M.Sc. (Chemistry) Part-II

Session: 2024-2025

Semester-II

Course code	Title of the paper	Hours per week			Total Credits	University Exams (hrs.)	Maximum marks		
		L	T	P			IA	SE	Total
Core Subjects									
MCHEM 1201T	Inorganic Chemistry	5	0	0	5	3	30	70	100
MCHEM1 202T	Organic Chemistry	5	0	0	5	3	30	70	100
MCHEM 1203T	Physical Chemistry	5	0	0	5	3	30	70	100
Elective Subjects									
MCHEM 1204 T	Computer Fundamental & Programming with C	5	0	0	5	3	30	70	100
Practical Subjects									
MCHEM1107L	Organic Chemistry Lab-II	0	0	6	3.75	6	30	70	100
MCHEM1108L	Physical Chemistry Lab-II	0	0	6	3.75	6	30	70	100

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SEMESTER-II
MCHEM 1201T
Inorganic Chemistry

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

65 hours
Time allowed- 3hrs
5 period/week
Credit: 05

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three sections: A, B, and C. Sections A and B will have four questions from the respective sections of the syllabus and will carry 12 marks each. Section C will consist of 11 short-answer questions from the entire syllabus and will carry 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt five questions selecting two questions from each of Section A and B and Section C will be compulsory.

Course Outcomes (C.O.):

1. Concepts of symmetry and group theory in solving chemical structural problems.
2. Enable the students tc predict the point group of important molecules. To understand the ideaof space groups and to learn the theory of molecular symmetry.
3. Use of character tables, Application of symmetry and group theory in spectroscopy.
4. To gainskill to apply group theory to vibrational and electronic spectroscopy.
5. The students will acquire knowledge of properties and applications of compounds of main group elements.

Section – A

Group Theory

Order, classes of group, representation of a group, transformation of coordinates matrices, matrix representation of symmetry operation, reducible and irreducible representations and C_{2v},C_{3v}, D_{4h}, Td, Oh, character tables, symmetry, the method of finding the number of irreducible representation in a reducible representation, separation of d orbitals under influence of octahedral, tetrahedral, sq. planar and trigonal bipyramidal symmetry, the separation of P, D, F etc. free ion terms into symmetry labelled electric field terms under the influence of octahedral field, the directed valence for Td and Oh symmetry, direct productfor Oh, Td, C3v, D4h and D5h and the method of descending symmetry for d^2 configuration.

Applications of Group Theory

Suitable metal orbitals and ligand or orbitals combination to form molecular orbitals in coordination complexes Oh, Td and square planar complexes, symmetry consideration regarding selection rules and spectral intensties,vibronic coupling, vibronic polarization in centrosymmetric complexes Oh and D4h and non – centro symmetric complexes C3v, Td polarization of electronically allowed transitions, selection rules, fundamentals, overtones and combinations in vibrational spectroscopy — the symmetry symbols for normal modes of vibrations. IR and Raman activity of their fundamentals and nature of vibrations in termsof change in internal coordinates in simple molecules like Trans N_2 F_2, SF_6, Fermi resonance.

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Section –B

Chemistry of Main Group elements

Hydrogen : transition metal hydrides, the group I A elements - organometallic compounds of alkali - metals. the group II A - organo- beryllium and organo-magnesium compounds, the group III A elements - structure and bonding of polyhedral boranes, structural study by NMR, Wade's rules, carboranes and other hetro-boranes, organoboron compounds, organoalumium compounds, compounds with C-N bonds, thiocarbonates, dithiocarbamates, zeolites, clays, silicates.

The group V A elements - Types of Covalence in nitrogen, stereochemistry, dinitrogen and nitrogen compounds as ligands, ammonia and amines, phosphorus-nitrogen compounds, the group VI A elements - chemical properties of dioxygen, singlet oxygen, dioxygen, superoxo and peroxo ligands, sulphur and sulphur - nitrogen compounds,sulphur - sulphur compounds as ligands, iso & heteropoly acids and anions of Mo and W. The group VII A Elements the charge — transfer complexes of halogens, polyiodide anions. pseudohalogens,the group VIII A elemrnts - the chemistry of xenon, krypton and radon.

Recommended Books

1. Inorganic chemistry: Principles of Structure and reactivity by James E. Huheey, E.A. Keiter, R.L.Keiter,
2. Advanced Inorganic Chemistry by Cotton and Wilkinson (5th edition.)
3. Chemical Applications of Group Theory – F. A. Cotton, 3rd edition.
4. Introductory Group Theory for Chemists – George Davidson.
5. Introduction to Ligand Fields – B. N. Figgis.
6. Inorganic Chemistry – Shriver, Atkins and Langford, 7th edition.
7. Advanced Inorganic Chemistry - Cotton and Wilkinson (3rd, 4th and 5th Ed.)
8. Theoretical Inorganic Chemistry - Day and Selbin

SEMESTER-II
MCHEM 1202T
Organic Chemistry

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

65 hours
Time allowed- 3hrs
5 period/week
Credit: 05

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three sections: A, B, and C. Sections A and B will have four questions from the respective sections of the syllabus and will carry 12 marks each. Section C will consist of 11 short-answer questions from the entire syllabus and will carry 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt five questions selecting two questions from each of Section A and B and Section C will be compulsory.

Course Outcomes (C.O.)

1. To know stereochemistry and various possible conformations of organic compounds and their effects on the rate of reaction.
2. To get an idea about the various kinetic and thermodynamic factors which control the organic reactions.
3. The students will get knowledge of mechanisms of addition reactions of C=C and C=O bonds and elimination reactions.

Section – A

Stereochemistry

Stereoisomerism: Introduction and different types of stereoisomers. Fischer, Newman and saw horse representations for organic Molecules.

Optical Isomerism: Requirement for a compound to be optically active, compounds with one asymmetric centre. Dissymmetry as a cause of optical activity. Compounds with two asymmetric centres. Racemic modification Racemisation: Thermal, anionic, cationic, free radical, epimerisation, Mutarotation. Racemic compounds, mixtures and solid solutions.

Diastereoisomerism: Resolution of acids, bases, aminoacids, alcohols, aldehydes and ketones. Absolute and Relative configuration, Different systems of rotation. 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, neighboring group participation.

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Elimination. Pyrolysis of acetate, xanthatesand amine oxide.Relation of conformation to reactivity. Optical isomerism due to restricted rotation in biphenyls, allenes, alkylidenes and spiranes.

Ring Systems: Conformational studies in cyclohexane; mono and disubstituted cyclohexane.Its stability and reactivity. 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 theisomers, Relative stability and interconversion of Geometrical isomers.

Section – B

Addition to carbon-carbon multiple bond

Mechanistic and stereochemical aspects of addition reactions involving electrophiles,nucleophiles andfree radicals. Regio and chemo selectivity. Orientation and reactivity. Addition to Cyclopropane ring, Hydrogenation of double and Triple bond, hydrogenation of aromatic rings. Hydroboration, Michael-reaction, sharpless asymmetric epoxidation.

Addition to Carbon – Hetero multiple bond

Mechanism of metal hydride reduction of carbonyl compounds and other functional groups. Dissolving metal reductions of carbonyl functions and conjugated systems. Addition of Grignard'sreagent, organozinc, organocopper and organo lithium reagents to carbonyl and unsaturated carbonyl compounds. Clemmenson reduction, and Meerwein Pondroff Verley reduction. Wittig's Reaction, Wolf Kishner reduction.

Recommended Books

1. Advanced Organic Chemsitry - Reaction, Mechanism and Structure, Jerry March, Johny Wiley. 4th edition
2. Stereochemistry of Carbon Compounds by Ernest, L. Eliel, Tata McGraw-Hill.
3. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International, 3rd edition.
4. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age, International, 5th edition.
5. Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.
6. A Guide Book to Mechanism in Organic Chemistry, Peer Sykes, Longman, 6th edition.
7. Structure and Mechanism in Organic Chemistry, C.K. Ingold, Cornell University, Press,2nd edition.
8. Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic &Professional.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukherjii and S.P. Singh, Macmillan

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SEMESTER-II
MCHEM 1203T
Physical Chemistry

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

65 hours
Time allowed- 3hrs
5 period/week
Credit: 05

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three sections: A, B, and C. Sections A and B will have four questions from the respective sections of the syllabus and will carry 12 marks each. Section C will consist of 11 short-answer questions from the entire syllabus and will carry 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt five questions selecting two questions from each of Section A & B and Section C will be compulsory.

Course Outcomes (C.O.):

1. To impart the students concepts of the fundamentals of quantum mechanics and its applicationsin the study of structure of atoms, bonding in molecules.
2. To understand the requirement of approximation methods in quantum mechanics.
3. To gain insight in to valance bond theory molecular orbital theory and the concept of hybridization.
4. To provide an insight into the thermodynamic and kinetic aspects of chemical reactions andphase equilibria. To derive some thermochemical equations and kinetic equations.

Section – A

Quantum Mechanics

Introduction to exact quantum mechanical result

Fundamental concepts of quantum mechanics, setting up of operators for different observables, Hermitian, unitary and linear operators, postulates of quantum mechanics. Discussion of solution of Schrodinger equation to some model systems. (Viz. particle in a box, the harmonic oscillator, the rigid rotator).

Hydrogen and hydrogen like atoms

Solution of Schrodinger equation for hydrogen and hydrogen like atoms, physical representation of *s* and *p* orbitals, radial plots, angular plots, probability functions and plots.

Approximate Methods

The variation principle, perturbation theory (first order and non-degenerate), applications of variation method and perturbation theory to the helium atom.

Angular Momentum

Ordinary angular momentum, the quantum mechanical operators for angular momentum. Eigen function and Eigen values of angular momentum using ladder operators, addition of angular momentum.

Electronic Structure of Atom

Electronic states of complex atoms, anti-symmetry and Pauli's exclusion principle, Hartree method, Russel Saunder's terms and coupling schemes.

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Molecular Orbital Theory

Huckel Theory of conjugated systems, bond order and charge density calculation, applications of Huckel molecular orbital theory to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene systems. Introduction to extended Huckel theory.

Section – B

Chemical Kinetics

Introduction: Rate of reaction, empirical rate-equation, order and molecularity of a reaction, effect of temperature on reaction rates.

Theories of reaction rates: Number of bimolecular collisions and derivation of rate constant from it, steric factor & its calculation, factors determining effectiveness of collisions. Lindemann mechanism, statistical derivation of rate equation (Eyring equation), transmission co-efficient, tunnelling effect, comparision of collision and transition state theories.

Fast reactions: Study of fast reactions by stopped flow technique, relaxation methods, magnetic resonance technique.

Thermodynamic treatment of reaction rates: free energy of activation, heat of activation and its relationship with various kinds of activation energies, relationship between steric factor and entropy of activation.

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

Complex reactions: Various types of complex reactions, parallel first order reactions producing a common product, parallel higher order reactions, reactions approaching equilibrium, Michaelis-Menten mechanism for enzyme catalysis, consecutive reactions, oscillating reactions.

Recommended Books

1. Kinetics and Mechanism by A.A. Frost & R.G. Pearson, John-Wiley & Sons, Inc., New York.
2. Physical Chemistry by P.W. Atkins, 8th edition.
3. Chemical Kinetics Methods by C. Kalidas, New Age International Publishers, 4th edition.
4. The Foundation of Chemical Kinetics by S.W. Benson.
5. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
6. Quantum Chemistry by I.N. Levine, Prentice Hall.
7. Quantum Chemistry by W. Kauzmann.
8. Quantum Chemistry by Eyring, Walter and Kimball.

SEMESTER-II
MCHEM 1204T
Fundamental & programming with C

65 hours
Time allowed- 3hrs
5 period/week
Credit: 05

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

INSTRUCTIONS FOR THE PAPER SETTER
The question paper will consist of three sections: A, B, and C. Sections A and B will have four questions from the respective sections of the syllabus and will carry 12 marks each. Section C will consist of 11 short-answer questions from the entire syllabus and will carry 2 marks each.

INSTRUCTIONS FOR THE CANDIDATES
Candidates are required to attempt five questions selecting two questions from each of Section A & B and Section C will be compulsory.

Course Outcomes (C.O.):

1. Understand the basic concepts of hardware & software, terminology of IT and familiar with various tools ofOffice.
2. Understand the basic terminology used in computer programming.
3. Foundation for the higher level of programming languages.
4. Develop confidence and ability for learning needed for Computer language.

Section – A

Organization of Computers: Block Diagram of Computer, Types of Computers, Characteristics, Applicationareas: Scientific Applications, Education, Health and E-commerce.

Word Processor: Introduction, Basic Editing, Formatting, Templates, Working with Graphics and Pictures, Tables, Mail Merge, Printing, and Publishing, Comparing, Merging, and Protecting Documents.

Presentation: Introduction, Using Themes and Layouts, Inserting Text and Using WordArt, Inserting Graphics,Working with Videos, Movie-Clips, Animations, and Transitions, Sounds, Editing, Saving.

Spreadsheet: Introduction, Worksheets and Workbooks, Entering data and texts, Formatting a Worksheet, Adding Elements to a Workbook, Charts, Formulas and Calculations, Statistical functions.

Section – B

Introduction to C: Problem Solving with Computers- Analysis, Design, Coding, Compilation, Testing and Debugging, Implementation and Maintenance. Character set, Constants, Variables, Rules for Defining Variables, identifier and Keywords, Data Types.
Operators and Expressions: Arithmetic, Relational, Logical, Assignment, Conditional, Unary, Bitwise, Comma, Operator Precedence and Associativity. Instructions – Type Declaration, Input/ Output Instructions. Control Statements: Decision Control Statements (if, if else, nested if else, switch), Jump Control Statements

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(break, continue, goto), Loop Control Statements (for, while, do-while), nested loops.

Functions: Function Declaration and Prototype, Call, Definition, Types of Functions, Methods of Parameter passing - Call by Value, Call by Reference, Recursion. Introduction to Array, String, Structure, Pointers.

Recommended Books

1. E. Balagurusamy, "Programming in C", Tata Mc GrawHill.
2. Kanetkar, "Let Us C", BPB Publications.
3. Rajaraman, V, "Fundamentals of Computers", PHI.
4. P.K Sinha, " Computer Fundamentals", BPB Publications.

SEMESTER-II
MCHEM 1207L
Organic Chemistry Practical-II

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

65 hours
Time allowed- 3hrs
7.5 period/week
Credit: 02

Course Outcomes (C.O.)

1. Students are able to synthesize some organic compounds.
2. Students are able to characterize synthesized organic compounds by spectral techniques.
3. To provide the knowledge to separate and purify components of organic binary mixtures.
4. Students are able to prepare suitable derivatives of different functional group compounds.

Qualitative Organic Analysis

Separation and purification of components of binary mixture (Solid/solid, solid/liquid and liquid/liquid) on the basis of solubility behaviour and solvent extraction and their identification andconformation by chemical tests and preparation of suitable derivative. Preparative TLC separation for IR and PMR spectral studies of the respective component.

Organic Synthesis

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

The products may be characterized byspectral techniques.

Recommended Books

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 LongmanLimited, 1986.
3. Advanced Practical Chemistry, Jagdamba singh, LDS Yadav, Pragati Prakashan.

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SEMESTER-II
MCHEM 1208L
Physical Chemistry Practical-II

Max Marks: 100
Semester paper 70
Internal Assessments 30
Pass Marks: 35%

65 hours
Time allowed- 3hrs
7.5 period/week
Credit: 02

Course Outcomes:

1. Students are able to determine density of given liquids using Pyknometer.
2. Students are able to determine molecular weight of different polymers by viscosity method.
3. Students are able to detect molar refractivity of given solid.
4. Students are able to determine equilibrium constant for various reactions by Partition method

Experiments:

1. To determine the Molecular weight of given polymer by viscosity method.
2. To find out the value of coefficient of expansion for the given liquid with the help of Pyknometer.
3. To determine the atomic Parachors of C, H & O.
4. To compare the cleansing powers of two samples of detergents by surface tension method.
5. To determine the interfacial tension between two immiscible solvents.
6. To find out the equilibrium constant for the reaction, $KI + I_2$ --- KI_3 by partition method.
7. To determine the rate constant of the hydrolysis of ethyl acetate catalysed by an acid andalso find out the half-life period of the reaction.
8. To determine the order of saponification of ethyl acetate with sodium hydroxide.
9. To find out the molar refractivities of homologous series of alcohols & also find out the atomic refractivities of C & H.
10. To find out the molar refractivity of the given solid.
11. To study the adsorption of acetic acid on activated charcoal & prove the validity of Freundlich Adsorption Isotherm.
12. To determine the density of given liquids with the help of Pyknometer.

Recommended Books

1. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman.
2. Advanced Physical Experiments, Gurtu - Gurtu, Pragati Prakashan, Meerut.
3. Practical Physical Chemistry, Alexander and Findley.

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