Record	04
Viva-Voce	05
Total :	34

Section - A

Error Analysis & Statistical Data Analysis

Errors, types of errors, minimization of errors distribution curves precision, accuracy & combination; statistical treatment for error analysis, student's t-test, null hypothesis, rejection criteria. F & Q - test; linear regression analysis, curve fitting. Calibration of volumetric apparatus : Burette, pipette & standard flask.

Adsorption : To study surface tension - concentration relationship for solutions (Gibb's equation).

Phase Equilibria :

- Determination of congruent composition & temperature of a binary system (e.g., diphenylamine - benzophenone system).
- Determination of glass transition temperature of given salt (e.g., CaCl_2) conductometrically.
- To construct the phase diagram for three component system (e.g., chloroform - acetic acid - water).

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Section – B

Chemical Kinetics :

- (i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant & catalyst & (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reaction.
- (ii) Determination of the velocity constant of hydrolysis of an ester / ionic reaction in micellar media.
- (iii) Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide. Study the kinetics as an iodine clock reaction.
- (iv) Flowing clock reactions (Ref : Experiments in Physical Chemistry by Showmaker).
- (v) Determination of the primary salt effect on the kinetics of ionic reaction & testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

Solution:

- (i) Determination of molecular weight of non – volatile & electrolyte/ electrolyte by cryoscopic method & to determine the activity coefficient of an electrolyte.
- (ii) Determination of the degree of dissociation of weak electrolyte & to study the deviation from ideal behavior that occurs with a strong electrolyte.

Books Suggested

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
2. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly. Prentice Hall.
3. Experiments and Techniques in Organic Chemistry, D.P. Pasto, C. Johnson and M. Miller. Prentice Hall.
4. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath.
5. Systematic Qualitative Organic Analysis, H. Middleton, Edward Arnold.
6. Handbook of Organic Analysis-qualitative and Quantitative. H. Clark, Edward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
9. Findley's Practical Physical chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.

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