M.Sc. (CHEMISTRY) Previous
(Annual Scheme)
(2017 – 18)
SCHEME OF EXAMINATION

Each Theory Paper : 3 Hrs. Duration

Dissertation/Thesis/ Survey Report/ Field Work, if any.

1. The number of papers and the maximum marks for each paper/ practical shall be shown in the syllabus for the subject concerned. It will be necessary for a candidate to pass in the theory part as well as in practical part (wherever prescribed) of a subject/paper separately.

2. A candidate for a pass at each of the Previous and the Final Examinations shall be required to obtain :
   1) Atleast 36% marks in the aggregate of all the papers prescribed for the examination, and
   2) Atleast 36% marks in practical(s) wherever prescribed at the examination, provided that if a candidate fails to secure atleast 25% marks in each individual paper at the examination and also in the dissertation/Survey report/field work, wherever prescribed, he shall be deemed to have failed at the examination notwithstanding his having obtained the minimum percentage of marks required in the aggregate for that examination. No division will be awarded at the Previous and the Final Examination. Division shall be awarded at the end of the Final Examination on the combined marks obtained at the Previous and the Final Examination taken together, as noted below :

First Division	60%	of the aggregate marks taken together of the
Second Division	48%	Previous and the Final Examination.

   All the rest will be declared to have passed the examination.

3. If a candidate clears any Paper(s)/ Practical(s)/ Dissertation prescribed at the Previous and/or Final Examination after a continuous period of three years, then for the purpose of working out his division the minimum pass marks only viz. 25% (36% in the case of practical) shall be taken into account in respect of such Paper(s)/Practical(s)/Dissertation as are cleared after the expiry of the aforesaid period of three years: provided that in case where a candidate required more than 25% marks in order to reach the minimum aggregate as many marks out of those actually secured by him will be taken into account as would enable him to make up the deficiency in the requisite minimum , aggregate.

4. The Thesis/Dissertation/Survey Report/Field Work shall be typewritten and submitted in triplicate so as to reach the office of the Registrar atleast 3 weeks before the commencement of the theory examinations. Only such candidates shall be permitted to offer Dissertation/ Field Work/Survey Report/Thesis (if provided in the scheme of examination) in lieu of a paper as have secured atleast 55% marks in the aggregate of all the papers prescribed for the previous examination in the case of annual scheme irrespective of the number of papers in which a candidate actually appeared at the examination.

N.B. Non-collegiate candidates are not eligible to offer dissertation as per provisions of O. 170-A

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2015

M.Sc. CHEMISTRY

(Two Year Course)

Note : In each question paper 10 questions will be set. Candidates have to answer any 5 questions selecting at least one question from each unit.

M.Sc. I Year (Previous)

Paper	Course No.	Course	Duration Hours	Max. Marks	Min Marks
Paper I	CH-401	Inorganic Chemistry	3	100	36
Paper II	CH-402	Organic Chemistry	3	100	36
Paper III	CH-403	Physical Chemistry	3	100	36
Paper IV	CH-404	Spectroscopy	3	75	27
Paper V	CH-405	(A) Mathematics for Chemists*	3	25	9
		(B) Biology for Chemists**			
Paper VI	CH-406	Computers for Chemists	3	50	18
Practical			14 hrs.	200	72
			Total Marks :	650	

* For students without Mathematics in B.Sc.

** For students without Biology in B.Sc.

M.Sc. I YEAR (PREVIOUS)

Paper I: CH- 401 Inorganic Chemistry

Duration : 3 hrs. Max. Marks: 100

Unit-I

Symmetry and Group Theory in Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by metrics (representation for the C_n, C_{nv}, D_{nh}, etc., groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their uses; spectroscopic derivation of character table for C_{2v} and C_{3v} point group. Symmetry aspects of molecular vibrations of H2O molecule.

Unit-II

Stereochemistry and Bonding in Main Group Element Compounds

VSEPR, Walsh diagram [tri-atomic (AH_2 type) and penta-atomic (CH_3I) molecules]. dπ-pπ bond. Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Metal-Ligand bonding

Limitations of crystal field theory. Molecular orbital theory: octahedral, tetrahedral and square planar complexes and π-bonding complexes.

Metal π-Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

Metal Clusters

Higher boranes, carboranes, metalloboranes and metallocarboranes, compounds with metal-metal multiple bonds.

Isopoly and Heteropoly Acids and Salts.

Unit-III

Electronic Spectra and Magnetic Properties of Transition Metal Complexes

Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), calculations of Dα, B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interactions, trends in stepwise constants, 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 pH-metry and spectrophotometry.

Unit-IV

Reaction Mechanism of Transition Metal Complexes

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, 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, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction.

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dox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere
oc reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Unit-V

Nuclear and Radiochemistry:
Laws of radioactive decay; Detection of radiations; Geiger-Nuttal rule; GM tubes and their characteristics; Ionization chamber, Proportional counters, Scintillation counters; Solid state detectors; Calibration of counting equipments; Determination of absolute disintegration rates.
Activation analysis: Principles; Various methods of activation; Methodology; Advantages, limitations and applications.

Books Suggested:

1. Chemical Applications of Group Theory. F A. Cotton.
2. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
3. Inorganic Chemistry, J.E. Huheey, Harper & Row.
4. Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.
5. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
6. Magnetochemistry, R.I. Carlin, Springer Verlag.
7. Comprehensive Coordination Chemistry eds., G. Wilkinson. R.D. Gillars and J.A. McCleverty, Pergamon.
8. Nuclear and Radiochemistry; G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller; 3rd Edn., Wiley: NY, 1981.
9. Essentials of Nuclear Chemistry, H. J. Arnikar; 4th Eds., New Age International: N Delhi, India, 2011.
10. Nuclear and Radiochemistry: Fundamental and Applications, 2 Vols., Jens-Volker Kratz and Karl Heinrich Lieser; 3rd Edn., John Wiley & Sons: UK, 2013.

Paper II: CH-402 Organic Chemistry

Max. Marks : 100

Duration : 3 hrs.

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, alternant and non-alternant 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 compounds, catenanes and rotaxanes.

Stereochemistry
Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral centre, 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 spiranes), chirality due to helical shape.
Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

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Unit-II

Reaction Mechanism : Structure and Reactivity

Types 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, isotope effects. 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, Taft equation.

Aliphatic Nucleophilic Substitution

The S_N2, S_Ni, mixed S_Ni-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 carbocation. The S_Ni mechanism. Nucleophilic substitution at the 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.

Unit-III

Aliphatic Electrophilic Substitution

Bimolecular mechanisms - S_E2 and S_Ei. The S_Ei mechanism - electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution

The S_NAr, S_Ni, benzyne and $S_{RN}i$ mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

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. Reactivity 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.

Unit-IV

Addition to Carbon-Carbon 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 to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction.

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anism of condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Elimination Reactions

The E2, El and ElcB mechanisms and their spectrum. Orientation of the double bond. Reactivity - effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Unit-V

Pericyclic Reactions

Molecular orbital symmetry. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions. 4n, 4n+2 and allyl systems. Cycloadditions - antarafacial and suprafacial additions. 4n and 4n+2 systems, 2+2 addition of ketenes. 1,3-dipolar cycloadditions and chelotropic reactions.

Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

Books Suggested

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure. Jerry March, John Wiley.
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. ROC Norman and J.M. Coxon. Blackie Academic & Professional.
8. Pericyclic Reactions, S.M. Mukherji. Macmillan, India.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
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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Paper III: CH-403 Physical Chemistry

Duration : 3 hrs. **Max. Marks : 100**

Unit-I

Quantum Chemistry

Introduction to Exact Quantum Mechanical Results : The Schrodinger equation and the postulates of quantum mechanics. Discussion of the solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate Methods: The variation theorem, linear variation principle. Perturbation theory (up to second order and non-degenerate). Applications of variation method and perturbation theory to Helium atom.

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, tunneling, spin, antisymmetry and Pauli's exclusion principle.

...ular Orbital Theory : Huckel theory of conjugated systems, bond and charge density calculations. ...lications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended ...ckel theory.

Unit-II

Thermodynamics

Classical Thermodynamics : Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. 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.

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 functions Application of partition functions. Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

Non Equilibrium Thermodynamics : Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction.

Unit-III

Chemical Dynamics

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain reactions (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical reactions (hydrogen-bromine and hydrogen-chlorine) and homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel- Marcus [RRKM] theories of unimolecular reactions).

Unit-IV

Surface Chemistry

Adsorption : Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation). Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomenon).

Micelles : Surface active agents, classification of surface active agents, micellization. hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion

binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

Macromolecules

Polymer - definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimension of various chain structures.

Unit-V

Electrochemistry

Electrochemistry of solutions. Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Graham Devanathan-Mottwatts, Tobin. Bockris, Devanathan models, Overpotentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot.

Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Semiconductor interfaces - theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface.

Polarography theory, Ilkovic equation, half wave potential and its significance.

Books Suggested

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

Paper IV: CH 404 - Spectroscopy and Diffraction Methods

Duration : 3 hrs. **Max. Marks : 75**

Unit-I

Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter - absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines.

Microwave Spectroscopy

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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.

Unit-II

Vibrational Spectroscopy

Infrared Spectroscopy: Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constantand bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. PQR 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.

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 antistokes Raman spectroscopy (CARS).

Applications of Vibrational Spectroscopy: Symmetry and shapes of AB2, AB3, AB4, AB5 and AB6, mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

Unit-III

Electronic Spectroscopy

Atomic Spectroscopy: Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

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; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

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.

Unit-IV

Magnetic Resonance Spectroscopy

Nuclear Magnetic Resonance Spectroscopy : General introduction, Nuclear spin, nuclear resonance, shielding mechanism, chemical shift and its measurements, factors influencing chemical shift, deshielding. Chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto). Spin-spin interactions, coupling constant '*J*', factors influencing coupling constant. Complex spin-spin interaction between two, three, four and five nuclei (ABX, AMX, ABC, A2B2, etc.). Spin decoupling, chemical exchange, effect of deuteration. Simplification of complex spectra - nuclear magnetic double resonance, NMR shift reagents, solvent effects. NMR of Paramagnetic substances in solution, the contact and pseudocontact shifts, factors affecting nuclear relaxation. Fourier transform technique (FT NMR), nuclear overhauser effect (NOE). NMR active nuclei other than proton - ^{13}C, ^{19}F and ^{31}P.

Electron Spin Resonance Spectroscopy : Basic principles, zero field splitting and Kramer's degeneracy, Isotropic and anisotropic Hyperfine coupling, spin-orbit coupling and significance of g-tensors, factors

affecting the 'g' value, application to transition metal complexes; spin Hamiltonian, spin densities and McConnell relationship, applications - spin polarization for atoms and transition metal ions.

Unit-V

X-ray Diffraction : Bragg condition, Miller indices, Laue Method, Bragg method Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules.

Electron Diffraction : Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron Diffraction : Scattering of neutrons by solids, measurements techniques. Elucidation of structure of magnetically ordered unit cell.

Books suggested

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis, Ed. H Windawi & 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. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
6. Basic Principles of Spectroscopy, R. Change, McGraw Hill.
7. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
8. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
9. Introduction to Magnetic Resonance, A Carrington and A.D. Maclachalan, Harper & Row.

Paper-V : CH-405 (a) Mathematics for Chemists
(For students without Mathematics in B.Sc)

Duration : 3 hrs. Max. Mark; : 25

Unit-I

Vectors and Matrix Algebra

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, special matrices (Symmetric, skew-symmetric, Hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations : Homogeneous, non- Homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants (examples from Huckel theory).

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

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Basic rules for integration, integration by parts, partial fraction 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 equations and their solutions.

Unit-V

Permutation and Probability

Permutations and combinations, probability and probability theorems, average, variance, root mean 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 Suicliffe, Longman.
3. Mathematical Preparation for Physical chemistry, F. Daniels. McGraw 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.

Paper-V : CH-405 (b) Biology for Chemists
(For students without Biology in B.Sc.)

Duration : 3 hrs. **Max. Marks : 25**

Unit-I

Cell Structure and Functions

Structure prokaryotic and eukaryotic cells, intracellular organelles 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 biomolecules, building blocks of bio-macromolecules.

Unit-II

Carbohydrates

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycoside, 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 or mucopolysaccharides, Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Carbohydrates metabolism - Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

Unit-III

Lipids

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.

Unit-IV

Amino-acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structure. 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).

Unit-V

Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via H bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of 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.

Paper-VI : CH-406 Computers for Chemists

Duration 3 hrs. Max. Marks: 50

Unit-I

Introduction to Computers and Computing

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS, principles of programming. Algorithms and flow-charts.

Unit-II

Computer Programming in FORTRAN/C/BASIC

(The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols. Expressions. Arithmetic assignment statement. Input and output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and

DIMENSION, DO statement, FUNCTION and SUBROUTINE, COMMON and DATA statements (students learn the programming logic and these language features by 'hands on' experience on a personal computer from the very beginning of this topic).

Unit-III

Programming in Chemistry

Developing of small computer codes (FORTRAN / C/ BASIC) involving simple formulae in Chemistry, such as Van der Waals equation, Chemical kinetics (determination of Rate constants), Radioactive decay (Half Life and Average Life). Determination of Normality, Molarity and Molality of solutions. Evaluation of Electronegativity of atom and Lattice Energy from experimental data. Determination of molecular weight and percentage of elements in organic compounds using data from experimental methods. Representation of molecules in terms of elementary structural features such as bond lengths, bond angles, dihedral angles, etc.

Unit-IV

Use of computer Programmes

Operation of PC, Data Processing. Running of standard Programs and Packages such as MS WORD, MS EXCEL - special emphasis on calculations and chart formations. X-Y plot. Simpson's Numerical Integration method.

Unit-V

Programmes with data preferably from physical chemistry Laboratory. Introduction of working of any one of the packages such as LOTUS / EXCEL / FOXPRO / MOPAC and Word Processing software such as WORDSTAR/ MS WORD.

Books Suggested:

1. Fundamentals of Computers - V. Rajaraman (Prentice Hall)
2. Computers in Chemistry - K.V. Raman (Tata McGraw Hill)
3. Computer Programming in FORTRAN IV - V Rajaraman (Prentice Hall)

M.Sc. (Prev.) PRACTICAL

Duration 14 hrs. (2 days) Max. Marks : 200

INORGANIC CHEMISTRY

Qualitative and Quantitative Analysis

a) Less common metal ions - Tl, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic/anionic forms)

b) Insolubles - oxides, sulphates and halides.

c) Separation and determination of two metal ions - Cu-Ni, Ni-Zn, Cu-Fe involving volumetric and gravimetric methods.

Chromatography

Separation of cations and anions by

a) Paper Chromatography

b) Column Chromatography - Ion exchange.

Preparations

Preparation of selected inorganic compounds and their studies by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements. Handing of air and moisture sensitive compounds.

1. $[VO(acac)_2]$
2. $TiO(C_9H_8NO)_2.2H_2O$

3. cis-$K[Cr(C_2O_4)_2(H_2O)_2]$
4. $Na_3[Cr(NH_3)_2(SCN)_4]$
5. $[Mn(acac)_2]$
6. $K_3[Fe(C_2O_4)_3]$
7. Prussian Blue, Turnbull's Blue.
8. $[Co(NH_3)_6]\ [CO(NO_2)_6]$
9. cis-$[Co(trien)(NO_2)_2]Cl.H_2O$
10. $Hg[Co(SCN)_4]$
11. $[Co(Py)_2Cl_2]$
12. $[Ni(NH_3)_6]Cl_2$
13. $[Ni(dmg)_2]$
14. $[Cu(NH_3)_4]SO_4.H_2O$

ORGANIC CHEMISTRY

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture, one liquid and one solid using TLC and column chromatography, chemical tests, IR spectra to be used for functional group identification.

Organic Synthesis (at least six to be carried out)

a) One step Preparations :

1. Acetylation : Acetylation of cholesterol and separation of cholesterol acetate by column chromatography.
2. Oxidation : Adipic acid by chromic acid oxidation of cyclohexanol / cyclohexene.
3. Aldol condensation : Dibenzal acetone from benazaldehyde.

b) Two step Preparations

1. Aniline → Sym. Tribromoaniline → Sym. Tribromobenzene
2. Benzoin → Benzil → Dibenzyl
3. Aniline → Dibenzoaminobenzene → p-Aminoazobenzene
4. Nitrobenzene → m-Dinitrobenzene → m-Nitroaniline
5. Phthalic anhydride → Fluorescein → Eosin

The products may be characterised by Spectral Techniques.

Quantitative Analysis (At least 3 to be performed)

1. Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
2. Estimation of amines / phenols using bromate bromide solution or acetylation method.
3. Estimation of Sulphur by Messenger or Fusion method.
4. Estimation of Nitrogen by Kjeldahl's method.
5. Determination of Iodine number and Saponification value of an oil sample.
6. Determination of DO, COD and BOD of water sample.

PHYSICAL CHEMSITRY

Number of hours of each experiment 3-4 hours. A list of experiment under different headings is given below. Typical experiments are to be selected from each type. Students are required to perform at least 30 experiments.

2-12-05

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2-3

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PART A

Error Analysis and Statistical Data Analysis

Errors; types of errors, minimization of errors distribution curves, precision, accuracy and combination: statistical treatment for error analysis, student 't' test, null hypothesis rejection criteria. F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask.

PART B

Adsorption

To study surface tension-concentration relationship for solutions (Gibbs equation).

Phase Equilibria

(i) Determination of congruent composition and temperature of a binary system (e.g., diphenylamine-benzophenone system)

(ii) Determination of glass transition temperature of a given salt (e.g. $CaCl_2$) conductometrically.

(iii) To construct the phase diagram for three component system (e.g. chloroform - acetic acid - water).

Chemical Kinetics

(i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant and catalyst and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester/ ionic reaction in micellar media.

(iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

(iv) Flowing clock reaction (Ref: Experiments in Physical Chemistry by Snowmaker)

(v) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

(vi) Oscillatory reaction.

Solutions

(i) Determination of molecular weight of non-volatile and non-electrolyte / electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

(ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry

A. Conductometry

(i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

(ii) Determination of solubility and solubility product of sparingly soluble salts (e.g., $PbSO_4$, $BaSO_4$) conductometrically.

(iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.

(iv) To study the effect of solvent on the conductance of $AgNO_3$ / acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.

Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Huckel's limiting law.

5. Potentiometry/pH metry
(i) Determination of strengths of halides in a mixture potentiometrically.
(ii) Determination of the valency of mercurous ions potentiometrically.
(iii) Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
(iv) Determination of temperature dependence of EMF of a cell.
(v) Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
(vi) Acid-base titration in a non-aqueous media using a pH meter.
(vii) Determination of activity and activity coefficient of electrolytes.
(viii) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
(ix) Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method.
(x) Determination of thermodynamic constants. ΔG, ΔS, and ΔH for the reaction by e.m.f. method.
$Zn + H_2SO_4 \rightarrow ZnSO_4 + 2H$

Polarimetry
(i) Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
(ii) Enzyme kinetics - inversion of sucrose.

Reference Books :

1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R.C. Denney, G.H. Jeffrey 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. Health.
5. Systematic Qaulitatitve Organic Analysis, H. Middleton, Adward Arnold.
6. Handbook of Organic Analysis-Qualitative and Quantitative, H. Clar, Adward Arnold.
7. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
8. Practical Physical Chemistry, A.M. James and F.E. Porichard, Longman.
9. Findley's Practical Physical Chemistry, B.P. Levitt, Longman.
10. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata-McGraw Hill.

INSTRUCTIONS TO THE EXAMINERS

M.Sc. (Previous) Chemistry Practical

Max. Marks: 200 **Duration of Exam: 14 hrs (spread in 2 days)** **Min. Marks: 72**

Inorganic Chemistry

Qualitative and Quantitative Analysis

(i) Analysis of mixture containing 8 radicals including one radical of rare elements. 30

Or

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24/2/05

Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe involving volumetric and gravimetric method.

(Both these exercises should be given in equal ratio by lots.)

(ii) Separation of cations and anions by paper chromatography or column chromatography. 20

Or

Preparation of one selected inorganic compound and its study by IR.

Organic Chemistry

(i) Qualitative and Quantitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group determination.

Or

Perform one of the quantitative analysis given in syllabus. 30

(Both these exercises should be given in equal ratio by lots.)

(ii) Organic synthesis 20

Perform one of the 8 organic syntheses as mentioned in the syllabus and may be characterized by spectral techniques.

Physical Chemistry

(i) One physical experiment (minor) from Part A of syllabus. 20

(ii) One physical experiment (major) from Part B of syllabus. 30

Viva 30

Record 20

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