

SYLLABUS

SESSION: (2018-19)

COURSE: M.Sc. I (Semester I and II)

FACULTY OF SCIENCES

P. G. DEPARTMENT OF CHEMISTRY



MATA GUJRI COLLEGE

Fatehgarh Sahib

(AN AUTONOMOUS COLLEGE)

Affiliated to Punjabi University, Patiala

Scheme of Course
M.Sc. CHEMISTRY Part I (Semester I and II)

Paper Code	Title of Paper	Credits	No. of Lectures	Max. Marks (External+Internal) Pass Percentage 35%	Time Allowed
<u>SEMESTER I</u>					
<u>Core Subjects</u>					
MCH 101	Inorganic Chemistry	5	65	75 (55+20)	3 Hrs.
MCH 102	Organic Chemistry	5	65	75 (55+20)	3 Hrs.
MCH 103	Physical Chemistry	5	65	75 (55+20)	3 Hrs.
<u>PRACTICALS</u>					
MCH 105	Inorganic Chemistry Practicals	3.75	100	100	6 Hrs.
MCH 106	Analytical Chemistry Practicals	3.75	100	100	6 Hrs.
<u>Elective Subjects</u>					
*MCH 104 (A)	Mathematics for Chemists	5	65	75 (55+20)	3 Hrs.
*MCH 104 (B)	Biology for Chemists	5	65	75 (55+20)	3 Hrs.
<u>SEMESTER-II</u>					
<u>Core Subjects:</u>					
MCH 201	Inorganic Chemistry	5	65	75 (55+20)	3 Hrs.
MCH 202	Organic Chemistry	5	65	75 (55+20)	3 Hrs.
MCH 203	Physical Chemistry	5	65	75 (55+20)	3 Hrs.
<u>PRACTICALS</u>					
MCH 205	Organic Chemistry Practicals	3.75	100	100	6 Hrs.
MCH 206	Physical Chemistry Practicals	3.75	100	100	6 Hrs.
<u>Elective Subject</u>					
MCH 204	Computer Fundamentals and Programming	5	65	75 (55+20)	3 Hrs.

INDUSTRIAL TRAINING: The candidates will be required to undergo training in an R & D Organizations and will submit project report followed by its presentation and viva-voce. Candidates will be awarded weightage for the project report and training in the internal assessment.

* **Note :** B.Sc. Non-medical students will take Biology for Chemists paper while B.Sc. Medical students will take the paper Mathematics for Chemists.

SEMESTER-I

PAPER-MCH 101: INORGANIC CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

OBJECTIVE OF THE COURSE

The syllabus pertaining to M.Sc. (1st Year Course) in Chemistry in the subject of Chemistry has been upgraded as per provision of the UGC module and demand of the academic environment. The course contents are revised from time to time as per suggestions of the members of the Board of Studies of the Chemistry. The syllabus contents are duly arranged unit wise and contents are included in such a manner so that due importance is given to requisite intellectual and laboratory skills.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 8 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 8.5marks each. Unit III will consist of 11 short answer questions that will cover the entire syllabus and will be of 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Chemical Bonding:

Ionic bond, covalent bond, polarization of ions, Fajan's rules, bond characteristics, wave mechanical treatment of covalent bond, the variation principle, ground state energy of hydrogen atom, the secular equations, valence bond theory, concept of resonance, resonance energy, molecular orbital theory, LCAO principle, Molecular Orbital treatment of H_2^+ ion, construction of MO and VB wave functions, electron charge densities in molecular orbitals of H_2^+ ion, hybridization, wave functions for sp^3 hybrid orbitals, the three centered bond, Linnett's double quartet approach, the Pauli exclusion principle, vander Waal 's forces, the hydrogen bond.

Introduction to Ligands and Complexes:

Types and classification of ligands, Acceptor character of CO, N₂, O₂, NO molecules in terms of molecular orbital energy level diagrams, Pi acid ligands: CO as prototype, other pi acid ligands-isocyanide ligands, dinitrogen, the CS ligands, the NO ligands, pi acid ligands: trivalent phosphorus compounds, multiple bonds from ligands to metals, semi-bridging in metal carbonyls, pi complexes of unsaturated organic molecules: alkene & alkyne, enyl, aromatic ring systems, hardness and softness of ligands, symbiosis and antisymbiosis. **33 Hrs.**

UNIT II

Main Group elements:

Molecular, ionic and metallic hydrides; organolithium, organosodium and organopotassium compounds; organoberyllium and organomagnesium compounds; boron-nitrogen compounds: borazine, substituted borazines, and boron nitride; boron clusters: metal borides, structure and bonding of polyhedral boranes, closo, nido and arachno structures, structural study by NMR, Wade's rules, metalloboranes, carboranes, metallocarboranes; organoboron and organoaluminium compounds; compounds with C-N and C-S bonds, carbides, silicates, zeolites, organosilicon compounds.

Nitrides, azides, dinitrogen and nitrogen compounds as ligands: nitrogen monoxide, ammonia and amines, chemical properties of dioxygen, singlet oxygen, dioxo, peroxy, superoxy ligands; Phosphorus-Nitrogen compounds: phosphazenes, cyclo and linear phosphazenes; chemistry and bonding of sulphur-nitrogen compounds, charge transfer complexes of halogens, interhalogen compounds, polyhalogen compounds, interhalogen cations, polyiodide anions. Noble gas compounds: synthesis, structure and reactions of xenon fluorides, xenon-oxygen compounds, compounds of Krypton and Radon.

32Hrs.

Books Recommended:

1. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry.
2. J.D. Lee, Concise Inorganic Chemistry, 4th edition.
3. Shriver and Atkins, Inorganic Chemistry, 5th edition.
4. L. Miessler, D.A. Tarr, Inorganic Chemistry, 3rd edition.
5. F.A. Cotton, Wilkinson, Advanced Inorganic Chemistry, 3rd, 5th and 6th edition.
6. F. Basolo and R.C. Johnson, Coordination Chemistry, 1st edition.

PAPER-MCH 102: ORGANIC CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures:65

Time: 3 hours

Pass marks: 35%

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INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Reactive Intermediates:

Carbocations: Generation, Structure, Stability, allylic and benzylic carbocations. Stereochemistry and reactions. Nonclassical carbocations, Phenonium ion, norbornyl system. Application of NMR spectroscopy in the detection of carbocations. Carbanions: Generation, Structure, stability, stereochemistry and general reactions. Carbenes: Formation, Structure, Singlet & Triplet carbene, Stereochemistry and reactions. Nitrenes: Formation, Structure Singlet & Triplet nitrene, Stereochemistry and reactions. Arynes: Formation, Structure and reactions. Free radicals: Formation, Structure, Stability, Stereochemistry and reactions.

Reactions of free radicals:

Polymerisation, Halogenation: Chlorination, Bromination by NBS, Iodination, Fluorination. Polar effects in halogenations. Addition reactions: Free radical addition of HBr, thiols and halogens. Auto-oxidation. Rearrangements.

Nature of Bonding in Organic Molecules:

Introduction to fullerenes, Aromaticity in benzenoid and non-benzenoid compounds, Alternant and non-alternant hydrocarbons, Huckel's rule, Anti-aromaticity, Homo-aromaticity, Annulenes. Bonding weaker than covalent: Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxanes.

Techniques used for determination of reaction mechanism:

Use of optical, stereochemical and isotope techniques. Reaction studies from identification of products. Trapping of intermediates, Crossover experiments. Use of Catalyst, use of isotopes in reaction mechanism studies in case of Favorskii, Claisen and Benzyne reactions. **32Hrs.**

UNIT-II

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 & PMO approach. Electrocyclic reactions: Conrotatory and disrotatory motions, $4n$, $4n+2$, and allyl systems. Cycloadditions: antarafacial and suprafacial additions, $4n$, $4n+2$ systems, $2+2$ addition of ketenes; 1,3-dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shift of hydrogen, Sigmatropic shifts involving carbon moieties. 3, 3- and 5, 5-sigmatropic rearrangements. Claisen, Cope rearrangements, Ene reactions.

Elimination Reactions:

E_2 , E_1 and E_{1cB} mechanism, stereochemistry, product ratio, orientation of double bond, Hoffman's rule, Saytzeff's rule, Factors governing E_2 and E_1 mechanism. Mechanism and orientation in pyrolytic elimination reactions.

Cyclic Elimination:

Amine Oxide, Esters, Xanthates, Free radical elimination. Elimination versus substitution. Effect of solvent, Temperature, Nature of Base, Structure of Reactant.

Aromatic Elimination:

Benzyne, Nucleophilic aromatic substitution, addition-elimination mechanism.

33 Hrs.

Books Recommended:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry- F.A. Carey & 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. Reaction Mechanism in Organic Chemistry, S.M. Mukherji& S.P. Singh. Macmillan.
8. Highlights of Organic Chemistry- An Advanced Text Book- W.J.L. Nobel.

PAPER-MCH 103: PHYSICAL CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

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UNIT-I

Basics of Chemical Thermodynamics:

Thermodynamic Properties: - state and path properties, first and second law of thermodynamics, Maxwell relations, thermodynamic equation of state, Joule Thomson effect, Nernst heat theorem, thermodynamic entropy, evaluation of absolute entropy, third law thermodynamics, Identification of statistical and thermodynamic entropy, determination of absolute entropies of solids, liquids and gases.

Non ideal system: Excess thermodynamic functions, determinations of partial molar properties, fugacity and activity, fugacity of gases, fugacity of mixture of gases, experimental determination of fugacity, determination of activity and activity coefficients of non-electrolytes.

Thermodynamics of living systems: Simultaneous or coupled reactions, coupled reactions and metabolism, free energy utilisation in metabolism, terminal oxidation chain overall metabolic plan general thermodynamic consideration of living systems.

Statistical Thermodynamics: Microstates and macrostates, concept of distribution, thermodynamic probability and most probable distribution. Ensembles, statistical mechanics for systems of independent particles and its importance in chemistry, Lagrange's undetermined multipliers, Sterling's approximation, types of statistics, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, derivation of distribution laws (most probable distribution) for the three types of statistics molecular partition function and its importance, translational, rotational, vibrational, electronic and nuclear partition functions, expression for internal energy, entropy, Helmholtz function, Gibb's free energy, pressure, work and heat in terms of partition function.

32 Hrs.

UNIT-II

Electrochemistry:

Ions in solution: Deviation from ideal behavior, ionic activity, Born model of ion-solvent interaction, Debye - Huckel theory of activity coefficients of strong electrolytes, Debye-Huckel limiting law, verification of Debye-Huckel limiting law, Bjerrum's theory of ion association in electrolyte solutions, ion-ion and ion-solvent interactions, mean ionic activity coefficients.

Conductance and Ionic Mobilities: Variation of equivalent conductance with concentration, Debye-Huckel Onsager equation, conductance at high frequencies and high potentials, modification of Debye-Huckel Onsager equation, some applications of conductance measurements, ion association and ion pair formation, ion triplets, ion triplets in electrolyte solutions, ion triplets and conductance.

Applied Electrochemistry:

Electrical Double Layer, electrokinetic phenomenon, null point and its determination, structure of electrical double layer, parallel plate condenser theory, diffuse layer theory and adsorption theory of double layer.

Electrocatalysis A chemical catalyst and an electrochemical catalyst, electro catalysis in redox reactions, electro catalysis in reaction involving adsorbed species, some specific features of electro catalysis.

Kinetics of electrode reactions: The ButlerVolmer equation, equilibrium current density, the diffusion over potential.

Bio electrochemistry: Cell membranes, membrane potentials and its Modern theory, The Hodgkin-Huxley theory of membrane potentials.

33 Hrs.

Books Recommended:

1. Bockris and Reddy, Modern Electrochemistry, Vol. I & II.
2. Glasstone Electrochemistry.
3. Dickerson, Molecular Thermodynamics .
4. Glasstone Thermodynamics for Chemists.
5. Peter Atkins, Julio Paula, Physical Chemistry.
6. Keith J. Laidler, Chemical Kinetics, 3rd Edition.

PAPER-MCH 104(A): MATHEMATICS FOR CHEMISTS

(For Students without Mathematics in B. Sc.)

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

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Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Matrix Algebra: Addition and multiplication, determinants (up to 4th order) 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 solutions, linear dependence and independence. Cayley Hamilton Theorem, Eigen values and Eigen vectors.

Trigonometry: Degree and radian measure of positive and negative angles, relation between degree and radian, Definition of trigonometric functions with the help of unit circle, Periodic functions, Concept of periodicity of trigonometric functions, values of

trigonometric functions for different angles, trigonometric functions of sum and differences of angles, additions and subtraction formulae .

Matrix Algebra: Addition and multiplication, determinants (up to 4th order) inverse of a matrix, special matrices (Symmetric, skew –symmetric, hermitian, skew-hermitian, unit, diagonal, unitary etc.) and their properties. **32 Hrs.**

UNIT-II

Calculus: Differential calculus: Differentiability, rules for differentiation, applications of differential calculus including maxima and minima.

Integral Calculus: Basic rules for integration, integration by parts, partial fraction and Substitution, definite integrals.

Elementary Differential Equations: Variables separable and exact, first order differential equations. Homogeneous exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc.

Permutation and probability: Permutations and combinations, probability, probability theorems examples from the Kinetic theory of gases. **33Hrs.**

Books Recommended:

1. The chemistry Mathematics Book, E. Steiner, Oxford University Press, 2nd Ed., 2008
2. Mathematics for chemistry, Doggett and Sucliffe, Longman, 1995
3. Mathematical preparations for physical chemistry, F. Daniels, McGraw Hill, 1958.

PAPER-MCH 104(B): BIOLOGY FOR CHEMISTS

(For Students without Biology in B. Sc.)

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

OBJECTIVE OF THE COURSE

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INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Origin of Life: Unique properties of Carbon, Chemical evolution and rise of living systems. Introduction of biomolecules, building blocks of biomolecules.

Cell Structure & Functions: Structure of prokaryotic & 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.

Cell Division: Cell division stages of mitosis & meiosis. Significance of cell division and fertilization

Carbohydrates: Conformation of monosaccharides, structure & functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars, N-acetyl muramic acid, Sialic acid, disaccharide & Polysaccharides. Structural

polysaccharides - cellulose and chitin. Storage Polysaccharides: starch and glycogen. Structure and Biological functions of glucosaminoglycans or muco polysaccharides, 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.

Lipids: Fatty acids, essential fatty acids, structure and function of triglycerols, 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. **32Hrs.**

UNIT -II

Structure of Proteins: Chemical and enzymatic hydrolysis of Proteins to peptides, amino acid. Secondary structure of proteins, forces responsible for folding of secondary structure, α -triple 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 (An overview), sequence determination: Edman degradation. Chemistry of oxytocin and thyroxine releasing hormone (TRH).

Enzymes: Enzymes as biological catalyst and mode of their action.

Structure of Nucleic Acids: Purines 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.

Replication of DNA: The chemical basis of heredity and overview of replication of DNA.

Protein synthesis & Genetic Code: Transcription, translation and genetic code.

33 Hrs.

Books recommended:

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

PAPER-MCH 105: INORGANIC CHEMISTRY PRACTICALS

Maximum Marks: 100

Time: 6 Hours

1. Oxidation Reduction titration:

- a) Standardisation of KMnO_4 and determination of nitrites.
- b) Standardization of $\text{K}_2\text{Cr}_2\text{O}_7$ and determination of Fe^{2+}
- c) Standardisation of $\text{Na}_2\text{S}_2\text{O}_3$ with KIO_3 and determination of I^-

2. Precipitation Titration:

- a) Standardisation of AgNO_3 by using adsorption indicator.
- b) Standardisation of thiocyanate solution and determination of Chloride by Volhard Method.

3. Complexometric Titrations:

- a) Determination of Ca^{2+} in milk
- b) Determination of Al^{3+} by back titration.
- c) Determination of Cu^{2+} and Ni^{2+} by using masking reagents.
- d) Determination of total hardness of water by EDTA titration

4. Gravimetric/titrimetric determination of mixed ions:

- a) Copper-Nickel
- b) Iron-nickel
- c) Copper-Zinc

5. Preparation of following compounds:

- a) Preparation of tetraamminecopper(II) sulphate
- b) Preparation of hexamminecobalt (III) chloride.
- c) Preparation of tris-thiourea cuprous chloride

PAPER-MCH106: ANALYTICAL CHEMISTRY PRACTICAL

Maximum Marks: 100

Time: 6 Hours

1. To determine the percentage purity of given sample of KBr using adsorption indicator (Eosin).
2. To determine the strength of ascorbic acid in the given solution of vitamin C tablet by titrating against (a) standard I_2 solution (b) standard sodium thiosulphate solution.
3. To determine the amount of H_2O_2 in the given solution by titrating against (a) standard $KMnO_4$ solution (b) Standard sodium thiosulphate solution.
4. To determine the percentage purity of given sample of KI by titrating against standard KIO_3 solution.
5. To determine the strength and composition of HCl and CH_3COOH solution by titrating it against NaOH pH metrically.
6. To determine the strength and composition of HCl and CH_3COOH solution by titrating it against NaOH conductometrically.
7. To determine the strength of $FeSO_4 \cdot 7H_2O$ solution by titrating it against standard $KMnO_4$ solution potentiometrically.
8. To determine the strength of strong acid by titrating it against strong base potentiometrically.
9. To determine the strength of unknown solution of $CuSO_4 \cdot 5H_2O$ colorimetrically.
10. To determine the strength of unknown solution of $K_2Cr_2O_7$ solution colorimetrically.
11. To determine the strength of unknown solution of $KMnO_4$ solution colorimetrically.
12. To determine the strength of Fe^{3+} in tap water spectrophotometrically (Record of λ_{max}).

SEMESTER-II

PAPER-MCH 201: INORGANIC CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

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UNIT-I

Group Theory:

The concept of group, order and classes of group, symmetry elements, symmetry operations and their matrix representation, multiplication tables, point group determination, determination of reducible and irreducible representations, character tables, construction of character tables for C_{2v} and C_{3v} point groups, application of group theory to chemical bonding, splitting of d-orbitals under the influence of octahedral, tetrahedral and square planar symmetry, the directed valence for O_h and T_d symmetry,

use of character tables to determine which metal orbitals are used in σ and π bond formation in octahedral, tetrahedral and square planar complexes, molecular orbital energy level diagrams for octahedral tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes.

Applications of Group Theory in Spectroscopy:

Symmetry considerations regarding selection rules and spectral intensities, vibronic coupling, vibronic polarization in centrosymmetric complexes and non-centrosymmetric complexes, polarization of electronically allowed transitions, selection rules regarding IR and Raman scattering spectroscopy, fundamentals, overtones and combinations in vibrational spectroscopy, mutual exclusion principle, symmetry symbols for normal modes of vibration, IR and Raman activity of their fundamentals and nature of vibrations in terms of change in internal coordinates in simple molecules like trans N_2F_2 , SF_6 .

32Hrs.

UNIT-II

Metal-Ligand Bonding in Coordination Complexes:

Crystal field theory, splitting of d-orbitals under the effect of octahedral, tetrahedral, tetragonal and square planar crystal fields, pairing energy, factors affecting the magnitude of crystal field splitting, use of CFT in explaining magnetic properties of transition metal complexes, the structural (ionic radii, Jahn-Teller effects) and thermodynamic effects (hydration and lattice energy) of crystal field splitting, the limitations of crystal field theory, the ligand field theory, molecular orbital theory, the comparison of VBT, CFT and MOT in case of transition metal complexes, the angular overlap model.

Atomic Spectroscopy:

Spin-spin coupling, orbital-orbital coupling, LS and j-j coupling schemes, determination of free ion terms for p^n and d^n configurations, determination of ground state terms-Hund's rule, hole formulism, spin-orbit coupling, the effect of octahedral and fields on S, P, D and F terms with the help of character tables, splitting patterns of G, H, I terms under the effect of weak octahedral and tetrahedral fields, Orgel diagrams

Free ions in Medium and Strong Crystal Fields:

Strong field configurations, transitions from weak to strong crystal fields, construction of correlation diagrams, spin cross over in coordination compounds, Tanabe Sugano diagrams (d^1 , d^2 , d^8 , d^9 octahedral and tetrahedral).

33 Hrs.

Books Recommended:

1. M.C. Day, J. Selbin, Theoretical Inorganic Chemistry.
2. F.A. Cotton, Wilkinson, Advanced Inorganic Chemistry, 5th edition
3. Shriver and Atkins, Inorganic Chemistry, 5th edition.

4. F.A. Cotton, Chemical Application of Group Theory.
5. G. Davidson, Introductory Group Theory For Chemists
6. B.N. Figgis, Introduction to Ligand Field.
7. A.B.P. Lever, Inorganic Electronic Spectroscopy.
8. R.S. Drago, Physical Method in Chemistry.

PAPER-MCH 202: ORGANIC CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

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UNIT-I

Stereochemistry:

Stereoisomerism: Introduction and different types of stereoisomerism. Fisher, Newman and Saw horse representations for organic compounds and their interconversions. Optical isomerism: Requirement for a compound to be optically active, compounds with one asymmetric centre. Dissymmetry as a cause of optical activity Molecules with two asymmetric centres. Racemic modification. Racemisation: Thermal, anionic, cationic, free radical, epimerization, Mutarotation, Racemic compounds mixtures and solid solutions.

Methods of resolution of acids, bases, amino acids, alcohols, aldehydes, ketones. Absolute and relative configuration, Different systems of notation. Asymmetric induction, Methods of determining the configuration: Cram's Rule and Prelog's Rule.

Conformational Isomerism:

Meaning of conformation. Conformation and reactivity in alicyclic compounds. Conformation and physical properties, dipole moment, NMR, IR and X-rays. Conformational effects on stability and reactivity. Ionic elimination. Intra molecular rearrangement, Neighbouring group participation. Pyrolysis of acetates xanthates and amine oxides. Relation of conformation to reactivity. Optical isomerism due to restricted rotation in biphenyls, allenes, alkylidenes and spiranes and determination of their absolute configuration.

Conformational studies in cycloalkanes, mono and disubstituted cycloalkanes- stability and reactivity. Energy determination in chair and boat form. Studies in fused systems: Decalins and Perhydrophenanthrenes.

Geometrical Isomerism:

Nomenclature (E & Z) Nature of geometrical isomerism and determination of Configuration. Curtin – Hammet Principle. Study of Physical properties of the isomers, Relative stability and interconversion of Geometrical isomers.

33 Hrs.

UNIT-II

Addition to Carbon-Carbon Multiple Bond:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regioselectivity and Chemoselectivity. Orientations and reactivity. Addition to cyclopropane ring. Hydrogenation of double bond and triple bond and aromatic rings. Hydroboration, Michael reaction, Sharpless Asymmetric Epoxidation.

Addition to Carbon-Hetero Multiple Bond:

Mechanism of Metal hydrides. reduction of carbonyl compounds and other functional groups, Dissolving metal reductions and conjugated systems.

Wolf-Kishner reduction, Clemmenson reduction, Meerwein Ponderoff Varley reduction, Wittig's reaction, Addition of Grignard's reagent, Organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds.

Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides.

Ammonolysis of esters.

32 Hrs.

Books Recommended:

1. Stereochemistry of Carbon compounds by Ernest L. Eliel, Tata McGraw Hill.

2. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
3. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.
4. Modern Organic Reactions, H.O. House, Benjamin.
5. Organic Chemistry, Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Oxford University Press.
6. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, John Wiley.

PAPER-MCH 203: PHYSICAL CHEMISTRY

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

OBJECTIVE OF THE COURSE

The syllabus pertaining to M.Sc. (1ST Year Course) in Chemistry in the subject of Chemistry has been upgraded as per provision of the UGC module and demand of the academic environment. The course contents are revised from time to time as per suggestions of the members of the Board of Studies of the Chemistry. The syllabus contents are duly arranged unit wise and contents are included in such a manner so that due importance is given to requisite intellectual and laboratory skills.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 8 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 8.5marks each. Unit III will consist of 11 short answer questions that will cover the entire syllabus and will be of 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Basics of quantum chemistry: Introduction of quantum chemistry, operators, postulates of quantum chemistry, eigen value and eigen function, normalization and orthogonality, Schrodinger wave equation.

Application of quantum chemistry to simple systems:

Translational motion: Particle in one dimensional box, particle in three dimensional box-rectangular and cubical box, particle with finite potential barrier, one finite potential barrier, two finite potential barrier, the quantum mechanical tunneling

Vibrational motion: Hooke's law, harmonic oscillator, the quantum mechanical derivation for a harmonic oscillator model of a diatomic molecule, a harmonic oscillator accounts for IR spectrum of a diatomic molecule, physical interpretation of ψ and ψ^2 .

Rotational motion: Rigid rotator, derivation of energy and wave function of rigid rotator, rotation in one plane, rotation in space.

Hydrogen and Hydrogen like atoms: Spherically symmetric potential and the Hamiltonian, spherical coordinates, Schrodinger wave equation in terms of r, θ, Φ , radial eigen functions, atomic orbitals of hydrogen like atoms, significance of the quantum numbers n, l, m . graphical representation of the orbitals (s, p).

Approximate methods: Variation principle-linear and non linear variation theory, Perturbation theory, application of variation and perturbation theory to He atom.

Theory of angular momentum: Angular momentum, quantum mechanical operator for angular momentum, ladder operator, eigen function and eigen values of angular momentum using ladder operator, orbital and spin motion, spin angular momentum, addition of angular momentum, coupled and uncoupled representation of angular momentum.

Molecular orbital theory (MOT): LCAO approximation, the H_2^+ ion, the LCAO MO wave function of H_2^+ ion, electron density and bonding in H_2^+ , physical representation, bond order, charge density calculation, free valence, conjugated molecules, Huckel MOT of conjugated systems, Huckel rule of aromaticity, applications of Huckel MOT to ethylene, butadiene, elementary idea of extended Huckel theory.

32 Hrs.

UNIT-II

Introduction of chemical kinetics: Introduction, factors influencing on reaction rates, influence of temperature on reaction rates, order and molecularity of reaction, methods of determination of order of reaction,

Theories of reaction rates: Arrhenius equation and its limitations, collision and absolute reaction rate theories, statistical derivation of rate equation (Eyring equation), thermodynamic formulation of reaction rates, free energy of activation, heat of activation and its relationships with various kinds of activation energies, relationship between steric factor and entropy of activation, transmission coefficient, unimolecular reactions, Lindmann theory, Hinshelwood theory, RRK theory, RRKM theory.

Complex reactions: Parallel reactions, reversible reactions, consecutive reactions, branching reactions, oscillating reactions, steady state treatment.

Fast reactions: Determination of fast reactions by NMR method, relaxation method, temperature jump method, pressure jump method, flow and stopped flow method.

Reactions in solution: Primary and secondary salt effects, effect of polarity and nature of solvent on rate of reaction.

Catalysis: Introduction, characteristics of catalytic reactions, types of catalysis, heterogeneous catalysis, electrocatalysts, homogeneous catalysts, organo catalysis, photocatalysts, nanocatalysts, tandem catalysis, autocatalysis, inhibitors, poisons, and promoters, acid base catalysis, enzyme catalysis, Michaelis-Menten equation, effect of temperature and pH on enzyme catalysis. **33 Hrs.**

Books Recommended:

1. Kinetics and mechanism by A.A Frost & R.G Pearson, John-Wiley, & sons Inc., N.York.
2. Physical Chemistry by P.W. Atkins.
3. Chemical kinetics methods by C.Kalidas, New Age International Publishers.
4. Introduction to Quantum Chemistry, A.K.Chandra, Tata McGraw Hill.
5. Quantum Chemistry by I.N. Levine, Prentice Hall.
6. Quantum Chemistry by R.K. Prasad.
7. Physical Chemistry by Puri, Sharma & Pathania
8. Physical Chemistry by Gurdeep Raj
9. Physical Chemistry by Gurtu & Gurtu
10. Quantum Chemistry by Donald A McQuarie

PAPER-MCH 204: COMPUTER FUNDAMENTALS AND PROGRAMMING

Maximum Marks: 75

(i) Semester Examination: 55

(ii) Internal Assessment: 20

Lectures: 65

Time: 3 hours

Pass marks: 35%

OBJECTIVE OF THE COURSE

The syllabus pertaining to M.Sc. (1st Year Course) in Chemistry in the subject of Chemistry has been upgraded as per provision of the UGC module and demand of the academic environment. The objective of this paper is for the students to understand the basics of computer and basics of programming so that they are able to solve computational problems. The syllabus contents are duly arranged unit wise and contents are included in such a manner so that due importance is given to requisite intellectual and laboratory skills.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 8 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 8.5marks each. Unit III will consist of 11 short answer questions that will cover the entire syllabus and will be of 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given on the basis of attendance, mid semester tests and assignments.

UNIT-I

Computer Fundamentals: Definition, Characteristics, Application of Computer, Number Systems: Binary, Octal and Hexadecimal Conversion, Binary Arithmetic, Computer Languages: Machine Language, assembly language, high level language, assembler, compiler and interpreter.

Programming Fundamentals: Algorithms, characteristics and Examples of algorithms, Flowcharts, symbols used in flowcharts, Examples of flowcharts, Pseudocode, character set, Identifiers and keywords, constants, variable.

Data Types: Declaring(integer, float and character), Defining and Initializing Variables, Scope of Variables, Using Named Constants, Casting of Data Types, Storage Classes

Operators and expressions: Arithmetic, Unary, Logical and Relational operators, assignment operators, Conditional operators. **32 Hrs.**

UNIT-II

Control statements: Branching constructs, looping constructs, nested control structures, switch, break and continue statements.

Functions: Declaration, Definition, Call, passing arguments, call by value, call by reference, Recursion, Use of library functions; Storage classes: automatic, external, register and static variables.

Arrays: Using one dimensional and two dimensional arrays, Passing array to a function, Solving matrices problem using arrays; Strings: input/output of strings, string handling functions. **33 Hrs.**

Books Recommended:

1. Let Us C by Yashavant Kanetkar, (BPB Publications, New Delhi).
2. Programming in ANSI by E. Balgurusamy, Tata McGraw-Hill Publishing Co. I.T., NewDelhi.

PRACTICAL / LAB WORK TO BE PERFORMED ON A COMPUTER: LIST OF PROGRAMS

- Use of input and output functions
- Use of data types and operators
- Use of conditional and loop statements
- Program to find the area of right angle triangle.
- Program to swap value of two variables without using third variable.
- P to test whether a given no. is even or odd.
- Program to check if a no. is divisible by 5 and or not.
- Program to calculate greatest of 3 numbers.
- Program to print n prime numbers.

- Program to print whether a given number is prime or not.
- Program to calculate factorial of a number.
- Program to calculate roots of a quadratic equation.
- Program to calculate the compound interest.
- Program to check the H.C.F of n numbers using recursion.
- Program to reverse a given number and check whether a given number is same as that of reverse number.
- Program to find the entered year is leap year or not.
- Program to find sum of first 20 odd natural numbers.

PAPER-MCH 205: ORGANIC CHEMISTRY PRACTICALS

Maximum Marks : 100

Time : 6 Hours

Qualitative Organic Analysis:

Separation and Purification of components of binary mixture (solid/solid, solid/liquid, liquid/liquid) on the basis of solubility behavior and solvent extraction and their identification and conformation by chemical tests and preparation of suitable derivative.

Organic Synthesis:

Benzoylation	:	Hippuric acid
Oxidation	:	Adipic acid/p-Nitrobenzoic acid
Aldol condensation	:	Dibenzalacetone/Cinnamic acid
Sandmeyer's reaction	:	p-Chlorotoluene
Benzfused Heterocycles	:	Benzimidazole
Cannizzaro's reaction	:	p-Chlorobenzaldehyde as substrate
Friedel Crafts reaction	:	β -Benzoylpropionic acid
Aromatic electrophilic Substitution	:	p-Nitroaniline / p-Iodoaniline

The products may be characterized by spectral techniques and checking the purity of prepared compounds by Thin Layer Chromatography.

Note: Subject to the availability of Instrument/Chemicals, the experiments can be substituted by alternate experiments.

Books Recommended:

1. Vogel's Textbook of Practical Organic Chemistry, 5th Edition ELBS (Longman), 1996.
2. Practical Organic Chemistry by F.G. Mann and B.C. Saunders, 5th Edition, Orient Longman Limited, 1986.

PAPER-MCH 206: PHYSICAL CHEMISTRY PRACTICALS

Maximum Marks: 100

Time: 6 Hours

1. To determine the molecular weight of given polymer by viscosity method.
2. To determine the percentage composition of solutions containing water-ethanol by viscosity method.
3. To determine the percentage composition of solutions containing water-ethanol by surface tension method.
4. To determine the atomic parachors of C, H and O.
5. To compare the cleansing powers of two samples of detergents by surface tension method.
6. To determine the interfacial tension between two immiscible solvents (water-benzene, water-toluene).
7. What is the effect of pH on the emission profile of a dye.
8. To find out the value of coefficient of expansion for the given liquid with the help of pyknometer.
9. To find out the molar refractivities of homologous series of alcohols and also find out the atomic refractivities of C and H.
10. To find out the molar refractivity of the given solid.
11. To find out the equilibrium constant for the given reaction, $KI + I_2 = KI_3$ by partition method.
12. To determine the rate constant of the hydrolysis of ethyl acetate catalysed by an acid and also find out the half life period of the reaction.
13. To determine the order of saponification of ethylacetate with NaOH.
14. To study the adsorption of acetic acid on activated charcoal and prove the validity of Freundlich adsorption isotherm.