SCHEME OF EXAMINATIONS

AND

SYLLABUS

M.Sc. (Previous) Chemistry

Effective from the Academic Session 2016-2017

This syllabus is for the Courses running under Annual Scheme at the affiliated Colleges of the University

Master of Science (M.Sc.)
Chemistry

Faculty of Science

UNIVERSITY OF KOTA

MBS Marg, KOTA (Rajasthan)-324 005

INDIA

M.Sc. (Previous) CHEMISTRY Examination

(Annual Scheme)

SCHEME OF EXAMINATION

Each Theory Paper 3 Hrs. duration

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 theory part as well as in the Practical part (Wherever prescribed) of a subject/paper separately.
2. A candidate for a pass at each of the Previous and the Final Examination shall be required to obtain (i) atleast 36% marks in the aggregate of all the papers prescribed for the examination and (ii) at least 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 test 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 the examination. No division will be awarded at the Previous Examination. Division shall be awarded at the end of the Final Examination on the combined marks obtained at the Previous and the Final Examinations taken together, as noted below :

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

3. All the rest will be declared to have passed the examination.
4. 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 requires 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 makeup the deficiency in the requisite minimum aggregate.
5. The Thesis/Dissertation/Serve Report/Field work shall be typewritten and submitted triplicate so as to reach the office of the Registrar at lest 3 weeks before the commencement of the theory examination. 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 paper prescribed for the previous examination in the case of annual scheme irrespective of the number of paper in which a candidate actually appeared at the examination.

   N.B.: Non-collegiate candidates are not eligible to offer dissertation as per provisions of 0.170-A.

M.Sc. (Previous) CHEMISTRY Examination

(Annual Scheme)

Distribution of Marks

Number of Paper	Code of Paper	Nomenclature of Paper	Duration of Exam.	Max. Marks	Min. Pass Marks
Paper-I	CH-401	Inorganic Chemistry	3 Hrs.	100	36
Paper-II	CH-402	Organic Chemistry	3 Hrs.	100	36
Paper-III	CH-403	Physical Chemistry	3 Hrs.	100	36
Paper-IV	CH-404	Group Theory & Spectroscopy	3 Hrs	50	18
Paper-V	CH-405A	Mathematics for chemists* or Biology for Chemists**	1.5 Hrs.	25	09
	CH-405B	Computers for Chemists	1.5 Hrs	25	09
Paper-VI	CH-406	Practical	14 Hrs.	200	72
		Seminar (Internal)	---------	25	09
			Total Marks	**625**	**225**

Note : *For students without Mathematics in B.Sc.
** For students without Biology in B.Sc.

M.Sc. (Previous) CHEMISTRY Examination

(Annual Scheme)

Paper-I: Inorganic Chemistry

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

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 10

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 250 words.

Total marks : 50

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 500 words, 2 questions to be attempted.

Total marks : 40

Unit-I Stereochemistry and Bonding in Main Group Compounds:

VSEPRT, Walsh diagram (tri- and penta-atomic molecules), d_{π}-p_{π} bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Metal-Ligand Equilibria 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 pH-metry and spectrophotometry.

Unit-II Reaction Mechanism of Transition Metal Complexes:
Energy profile of a reaction, reactivity of metal complex, 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, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Unit-III Metal-Ligand Bonding:
Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.

Unit-IV Electronic Spectra and Magnetic Properties of Transition Metal Complexes:
Spectroscopic ground states, correlation. Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1-d^9 states), calculations of Dα, β and β parameters, charge transfer spectra, spectroscopic method of assignmetnt of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

Unit-V Metal π-Complexes:
Metal carboynl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxgen complexes; tertiary phosphine as ligand.

Metal Clusters:
Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal metal multiple bonds.

Books Suggested :

- *Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.*
- *Inorganic Chemistry, J.E. Huhey, Harpes & Row.*
- *Chemistry of the Elements. N.N. Greenwood and A. Earnshow, Pergamon.*
- *Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.*
- *Magnetio chemistry, R.1. Carlin, Springer Verlag.*
- *Comprehensive Coordiantion Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. Mc Cleverty, Pergamon.*

Paper-II: Organic Chemistry

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

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 10

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 250 words.

Total marks : 50

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 500 words, 2 questions to be attempted.

Total marks : 40

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. Hűckel's rule, energy level of π-molecular orbitals, annulenes, anti-aromaticity, ψaromaticity, 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 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-II 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 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, subsistent and reaction constants, Taft equation.

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 systems, 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.

Unit-III Aliphatic Electrophilic Substitution:

Bimolecular mechanisms S_E2 and S_E1, The S_E1 mechanism, electrophilic substution accompanied by double bond shifts. Effect of substrates, leaving groups 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 reactiion, Gatterman-Koch reaction.

Aromatic Nucleophilic Substitution:
The S_NAr S_N1, benzyne and $S_{RN}1$ mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richte, 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 carboyxlic 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, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and usaturated carbonyl compounds. Witting reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Unit-V Elimination Reactions:
The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactitivty-effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

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 ally systems. Cycloadditions-antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.

***Books Suggested**:*

- *Advanced Organic Chemistry: Reactions, Mechanism & Structure, Jerry March, J. Wiley.*
- *Advanced Organic Chemistry, F.A. Carey and R.J. Sunderg, Plenum.*
- *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.*
- *Structure and Mechanism in Organic Chemistry, C.K. Ingold, Comell University Press.*
- *Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice-Hall.*
- *Modern Organic Reactions, H.O. House, Benjamin.*
- *Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professionsl.*
- *Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, McMillan.*
- *Pericyclic Reactions, S.M. Mukherji, McMillan, India*
- *Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.*
- *Stereochemisty of Organic Compounds, P.S. Kalsi, New Age International.*
- *Pericyclic Reactions: Ameta, Sharma,Vardia, Vyas, Sadguru Publications*

Paper-III: Physical Chemistry

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

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 10

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 250 words.

Total marks : 50

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 500 words, 2 questions to be attempted.

Total marks : 40

Unit-I Quantum Chemistry:

Introduction to Exact Quantum Mechanical Results:

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systesm viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

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.

Angular Momentum:

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators addition of angular momentum, spin, antisymmetry and Pauli's exclusion principle.

Molecular Orbital Theory:

Hűckel theory of conjugated systems bond and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Hűckel theory.

Unit-II Thermodynamic:

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 Hűckel 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 microcanonical 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.

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, irreversible thermodynamics for biological systems, coupled reactions.

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 (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogenous 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), catalytic activity at surfaces.

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, solublization, 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-Hückel-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, Grahmam Devanatham-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.

Electocatalysis:
Influence of various parameters. Hydrogen electrode. Bioelectrochemistry, threshold membrane phenomena, Nernst-Planck equation, hodges-Huxley equation; core conductor models, electrocardiography.

Polarography:
Theory, Ilkone equation; half wave potential and its significance. Introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods.

Books Suggested:

- *Physical Chemistry, P.W. Atkins, ELBS.*
- *Introduction to Quantum Chemistyry, A.K. Chandra, Tata Mc Graw Hill.*
- *Quantum Chemistry, Ira N. Levine, Prentice Hall.*
- *Coulson's Valence, R.Mc Weeny, ELBS.*
- *Chemical Kinetics. K.J. Laidler, McGraw-Hill.*
- *Kineties and Mechanism of Chemical Transformation J.Rajaraman and J. Kuriacose, McMillan.*
- *Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.*
- *Modern Electrochemistry Vol. 1 & Vol II J.O.M. Bockris and A.K.N. Reddy, Planum.*
- *Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.*

Paper-IV: Group Theory, Spectroscopy and Diffraction Methods

Duration : 3 Hours **Max. Marks : 50**

Note : The question paper will contain three sections as under –

Section-A: One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 05

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 250 words.

Total marks : 25

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 500 words, 2 questions to be attempted.

Total marks : 20

Unit-I Symmetry and Group Theory in Chemistry:

Symmetry elements and symmetry operation, definition of group, subgroup, relation between orders of a finite group all its subgroup. Conjugacy relation and classes. Point symmetry group. SchÖnflies symbols, representations of groups by matrices (representation for the C_n, C_{nv}, C_{nh}, D_{nh}, etc, group to be worked out explicitly). Character of representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy

Unifying Principles:

Electrogmagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainity 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, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

Unit-II Microwave Spectroscopy:

Classification of molecules, rigid rotator 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.

Vibrational Spectroscopy:

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.

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).

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: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant "J" Classification (AVB, AMX, ABC, A_2B_2 etc.). spin decoupling; basic ideas about instrument, NMR studies of nuclei other than proton-^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FT NMR, use of NMR in medical diagnostics.

Electron Spin Resonance Spectroscopy: Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyper fin coupling constants, spin Hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications.

Nuclear Quadrupole Resonance Spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradients, coupling constant, splitting, applications.

Unit-V Difraction Methods:

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 v/s 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 and liquids, magnetic scattering measurement techniques. Elucidation of structure of magnetically ordered unit cell.

Books suggested:

- *Modern Spectroscopy, J.M. Hollas, John Wiley.*
- *Applied Electron Spectroscopy for chemical analysis ed. H.Windawi and F.L.Ho,Wiley Intersci.*
- *NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.*

- *Physical Methods in Chemistry, R.S. Drago, Saunders College.*
- *Chemical Applications of Group Theory, F.A. Cotton.*
- *Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.*
- *Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.*
- *Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.*
- *Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.*
- *Introduction to Magnetic Resonance. A Carrington and A.D. McLachalan, Harper & Row.*

Paper-V (a1)- Mathematics for Chemists

(For students without Mathematics in B.Sc.)

Duration : 1½ Hours **Max. Marks : 25**

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 2.5

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 150 words.

Total marks : 12.5

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 300 words, 2 questions to be attempted.

Total marks : 10

Unit-I Vectors:

Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus, Gauss'theorem, divergence theorem etc.

Unit-II Matrix Algebra:

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, Skey-Harmitian, 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 Hückel theory). Introduction to tensors; polarzability and magnetic susceptibility as examples.

Unit-III 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.). exact and inexact differentials with their applications to thermodynamic properties.

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) curve sketching.

Unit-IV Elementary Differential Equations:

Variables-separable and exact first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. solution of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and legendre equation etc., spherical harmonics, second order differential equation and their solutions.

Unit-V Permutation and Probability:

Permutations and combinations, probability and probability theorems, average, probability curves, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.

Books Suggested

- *The Chemistry Mathematics Book, E.Steiner, Oxford University Press.*
- *Mathematics for Chemistry, Doggett and Sucliffe, Longman.*
- *Mathematical for Physical Chemistry : F. Daniels, Mc Graw Hill.*
- *Chemical Mathematics D.M. Hirst, Longman.*
- *Applied Mathematics for Physical Chemistery, J.R. Barrnte, Prentice Hall.*
- *Basic Matchematics for Chemists, Tebbutt, Wiley.*

OR

Paper-V (a2) : Biology for Chemists

(For students without Biology in B.Sc.)

Duration : 1½ Hours **Max. Marks : 25**

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 2.5

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 150 words.

Total marks : 12.5

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 300 words, 2 questions to be attempted.

Total marks : 10

Unit-I Cell Structure and Functions:

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparisons 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 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 functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate 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. Liproproteins-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 peptidies, 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).

Unit-V Nucleic Acids:

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 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

- *Principles of Biochemistry, A.L. Lehnigher, Worth Publishers.*
- *Biochemistry, L. Stryer, W.H. Freeman.*
- *Biochemistry, J. David Rawn, Neil Patterson.*
- *Biochemistry, Voet and Voet, John Wiley.*
- *Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.*

Paper-V (b) : Computer for Chemists

Duration : 1½ Hours **Max. Marks : 25**

Note : The question paper will contain three sections as under –

Section-A : One compulsory question with 10 parts, having 2 parts from each unit, short answer in 20 words for each part.

Total marks : 2.5

Section-B : 10 questions, 2 questions from each unit, 5 questions to be attempted, taking one from each unit, answer approximately in 150 words.

Total marks : 12.5

Section-C : 04 questions (question may have sub division) covering all units but not more than one question from each unit, descriptive type, answer in about 300 words, 2 questions to be attempted.

Total marks : 10

(This is a theory cum-laboratory course with more emphasis on laboratory work)

Unit-I Introduction to Computers and Computing:

Basic structure and functioning of computer 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. Data processing, 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 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.

Unit-III

LOGICAL variables. Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the very beginning of this topic.)

Unit-IV Programming in Chemistry:

Development of small computer codes involving simple formulae in Chemistry, such as Van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Hűckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles, etc. of molecules extracted from a database such as Cambridge data base.

Unit-V Use of Computer Programmes:

The student will learn how to operate a PC and how to run standard programmes and packages, execution of linear regression, X-Y plot, Numerical Integration and differentiation as well as differential equation solution programmes. Monte Carlo and Moleculuar dynamics, programmes with data preferably from physical chemistry laboratory. Further the student will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO and word processing software such as WORDSTAR / MS WORD.

Book Suggested :

- Fundamentals of Computer : V. Rajaraman (Prentice Hall)
- Computers in Chemistry : K.V. Raman (Tata Mc Graw Hill)
- Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)
- Computational Chemistry, A.C.Norris.

M.Sc. (Previous) CHEMISTRY Practical
(Annual Scheme)

Contact Hrs.: 18 Hrs./Week **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 etc. 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 I.R. electronic spectra, Mőssbauer, E.S.R. and magnetic susceptibility measurements. Handling 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. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Mn(acac)_3$
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. $[Cu(NH_3)_4]SO_4H_2O$

Organic Chemistry:

Qualitative Analysis:

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

Organic Synthesis:

Acetylation: Acetylation of cholesterol and sepration of cholesteryl acetate by column chromatography.
Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol
Grignard reaction: Synthesis of triphenylmethanol from benzoic acid
Aldol condensation: Dibenzal acetone from benzaldehyde.
Sandmeyer reactuion: p-Chlorotoluene from p-toluidine.
Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E..
Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate.

Friedel-Crafts reaction: β-Benzoyl propionic acid from succinic anhydride and benzene.
Aromatic electrophilic sustitutions: Synthesis of p-nitroaniline and p-bromoaniline.

The Products may be Characterized by Spectral Techniques.

Quantitative Analysis:

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
Estimation of amines/phenols using bromate bromide solution/or acetylation method. Determination of lodine and Saponification values of an oil sample.
Determination of DO, COD and BOD of water sample.

Physical Chemistry:

Number of hours for 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.

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.

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 transition temperature of given salt (e.g.,$CaCl_2$) conductmetrically.
iii. To construct the phase diagram for three component system (e.g. chloroform-acetic acid-water).

Chemical Kinetics:

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 reaction.

i. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
ii. Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide studing the kinetics as an iodine clock reactions.
iii. Flowing clock reactions (Ref : Experiments in Physical Chemistry by Showmaker)
iv. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion).
v. Oscillatory reaction.

Solution:

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

2. Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behavior 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 acid 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 equilibirum constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Hűckel-Onsager theory.
v. Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulphate using Debye Hűckel's limiting law.

B. Potentiometry/pH metry:

1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the valency of mercurous ions potentiometrically.
3. Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
4. Determination of temperature dependence of EMF of a cell.
5. Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
6. Acid-base titration in a non-aqueous media using a pH meter.
7. Determination of activity and activity coefficient of electrolytes.
8. Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
9. Determination of the dissociation constant of monobasic/dibasic acid by albert-Serjeant method.
10. Determination of thermodynamic constants, DG, DS, and DH for the reaction by e.m.f. method. $Zn + H_2SO_4 \longrightarrow ZnSO_4 + 2H$

Polarimetry:

1. Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
2. Enzyme kinetics-inversion of sucrose.

Books Suggested

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

M.Sc. (Previous) CHEMISTRY Practical Examination

(Annual Scheme)

Distribution of Maximum Marks

Duration of Examination : 14 Hrs. (Spread over 2 days) **Max. Marks : 200**

S. No.	Exp. No.	Details of Experiment	Marks Alloted
1.		**Inorganic Chemistry** (Qualitative and Quantitative Analysis)	
	(i)	Analysis of mixture contain 8 radicals including two radicals of rare elements.	24
	(ii)	Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.	06
	(iii)	Separation of cations and anions by Paper Chromatography or Column Chromatography. **or** Preparation of selected inorganic compounds and their studies by I.R. electronic spectra, Mőssbauer, E.S.R. and magnetic susceptibility measurements.	20
		Total Marks (Inorganic Chemistry)	**50**
2.		**Organic Chemistry**	
	(i)	**Qualitative Analysis:** Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using chromatography, chemical tests. IR spectra to be used for functional group identification.	20
	(ii)	**Quantitative Analysis:** Perform any one of the following exp. a. Estimation of amines/phenols using bromate bromide solution / acetylation method. b. Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method. c. Determination of iodine and Saponification values of an oil sample. d. Determination of DO, COD and BOD of water sample.	15
	(iii)	**Organic Synthesis:** Perform any one of the 9 organic syntheses as mentioned in the syllabus and Products may be Characterized by Spectral Techniques.	15
		Total Marks (Organic Chemistry)	**50**
3.		**Physical Chemistry**	
	(i)	Perform any one physical experiments	25
	(ii)	Perform any one physical experiments A list of experiment under different headings is given in the syllabus, Typical experiments are to be selected from each type. Students are required to perform at least 30 experiments	25
		Total Marks (Physical Chemistry)	**50**
4.		**Viva-voce**	**30**
5.		**Practical Record**	**20**
		Grand Total of Maximum Marks	**200**

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