

**M.Sc. CHEMISTRY
(FOUR SEMESTER COURSE)**

SCHEME OF EXAMINATION

M.Sc. (Previous)

SEMESTER I

Paper	Course No.	Course	Hrs	Marks
				Theory + CCE
✓ Paper I	MCH-401	Inorganic Chemistry I	60	35 + 15 = 50
✓ Paper II	MCH-402	Organic Chemistry I	60	35 + 15 = 50
✓ Paper III	MCH-403	Physical Chemistry I	60	35 + 15 = 50
Paper IV	MCH-404	Group Theory & Spectroscopy I	60	35 + 15 = 50
✓ Paper V	MCH-405	✓ a) Mathematics for Chemists*	60	35 + 15 = 50
		✓ b) Biology for Chemists**	60	35 + 15 = 50
Practical			270	100
Total Marks				350

* For student without Mathematics in B.Sc.

** For student without Biology in B.Sc.

SEMESTER II

Paper	Course No.	Course	Hrs	Marks
				Theory + CCE
Paper VI	MCH-406	Inorganic Chemistry II	60	35 + 15 = 50
Paper VII	MCH-407	Organic Chemistry II	60	35 + 15 = 50
Paper VIII	MCH-408	Physical Chemistry II	60	35 + 15 = 50
Paper IX	MCH-409	Spectroscopy II	60	35 + 15 = 50
Paper X	MCH-410	Computers for Chemists	60	35 + 15 = 50
Practical			270	100
Total Marks				350

SEMESTER I
Class - M.Sc. Prev. (Chemistry)

Paper-I
MCH-401: INORGANIC CHEMISTRY I

MM - 35

Unit-I

Stereochemistry and Bonding in Main Group Compounds :
VSEPR, Walsh diagram (triatomic and penta-atomic molecules), $d\pi-p\pi$ bond, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Unit-II

Metal-Ligand Equilibrium in Solution
Stepwise and overall formation constants and their interaction, trends in stepwise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by potentiometry and spectrophotometry.

Unit-III

Reaction Mechanism of Transition Metal Complexes
Energy profile of a reaction, reactivity of metal complex, inert and labile 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, anion 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-IV

Metal-Ligand bonding
Limitation of crystal field theory, molecular orbital theory for bonding in octahedral, tetrahedral and square planar complexes, π -bonding and molecular orbital theory.

Unit-V

HSAB Theory : Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; donor and acceptor numbers, E and C equation; applications of HSAB concept.

Books Suggested :

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

SEMESTER I

Class - M.Sc. Prev. (Chemistry)

Paper-II

MCH-402: ORGANIC CHEMISTRY I

MM - 35

Unit-I

Nature of Bonding in Organic Molecules

Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy. Level of π -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, catenanes and rotaxanes.

Unit-II

Stereochemistry

Strain due to unavoidable crowding Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

Unit III

Conformational analysis and linear free energy relationship

Conformational analysis of cycloalkanes, decalines, effect of conformation on reactivity, conformation of sugars.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. The Hammett equation and linear free energy relationship, substituents and reaction constants, Taft equation.

Unit-IV,

Reaction Mechanism : Structure and Reactivity

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects

Unit-V

Aliphatic Nucleophilic Substitution

The SN₂, SN₁ mixed SN₁ and SN₂ and SET mechanism. The neighboring group mechanism, neighboring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The SN₁ mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

Book 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, R.O.C. Norman and J.M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.
9. Pericyclic Reactions, S.M. Mukherji, Macmillan, India
10. Stereochemistry of Organic Compounds, D.Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

SEMESTER I

Class - M.Sc. Prev. (Chemistry)

Paper-III MCH-403: PHYSICAL CHEMISTRY I

MM - 35

Unit-I

Introduction to Exact Quantum Mechanical Results

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

Unit-II

Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

Molecular Orbital Theory

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

UNIT III

Angular Momentum

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

Unit-IV

Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems : Excess functions for non-ideal solutions. Activity, activity coefficient, Debye Huckel theory for activity coefficient for electrolytic solutions; determination of activity and activity coefficients; ionic strength. Application of phase rule to three component systems; second order phase transitions.

Unit-V

Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of

undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Fermi-Dirac Statistics, distribution law and applications to metal. Bose-Einstein statistics distribution Law and application to helium.

Books Suggested

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

SEMESTER I

Class - M.Sc. Prev. (Chemistry)

Paper-IV

MCH-404: Group Theory & Spectroscopy I

MM - 35

Unit-I

Symmetry and Group theory In Chemistry

Symmetry elements and symmetry operation, definition of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schoenflies symbols, representations of groups by matrices (representation for the C_n , C_{nv} , C_{nh} , D_{nh} group to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Derivation of character table for C_{2v} and C_{3v} point group Symmetry aspects of molecular vibrations of H_2O molecule.

Unit-II

Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. applications.

Unit-III

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.

Unit-IV

Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman spectroscopy, coherent anti stokes Raman spectroscopy (CARS).

Unit-V

Electronic Spectroscopy

Molecular Spectroscopy

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radio-active and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

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.

Books suggested

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

SEMESTER I
Class - M.Sc. Prev. (Chemistry)

Paper-V
MCH-405 (a) : MATHEMATICS FOR CHEMISTS
(For students without Mathematics in B.Sc.)

MM - 35

Unit-I

Vectors

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

Matrix Algebra

Addition and multiplication; inverse, adjoint and transpose of matrices.

Unit-II

Differential Calculus

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).

Unit-III

Integral calculus

Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

Unit-IV

Elementary Differential equations

First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Unit-V

Permutation and Probability

Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit.

Book Suggested

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclicic, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw 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.

SEMESTER I
Class - M.Sc. Prev. (Chemistry)

Paper-V
CH-405 (b) BIOLOGY FOR CHEMISTS
(For students without Biology in B.Sc.)

MM- 35

Unit-I

Cell Structure and Functions

Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP - the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of bio-macromolecules.

Unit-II

Carbohydrates

Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Unit-III

Lipid

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-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. 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 acid (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.

(81)

Some Oxidation Reaction Solid State Reactions using Solid support-Protection-deprotection Reactions, Oxidations, Reductions, Isomerisations.

Photo Induced Organic Synthesis- Introduction, Photochemical reactions- Industrial application of Photochemistry- The Barton Reactions, Photochemical synthesis of Vitamin D and related compounds, Photo-Oxygenation, Photonitrosation.

Reference Books :-

1. V.K. Ahluwalia & M.R. Kidwai : "New Trends in Green Chemistry", Anamalya Publishers, 2005.
2. V.K. Ahluwailia : "Green Chemistry A Textbook", Narosa Publishers.
3. P.T. Anastes & J.K. Warner : "Oxford Green chemistry theory & Practical", University Press, 1998.
4. M.C. Cann & M.E. Connely : "Real world cases in Green Chemistry Americal Chemical Society, Washington, 2000.
5. M.A. Ryan & M. Tinnesand : "Introduction to Green Chemistry", Americal Chemical Society, Washington, 2002.

BARKATULLAH UNIVERSITY, BHOPAL
SESSION- 2013-14

Class - M.Sc.
Subject - Chemistry
Course Code -
Paper name - Practical
Semester - I

Max. Marks : 100

(Duration: 6-8 hrs in each branch)

Practical examination shall be conducted separately for each branch.

Inorganic Chemistry	8
Qualitative Analysis	8
Chromatography	8
Preparation	4
Record	5
Viva Voce	5
Total	33

Qualitative analysis of inorganic mixture containing eight radicals. (Including insoluble and rare earth)

Chromatography Separation of cations and anions by Column Chromatography : Ion exchange.

Chromatography Separation of cations and anions by Paper Chromatography.

Preparations

Preparation of selected inorganic compounds and their studies by I.R. electronic spectra, mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds.

1. VO(acac)₂
2. TiO(C₉H₈NO)₂H₂O
3. cis-K[Cr(C₂O₄)₂(H₂O)₂]
4. Na[Cr(NH₃)₂(SCN)₄]
5. Ni(acac)₂
6. K₃[Fe(C₂O₄)₃]
7. Prussian Blue, Turnbull's Blue.

Organic Chemistry	12
Qualitative Analysis	12
Organic Synthesis	4
Record	5
Viva Voce	5
Total	33

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid or 2 solids) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis

Synthesis of organic compounds by applying following methods.

- (i) Acetylation
- (ii) Oxidation
- (iii) Halogenation
- (iv) Benzoylation
- (v) Reduction

The products may be characterized by spectral techniques.

Physical Chemistry

Error Analysis and Statistical Data Analysis	8
Conductometry	9
Solution	8
Record	4
Viva Voce	5
Total	34

1. **Error Analysis and Statistical Data Analysis**
 Errors, types of errors, minimization of errors distribution curves precision, accuracy and combination; statistical treatment for error analysis 't test, null hypothesis, rejection criteria. F & Q test; linear regression analysis, curve fitting. Calibration of volumetric apparatus, burette, pipette and standard flask.

2. **Conductometry**
 - i. Determination of velocity constant, order of 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 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 equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone, water) and to test the validity of Debye-Huckel-Onsager theory.
 - v. Determination of the activity coefficient of zinc ions in the solution of 0.002-M-zinc sulphate using Debye Huckel's limiting law.

3. Solution

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

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

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

Books Suggested

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