2015-16

Multani Mal Modi College, Patiala

Unit Planning M.Sc Chemistry

Department of Chemistry

MSc Chemistry-I(SEMESTER-Ist)

Paper: 101

(2015-16)

Subject: Inorganic Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I
Chemical Bonding:- The ionic bond, covalent bond, the variation method, groundstate energy of hydrogen atom, the secular equations, the molecular orbital theory, electron distribution in hydrogen molecule ion, symmetric and antisymmetric energy states, the classical interaction energy, resonance, contribution of ionic terms, sp3 hybridisation, three centered bond, Linnetts doublet - quartet approach, the Pauli's exclusion principle. Pi Bonding Ligand Complexes:- Pi Acid Ligands: CO as prototype, other pi acid ligands-isocyanide ligands, dinitrogen, the CS ligands, the NO ligands, pi acid ligands : trivalent phosphorus compound, multiple bonds from ligands to metal, pi complexes of unsaturated organic molecules : alkene & alkyne, enyl ligands, aromatic ring systems. Theories of Bonding in Transition Metal complexes – Qualitative Approach :Qualitative introduction to the molecular orbital theory, complexes with no pi bonding, complexes with pi-bonding, the crystal field & ligand field theories, orbital splitting and magnetic properties, the angular overlap model.
TILLMST-II
Structural and Thermodynamic Consequences of Partly Filled- shells:- Ionic radii, Jahn-Teller effects, thermodynamic effects of d-orbital splitting, magnetic properties of chemical compounds, origin of magnetic behavior, magnetic susceptibility and types of magnetic behavior : diamagnetism, paramagnetism, ferromagnetism : types of paramagnetic behavior : Large multiplet separation, small multiplet separations, spin only, heavy atoms, high spin-low spin cross overs. Spectral Properties:- Russel - Saunder's term, selection rules, break down of selection rules, band widths & shapes, energy level diagrams and d-d complex spectra, Orgel diagrams - weak fields, charge - transfer spectra, photochemical reactions of chromium & ruthenium complexes. Bioinorganic Chemistry:-Introduction, the biochemistry of Iron : iron storage and transport ferritin, transferrin, bacterial iron transport, hemoglobin and myoglobin, nature of the heme-dioxygen binding, model systems, cooperativity in hemoglobin cytochromes, other iron - porphyrin bimolecule peroxidases & catalases, cytochrome P450 enzymes, other natural oxygen carriers - hemerythrins, iron - sulfur proteins.
TILLFINAL EXAM
The biochemistry of other metals : zinc (carboxypetidase A, carbonic anhydrase, metallothioneins), copper (superoxide dismutase (CuZn SOD), hemocyanins, oxidases), cobalt (cyanocobalamin), molybdenum (nitrogenases) & tungsten. Miscellaneous other elements : vanadium, chromium & nickel metal ions, chelates in chemotherapy, synthetic metal chelates as antimicrobial agents, lithium and mental health, gold and its compounds, metal complexes as antitumour agents, chelation therapy.

Mode of Assessment

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

MSc Chemistry-I(SEMESTER-Ist)

Paper: 102

(2015-16)

Subject: Organic Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I

Carbocations : Generation, Structure, Stability, Application of NMR spectroscopy in the detection of Carbocation, allylic and benzyllic carbocations. Stereochemistry and reactions. Nonclassical carbocations : Phenonium ion, norbornyl system, explaination based on rearrangement.

Carbanions : Generation, Structure, stability, stereochemistry, Tautomerism, Prototropy and general reactions.

Carbenes : Formation, Structure, Singlet & Triplet carbene, Stereochemsitry and reactions.

Nitrenes : Formation, Structure Singlet & Triplet nitrene, Stereochemsitry and reactions

Arynes : Formation, Structure and reactions.

Free radicals : Formation, Structure, Stability, Stereo-chemistry and reactions.

Reaction of Free Radicals:- Polymerisation Halogenation : Chlorination, bromination, Bromination by NBS, Iodination, Fluorination, Polar effects in halogenation.

Addition Reactions : Free radical addition of HBr, Hcl, HI thiols and halogens.Auto-oxidation Rearrangements

Nature of Bonding in Organic Molecules Introduction to fullernes Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's Rule, anti-aromaticity, homo-aromaticity, PMO - approach.

Bonding weaker than Covalent bond Addition compounds, Crown ether complexes and Cryptands, inclusion compounds, Cyclodextrins, Catenanes and rotaxane.

Techniques used.for determination of reaction mechanism(Non-kinetic method) :Use of optical, Stereochemical and isotopic techniques. Reaction studies from identification of products. Trapping of intermediate, crossover experiments, use of Catalyst, use of isotopes in reaction mechanism studies in case of Favorskii, Claisen's and Benzyne reactions.

TILLMST-II

Elimination Reactions:- E2, E1 and E1 CB mechanism, Stereochemistry Product ratio, Orientation of double bond, Hofman Rule, Saytzeff Rule. Factors Governing E2 & E1 Mechanism.

Cyclic Elimination : Amine Oxide, Esters, Xanthate, and Free radical elimination.

Dehalogenation by zinc. Triple bond by elimination. Elimination versus substitution. Effect of solvent, temperature, Nature of Base, Structure of the reactants.

Aromatic Elimination : Benzyne, Nucleophillic aromatic substitution, addition elimination.

Pericyclic Reactions

Molecular Orbital symmetry, Frontier Orbitals of ethylene, 1,3 - butadiene, 1, 3, 5-hexatrience and allylsystem. Classification of Pericyclic reactions. Woodward-Hoffman rule,

correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatorymotions 4n, 4n+2 and allylsystems.Cycloadditions - antarafacial and suprafacial additions 4S+2S Systems and 2S+2S additions of alkene.

TILLFINAL EXAM

Sigmatropic rearrangement - suprafacial and antarafacial shift involving carbon moieties. 3, 3-and 5, 5-sigmatropic rearrangement Claisen, Cope-rearrangement reactions.

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3	Attendance	20%

MSc Chemistry-I (SEMESTER-Ist)

Paper: 103

(2015-16)

Subject: Physical Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I

Thermodynamics:- Recall : Concepts involved in first and second law of thermodynamics, Entropy, free energy and chemical equilibrium. Thermodynamic equation of state. Maxwell relations.

Non-ideal systems : Excess functions for non-ideal systems. Activity and activity coefficients and their determination. Concept of fugacity and its experimental determination. Partial molal properties and their determination.

Third law of the thermodynamics : Indentification of statistical and thermodynamic entropy. Nernst postulate, Plank's contribution. Alternate formulation of third law. Cooling by adiabatic and demagnetisation. Evaluation of absolute entropy.

Thermodynamic and 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 systms.

Statistical Thermodynamics General introduction : Phase space, microstates, macrostates, thermodynamic probability. Brief introduction to different types of statistics. Ensemble concept. Canonical, grand canonical and microcanocical ensembles. Stirling approxination, Maxwell Baltzmann distribution law.

(Partition function and thermodynamic properties : Partition function and its factorization. Translational, rotational, vibrational; electronic and nuclear partition functions. Expressions for internal energy, entropy, Helmholtz function, Gibb's function, pressure, work and heat in terms of partition function. Thermodynamic properties of ideal gases. Vibrational, rotational, electronic and nuclear contributions to the thermodynamic properties.

TILLMST-II

Ion-solvent interactions : Born model of ion-solvent interactions, Structural models of ion -

solvent interations. Experimental determination of salt-solvent interactions. Relative heats of solvation of ions in the hydrogen scale. Evaluation of ion-solvent interactions from experimental data of salt-solvent interactions.

Ion - ion interactions : Debye - Huckel theory of ion - ion interactions. Verification of Debye - Huckel limiting law. Activity, coefficients at moderate concentrations and higher concentrations. Activity coefficients as a function of ion-ion and ion-solvent interactions. Mean activity coefficients and their experimental determination.

Conductance and Ionic mobilities : Conductance of electrolytic solution. Variation of equivalent conductance with concentration. Debye - Huckel - Onsager theory. Modification of Debye - Huckel - Onsager equation. Ionic conductances. Ion-association and ion-pair formation. 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, Electrocatalysis in redox reactions. Electrocatalysis in reactions involving adsorbed species. Some specific feature of electrocatalysis.,

TILLFINAL EXAM

Electrochemical Energy Conversion and Electricity storage : Direct energy convertors. Efficiency of electrochmical energy convertors. Some typical examples of electrochemical energy convertors. Advantages and applications of fuel cells. Electricity storage density and energy density. Various electricity storers and their applications.(Corrosion of Metals : Classification of corrosion processes, theories of corrosion processes, passivation of metals. Corrosion monitoring and methods of corrosion prevention

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MSc Chemistry-I (SEMESTER-Ist)

Paper: 104 (A)

(2015-16)

Subject: Mathematics for chemists

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I
Vectors and Matrix Algebra Vectors :Vectors, dot, cross and triple products. The gradient, divergence and curl. Matrix Algebra :Addition and multiplication, determinants (upto 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 solution, linear dependence and independence. Cayley Hamilton theorem, matrix eigenvalues and eigenvectors. Coordinate Geometry:- Cartesian system of co-ordinates in the plane, slope of a line, parallel and perpendicular lines, intercepts of a line on the co-ordinate axes, Various forms of equations of a line-parallel to axis, slope intercept form, the point slope form, two point form, intercept form, normal form and general forms. 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, addition and subtraction formulae.
TILLMST-II
Differential Calculus : Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima. Functions of several variables, partial differentiation, Euler's theorem co-ordinate transformations (e.g. cartesian to spherical polar). Integral calculus : Basic rules for integration, integration by parts, partial fraction and substitution definite integrals. Reduction formulae. Elementary Differential Equations:- Veriables - separable and exact, first order defferential equations. Homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and Legendre equation, spherical harmonics.
TILLFINAL EXAM
Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases, curve fitting (including least square fit) with a general polynomial fit.

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MSc Chemistry-I (SEMESTER-Ist)

Paper: 104 (B)

(2015-16)

Subject: Biology for chemists

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-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 and divisions:- Structure of prokaryotic .& eukaryotic cells, Intracellular organelles and their functions, Comparison of plant and animal cells. Overview of metabolic process - catabolism and Anabolism. ATP - the Biological energy currency. Cell division stages of mitosis & meiosis. Significance of cell division and fertilization.

Carbohydrates:- Monosaccharides, structure & functions of important derivatives of monosaccharides(Enantiomers, Epimers, Hemiacetal, Hemiketalepanomers). O-glycosidic bond disaccharide & Polysaccharides. Structural polysaccharides. Reducing and non-reducing sugars. Structural Polysaccharides - cellulose and chitin. Storage Polysaccharides - starch and glycogen

Structure and Biological functions. Carbohydrate metabolism - Kreb's Cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, Pentose phosphate Pathway.

Lipids, Fatty acids, essential fatty acids, structure and function. Storage lipids. Triacyl glycerols. Structural lopids-phospholipids, Glycolopids & Archae bacterial ether lipids. Lipoproteins — composition and function. Lipids as Signals, Co factors and pigments, Lipid and cell memberane. Properties of lipid aggregates — micelles, bilayers, liposomes and their possible biological functions, Biological membranes and transport.. Fluid mosaic model of membrane structure.

Lipid metabolism - b - oxidation of fatty acids.

TILLMST-II

Structure of ProteinsAmino acids, essential and non essential, Iminoacids their structure, properties and classification, Ionic properties of amino acids. pka and zwitterion form,

Peptide bond chemical properties of amino acids. Primary structure - peptide chain.

Secondary structure of proteins, forces responsible for holiding of secondary structure - α halix, beta sheets, Tilius & loops., triple helix structure of collagen. Tertiary structure of protein. Quarternary structure of homoglobin.

Degradation and biosynthesis of amino acids, sequence determination: chemical/ enzymatic/mass spectral, racemization/detection.

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 ribonuclic acids (RNA) and deoxyribonucleic acids (DNA), Types of DNA and RNA, double helix model of DNA and forces responsible for holding' it Chemical and enzymatic hydrolysis of Nucleic acids.

TILLFINAL EXAM

Replication of DNA

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

Protein synthesis & Genetic CodeTranscription, translation and genetic code, chemical

synthesis of mono and trinucleoside.

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MULTANI MAL MODI COLLEGE, PATIALA

UNIT PLAN

MSc Chemistry-I (SEMESTER-IInd)

Paper: 201

(2015-16)

Subject: Inorganic Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I

Chemistry of Main Group Elements:- Group I A to IV A Group Elements:- Hydrogen : transition metal hydrides, the group IA 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, the group IV A element - compounds with C-N bonds, thiocarbonates, dithiocarbamates, zeolites, clays.

Chemistry of Main Group Elements

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

TILLMST-II

Group Theory Order, classes of group, representation of a group, transformation of coordinates matrices, matrix representation of symmetry operation, reducible and irreducible representations and C2v,C3v, D4, 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 octaheral, 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 & Oh symmety, direct product for Oh, Td, C3v, D4h & D5h and the method of descending symmetry for d2 configuration.

- Applications of Group Theory:- Suitable metal orbitals and ligand or orbitals

combination to form molecular orbitals in coordination complexes Oh, Td & square planar complexes, symmetry consideration regarding selection rules and spectral intensties, vibronic coupling, vibronic polarization in centrosymmetric complexes Oh & D4h and non centro symmetric complexes C3v, Td
TILLFINAL EXAM
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 terms of change in internal coordinates in simple molecules like trans N2F2, SF6, Fermi resonance.

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MULTANI MAL MODI COLLEGE, PATIALA

UNIT PLAN

MSc Chemistry-I (SEMESTER-IInd)

Paper: 202

(2015-16)

Subject: Organic Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I
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. (b) Disastereoisomerism : Resolution of acids, bases, aminoacids, alcohols, aldehydes and ketones, Absolute and Relative configuation, Different systems of rotation. Assymetric induction, methods of determining the configuration. Cram's Rule and Prelog's Rule. Conformation 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. Elimination. Pyrolysis of acetate, Xanthates and amine oxide. Relation of conformation to reactivity. Optical Isomerism due to restricted rotation in biphenyls allenes, Alkylidenes and spiranes. Systems : Conformational studies in Cyclohexane; mono and disubstituted Cyclohexane. Its stability and reactivity. Energy determination in chair and boat form. Studies in fused systems. Decalins and Perhydrophenanthrenes..

TILLMST-II
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. Addition to carbon – carbon multiple bond : Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and freeradicals. Regio and chemoselectivity. 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.
TILLFINAL EXAM
Wolf Kishner reduction; Clemmenson reduction, and Meerwein Pondroff Varley reduction. Wittig's Reaction. Addition of Grignard's reagent, organozinc and organo lithium reagents to carbonyl and unsaturated carbonyl compounds.Mechanism of condensation reactions involving enolates – Aldol, knoevengel, Claisen, Mannich, Benzoin, Perkin and stobbe reactions, Hydrolysis of esters and amides. Ammonloysis of esters.

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MULTANI MAL MODI COLLEGE, PATIALA
UNIT PLAN
MSc Chemistry-I (SEMESTER-IInd)
Paper: 203
(2015-16)
Subject: Physical Chemistry

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I

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 atomsSolution 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 MomentumOrdinary 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, term separation energies for p2 and d2 configurations.Molecular Orbital TheoryHuckel 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.

TILLMST-II

Ion-solvent interactions : Born model of ion-solvent interactions, Structural models of ion - solvent interations. Experimental determination of salt-solvent interactions. Relative heats of solvation of ions in the hydrogen scale. Evaluation of ion-solvent interactions from experimental data of salt-solvent interactions.
Ion - ion interactions : Debye - Huckel theory of ion - ion interactions. Verification of Debye - Huckel limiting law. Activity, coefficients at moderate concentrations and higher concentrations. Activity coefficients as a function of ion-ion and ion-solvent interactions. Mean activity coefficients and their experimental determination.
Conductance and Ionic mobilities : Conductance of electrolytic solution. Variation of equivalent conductance with concentration. Debye - Huckel - Onsager theory. Modification of Debye - Huckel - Onsager equation. Ionic conductances. Ion-association and ion-pair formation. 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, Electrocatalysis in redox reactions. Electrocatalysis in reactions involving adsorbed species. Some specific feature of electrocatalysis.

TILLFINAL EXAM
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, partition functions for translation, rotation & vibration, 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.

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MULTANI MAL MODI COLLEGE, PATIALA
UNIT PLAN
MSc Chemistry-I (SEMESTER-IInd)
Paper: 204
(2015-16)
Subject: FUNDAMENTALS AND PROGRAMMING WITH C

Max Marks: 75
Theory: 55
Internal Assessment: 20 **Maximum Time: 3 Hrs.**

TILLMST-I
Computer organization : Hardware, Software, Programming languages with special reference to BASIC, Fortran and C. Binary representation : Binary numbers, Conversion of decimal to binary and binary to decimal, Idea of Octal and hexa-decimal numbers. Problem solving : Problem analysis, Algorithm development, Program Coding, Program Compilation and execution. Introduction to C : Historical development of C, The C character set, Constants, variables and keywords, Types of C constants and variables, C keywords. C instructions : Type declaration instruction, Arithmetic instructions, Integer and float conversion, Type conversion in assignment, Hierarchy of operations, Writing of a first program in C, Control Instructions in C. Simple problems with sequential structure.

TILLMST-II
Decision and control structure : The if statement, The if-else statement, The nested if-else statement, Use and hierarchy of logical operators, Conditional operators. Loop control structure : The while loop, The for loop, Nesting of loops, The do-while loop, Break and continue statements. Case control studies : Decision using switch, The go to statement, Simple problems with Selective and repetitive structures. Functions : What is function, why use functions, Passing values between a functions, Role of functions.
TILLFINAL EXAM
Advanced features of functions : Function declaration and prototypes, Call by values and call by reference, An introduction to pointer, Pointer notion. Arryas : What are arrays, Initialization of arrays..

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Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 301

Subject: ANALYTICAL CHEMISTRY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

1. Introduction to analytical chemistry, Methods of quantitative analysis, chemical analysis with its scale of operation, various steps in quantitative analysis.

2. Sampling in analysis, Theory of sampling importance of selecting a representative sample, criterion of a good sampling plan, Stratified sampling Vs. random sampling. Minimisation of variation in stratified sampling, sampling plan for solids, liquids and gases.

3. Reliability of analytical data, Errors in chemical analysis, classification of errors, Minimisation of errors, accuracy and precision. Improving accuracy of analysis, correlation and Regression, linear regression. Analysis of variance.

Polarography: Principle, residual, Migration, diffusion currents, polarographic maximum, advantages and disadvantages of D.M.E. Reversible & irreversible processes, fundamental equation of polar graphic wave. Derivation of Ilkovic equation & deviations, Quantitative technique & evaluation of quantitative results, Amperometric titrations & Biampometric titrations.

TILLMST-II

5. Basic Principles of related technique of Polarography, Alternating current, Square Wave, pulse (normal and Differential) Tensometry, radio frequency and computer controlled polarograph.

6. Chronoptentiometry theory, circuit and applications & comparison with polarography

Thermo Analytical Methods

1. Thermogravimetric analysis, Introduction, Instrumentation, Factors affecting thermogravimetric results, applications of Thermogravimetry.

2. Differential Thermal analysis and differential scanning calorimetry on line analysis.

3. Thermometric titrations Introduction theory and applications.

Spectrophotometry and Colorimetry

Theory of spectrophotometry and colorimetry, Beer's law, Deviation from Beer's law, absorptivity, Photometric accuracy. Spectrophotometric titrations and titration curves and applications to quantitative analysis.

Solvent extraction: Distribution constant and distribution ratio and their importance in solvent extraction, synergistic extraction, extraction by solvation, Ion pair formation Methods of

extraction and their applications in analytical chemistry.
TILL FINAL EXAM
Ion Exchange Resins: Different types of Ion exchangers and their synthesis. Ion exchange chromatography. Applications in analytical chemistry (a) Total cation Conc. in tap water (b) Cu (II) from a brine solution U (VI) by liquid ion exchanger (d) use of mixed solvents.

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Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 311

Subject: LIGAND FIELD THEORY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

Introduction:

(a) Concept of Ligand Field

(b) Scope of Ligand Field

(c) The d and other orbitals.

(d) Qualitative Demonstration of Ligand Field Effect.

(e) The Physical Properties Affected by Ligand Field.

(f) Ionic Model of Coordination Compounds.

(g) Crystal Fields and Ligand Fields

Atomic Spectroscopy

(a) The Free Ion

(b) Free Ion Terms

(c) Term Wave Functions

(d) Spin-Orbit Coupling

Free Ions in Weak Crystal Fields

(a) The Effect of a Cubic Crystal Field on S and P terms.

(b) The effect of a Cubic Crystal Field on D terms.

(c) The effect of a Cubic Crystal Field on F terms.

(d) The effect of a Cubic Crystal Field on G, H and I terms.

TILLMST-II

Thermodynamic Aspects of Crystal Fields

(a) Crystal Field Stabilization Energy.

b) Lattice energy and C.F.S.E.

Free ions in medium and strong Crystal fields:

(a) Strong field configuration.

(b) Transition from weak to strong crystal fields.

(c) Term energy level diagrams.

(d) Tanabe-Sugano diagrams.

Molecular orbital theory for complex ions:

(a) Elementary Molecular Orbital Theory.

(b) Bonding in octahedral complexes.

(c) Bonding in tetrahedral complexes.

TILL FINAL EXAM

Electronic Spectra of complex ions:

(a) Selection rules and band widths.

(b) Spectra of aqueous solutions of $[M(H_2O)_6]^{n+}$.

(c) Spectra of spin free ML_6^{n+}.

(d) Spectra of spin paired ML_6^{n+}.

(e) Spectra of distorted octahedral complexes.

(f) Spectra of tetrahedral complexes

(g) The spectrochemical and nephelauxetic series.

(h) Charge transfer spectra

4. **Spectral and Magnetic properties of Complexes of Non-Cubic Stereochemistry:**

(a) General

(b) Square Planar Complexes.

(c) Square Pyramidal Complexes.

(d) Dodecahedral Complexes

Quantitative Basis of the Crystal Fields:

(a) Crystal Field Theory.

(b) The Octahedral Crystal Field Potential, Voct.

(c) The Effect of Voct on d Wave Functions.

(d) Evaluation of 10 Dq.

(e) The Tetrahedral Potential.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 312

Subject: REACTION MECHANISM OF TRANSITION METAL COMPLEXES

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

Ligand replacement reaction: Labile and inert complexes, crystal field stabilization, general aspects, dissociation or displacement, classification of mechanism, water exchange rates, formation of complexes from aqueous ions, equation and base hydrolysis, attack on ligands.

Reaction of Square complexes: mechanism of ligand displacement reactions, the trans effect, cis-effect.

Oxidative addition and migration (insertion) Reactions: General comments, the acid base behaviour of metal atom in complexes, Lewis acidity of complexes, oxidative addition: addition of specific molecules (hydrogen addition, HX additions, Organic halides, additions of some other molecules), reductive elimination, insertion reactions, insertion of carbon monoxide, insertions of alkenes and C-C unsaturated compounds, cleavage of C-H bonds; Alkane "activation", cyclometallation reactions

TILLMST-II

Stability Constants of Metal complexes

(i) Slope ratio method
(ii) Job's method of continuous variation
(iii) Solubility method
(iv) Mole- Ratio method.

General methods:

(a) Bjerrum's potentiometric method

(b) Leden's method

(c) Ion Exchange method.

(d) Polargraphic methods: Lingane's method, Deford & Hume's method.

TILL FINAL EXAM

Factors affecting the stability constants

(i) Statistical effect
(ii) Electrostatic effect
(iii) Chelate effect

Metal Cabonyl reactions: Reactions of octahedral, reactions of binuclear carbonyl, associative reactions, species with 17 electrons,

Electron transfer processes: Electron transfer theory outersphere reactions, ligand-bridged reactions, iron-(II) iron-(III) exchange, two electron transfer, non-complementary reactions, replacement through redox mechanism.

Stereochemical nonrigidity: Metal carbonyl scrambling, Fluxionality in organometallic compounds.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 313

Subject: INORGANIC SPECTROSCOPY-I

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

General Introduction to Spectroscopy

Nature of radiation energies corresponding to various kinds of radiations, atomic and molecular transitions, selection rules & chemical processes effecting the natural line width of a spectral line, general applications; determinations of concentration, isobestic points, finger printing, Job's method of Isomotal solutions.

Electronic Absorption Spectroscopy

Vibrational and electronic energy levels in a diatomic molecule, relationship of Potential energy curves to electronic spectra. Nomenclature, Assignment of transitions, Spin-orbit coupling, criteria to aid in Bond assignment, Intensity of Electronic Transition i) Oscillator Strengths, Transition moment Integral Derivation of some selection rules, spectrum of formaldehyde, Spin-Orbit & vibronic coupling contribution to Intensity, mixing of d & p orbital's in certain symmetries, higher state mixing, Intensity of electronic transitions, charge transfer transitions, polarised absorption spectra. Applications, finger printing, molecular addition compounds in Iodine, effect of solvent polarity on charge transfer spectra.

TILLMST-II

Spectra of Transition Metal Complexes

Spectra of transition metal complexes : Selection rules and intensities of transition, nature of electronic transitions in complexes, use of Orgel diagrams.

Vibration & Rotation Spectroscopy

anharmonic vibrations, absorption of radiation by molecular vibrations, selection rules, force constant, vibration in polyatomic molecules, effects giving rise to absorption bands, Group vibrations, limitation of group vibration concept.

Raman Spectroscopy : Introduction, selection rules, polarised and depolarised Raman lines, significance of nomenclature used to describe number of IR active and Raman active line. Symmetry requirements for coupling, combination bands and Fermi Resonance. Microwave Spectroscopy, measurement of bond angles and bond distance.

TILL FINAL EXAM

Application of Electronic Absorption and IR Spectroscopy

Calculations of Dq and β for octahedral Ni (II) complexes, structural evidence from electronic spectra. Miscellaneous applications of the principles related to electronic transitions.

Applications of Infrared and Raman Spectroscopy: Procedure Finger printing, applications of Raman and Infrared selection rules to the determination of Inorganic structures, hydrogen bonding systems, change in spectra of donor molecules upon coordination, Change in the spectra accompanying change in symmetry upon coordination.

Mossbauer Spectroscopy

Introduction Interpretation of Isomer Shift, Quadrupole Interactions, Magnetic interactions, applications.

Nuclear Quadrupole Resonance Spectroscopy

Introduction, energies of quardrupole transitions, effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure, applications, interpretations of structural information from NQR spectra

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 321

Subject: PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I
Photochemical Excitations Light absorption. Electronic transitions/excitations. Singlet and Triplet states "Forbidden" transitions. **Types of excitation** Molecular orbital view of excitations. Study of Mechanism of Photochemical Reactions Detection of intermediates Low temperature photochemistry. Quantum efficiency. Sensitisation and Quenching. **The Fate of Excited Molecules : Photophysical Processes** Jablonski diagram Intersystem crossing Energy transfer. **The Frontier Molecular Orbital Approach** **Cycloadditions** Cheletropic reactions. Dipolar cycloadditions. **Sigmatropic reactions** Peripatetic cyclopropane bridge Fluxional molecules-Degenerate Cope rearrangements **Pericyclic Reactions Involving Ionic Transition States** Cycloaddition reactions Electrocyclic reactions Sigmatropic reactions Peripatetic cyclopropane bridge Group transfers and Group eliminations **The Perturbational Molecular Approach** Aromatic and Antiaromatic Transition States, Evan's and Dewar's rules. **Applications of Evan's and Dewar's rules to Pericyclic Reactions** Pericyclic reactions involving ionic transition states Cycloaddition reactions Electrocyclic reactions Sigmatropic reactions Peripatetic cyclopropane bridge Cheletropic reactions Dipolar cycloadditions Group transfers and Group eliminations
TILLMST-II
The Fate of Excited Molecules : Photochemical Processes Photoadditon and Substitution Reactions Photoreduction of carbonyl compounds-Linear addition initiated by hydrogen abstraction reaction

Synthetic applications of photochemical hydrogen abstraction reactions.
Intramolecular hydrogen abstraction: The type-II family of reactions.Addition reactions of cyclic conjugated enones.
Cycloadditions
Intermolecular [2+2] cycloadditons of alkenes and conjugated dienes.
Photosensitised intermolecular cycloadditions of conjugated dienes.
Photosensitised cyclodimerisation of 1,3-Dienes.
[2+2] photocycloaddition reactions of carbonyl compounds.
Oxetane formation by photoaddition of excited carbonyl compounds with "electron rich" substrates : alkenes and enol ethers.
Oxetane formation by photoaddition of excited carbonyl compounds with "electron poor" substrates cyanoethylenes.
Photocyclodimerisation of aromatic compounds.
Photocycloaddition reactions of conjugated enones.
Synthetic applications of the [2+2] photochemical cycloadditons of enones.

TILL FINAL EXAM

Isomerisations and Rearrangements
Photochemical cis-trans isomerisation of alkenes.
Photochemical cis-trans isomerisation of conjugated dienes.
cis-trans isomerisation of cycloalkenes.
Photovalence isomerisation reactions of benzene : Photochemistry of benzene valence isomers
Photorearrangements of 2,4-cyclohexadienones.
Sigmatropic isomerisations of □ ,□unsaturated enones.
Photofragmentation Processes
Homolytic α-cleavage of ketones
Photochemical reactions of cyclobutanones
Sigmatropic rearrangements of □ ,□ unsaturated ketones initiated by □ - cleavage.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
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M.Sc.-II Chemistry SEMESTER-III

Paper: 322

Subject: CHEMISTRY OF NATURAL PRODUCTS

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

General methods and basic techniques used in structure determination

Dehydrogenation : Dehydrogenation with high potential quinones, D.D.Q., mercuric acetate, selenium dioxide and zinc distillation with suitable examples and mechanism.

Catalytic and Chemical Dehydrogenation : Dehydrogenation with, S, Se, Pt, Pd-C as involved in C-H, C-C, C-O, C-N bonds codinine, Morphine to Apomorphine, Zinziberene, Himachalene, Cedrene, Santonin, Abietic acid, Cholesterol, Bile acids, Conessine, Yohimbine, Reserpine Atisine veatichin, Kobusine Sangorine.

II. **Degradation of Carbon Skeleton :** Hoffmann degradation, mechanism, direction of elimination as involved in morphine group alkaloids, conessine, kobusine, narcotine, launadosine, hetisine atisinium hydroxide.

Emde degration : Conessine, Thebaine, Quinoline.

Von Braun Reaction : Fission of C-N bond in cocaine, dihydroatisin, morphine, thebaine, codeine.

Alkalifusion : Alkalifusion of carboxylic function, alcohols carbonyl functions, as illustrated in geraniol, mangostein estradiol, estrone, querectine, terramycin formation α, β– apoteramycin.

TILLMST-II

Oxidation Method :

(i) Oxidation by $KMnO_4$, Chromic acid, methinic H, allylic methylene, α-ionone, camphene

(ii) Ozonolysis : Mechanism, α, β - unsaturated carbonyl compounds, aromatic, heterocyclic, fenchene, camphene, α-pinene, atisine veatichin, parasantoid codine and indoles.

(iii) Indirect Oxidation : (a) Hydroxylation with peracids. O_sO_4, silver acetate and Iodine, oxidation with HIO_4LTA, sodium bismuthate. (b) Haloform reaction : Methyl ketone, a ionone cedrene, caryophyllene and cholesterol. (c) HNO_3 oxidation : Degradation of strychnine and determination of ring size A, B, C in steroids. (d) Nitrous acid oxidation : Mechanism, cyclic ketone, ketocineoles, sangorine, methinic ketone camphor, menthone.

IV. Structure and synthesis of some natural products based on chemical and spectroscopic methods :

Ascorbic Acid, α-pinene camphor and longofolein.

TILL FINAL EXAM

Terpenes and Caretenoids : Isoprene Rule MVA. conversion to borneol, thujene and allied derivatives. Formation of F.P.P., G.G.P.P. conversion to codinine, abietic acid, cambrene Farnesal and Noralidols

to cyclic sesquiterpenes, lanosterol cholesterol.

Biogenetic Approach : Acetate pathways bio-genesis of macrolide, erythromycin, muscone muscopyridine, shikmic acid pathways biogensis of coumarine, flavonoid isoflavones.

II. Structure elucidation of following by chemical means and spectral studies, confirmation of structure by synthesis. Himachalene, Santonin, abietic acid, β-caryophylene, cedrene cedrol, α–Terpene, menthol, β–carotene vitamin–A.

Structure elucidation with synthesis of the followings :

I. Alkaloids : Quinine, Morphine.

II. Steroid : Bile acids, cholesterol Andosterone Testosterone, Progestrone.

III. Antibiotic : Penicillin, Cephalosporin and Mangostein (Structure Only).

Mode of Assessment	
Component	**Weightage**
Mid Semester Test (MST)	40% (Average of 2 MST)
Written Assignments	40%
Attendance	20%

M.Sc.-II Chemistry SEMESTER-III

Paper: 323

Subject: HETEROCYCLIC CHEMISTRY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I
Three membered ring with one heteroatom : Oxirane, Aziridine, Thirane : Introduction, synthetic methods, Direct insertion of heteroatom into carbon-carbon-double bond, methylene insertion reaction, cyclisation method, condensation reaction, Nucleophillic and Electrophillic ring opening. Reaction involving extrusion of the heteroatoms. **II. Four membered Heterocyclics with one Heteroatom :** Oxetane, Oxetene, thitenes, thitanes, Azitidines : Introduction, Synthetic method, Cyclisation reaction, Direct combination method, Reaction electrophillic, Nucleophillic ring opening and General chemical reactions. **III. Five membered Heterocyclics with two heteroatoms :** Pyrazole and Imidazoles : Introduction, Physical properties, Structure, Synthetic method, Electrophillic and Nucleophillic reactions. IV. (a) Isoxazole and Oxazole : Introduction, Physical and chemical properties of isoxazole and oxazoles and their derivatives. Isothiazole and Thiazoles : Physical and chemical properties, synthetic reactions.
TILLMST-II
Three membered ring with one heteroatom : Oxirane, Aziridine, Thirane : Introduction, synthetic methods, Direct insertion of heteroatom into carbon-carbon-double bond, methylene insertion reaction, cyclisation method, condensation reaction, Nucleophillic and Electrophillic ring opening. Reaction involving extrusion of the heteroatoms. **II. Four membered Heterocyclics with one Heteroatom :** Oxetane, Oxetene, thitenes, thitanes, Azitidines : Introduction, Synthetic method, Cyclisation reaction, Direct combination method, Reaction electrophillic, Nucleophillic ring opening and General chemical reactions. **III. Five membered Heterocyclics with two heteroatoms :** Pyrazole and Imidazoles : Introduction, Physical properties, Structure, Synthetic method, Electrophillic and Nucleophillic reactions. IV. (a) Isoxazole and Oxazole : Introduction, Physical and chemical properties of isoxazole and oxazoles and their derivatives. Isothiazole and Thiazoles : Physical and chemical properties, synthetic reactions.
TILL FINAL EXAM
Ring Expansion : (a) Pyrrole to Pyridines. (b) Benzylidene Coumaranones to flavonones and flavonols. (c) Tetrahydro furfurylalcohol to Dihydropyran. iii. 1, 2 Rearrangements in Heterocyclic system. (a) 1,2 - Rearrangement in catechin derivatives. (b) 1,2 - Rearrangement of indole derivatives.

(c) 1,2 - Rearrangement during Clemmenson's Reduction.

iv. Aromatic Rearrangements

(a) Jacobsen Rearrangement

(b) Migration of Alkyl group during Fisher's Indole Synthesis

(c) Rearrangement of N-substituted aniline, N-oxides

(d) Rearrangement of Benzidine.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
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3	Attendance	20%

Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-III

Paper: 331

Subject: Fundamentals of Spectroscopy **Max Marks: 75**

Maximum Time: 3 Hrs.

TILLMST-I

Molecular Spectra

Electromagnetic radiation, interaction of electromagnetic radiations with molecules and quantization of different forms of energies in molecules. Regions of the electromagnetic spectrum. Units of energy. Representations of spectra. Time dependent Schrodinger equation. Induced quantum transition, derivation of an equation giving the rate of transition. Basis of selection rules.

Rotational Spectra

Symmetry of molecules and angular momenta in three coordinates. Rigid rotor model, Intensities of spectral lines, Effect of isotopic substitution. Determinations of moments of intertia and bond length. Non-rigid rotor.

Vibrational Spectra

Classical equation of vibration (Hook's law) of linear molecules, simple harmonic oscillator, vibrational energies of diatomic molecules, zero-point energy. Anharmonic oscillator. Vibrations of polyatomic molecules (H_2O and CO_2) Fundamental frequencies, overtones, combination bands and hot bands of polyatomic molecules. Effect of Various Parameters on the Vibrational Frequency. Application of vibration spectra in elucidation of molecular structure from Vibration Frequency.

Vibrational-Rotation Spectra

Selection rules and transitions for the rigid rotor - Harmonic oscillator model, relative intensities, coupling of rotation and vibrations.

Raman Spectra

Classical and quantum theory of Raman effect. Pure rotational spectra of linear molecules. O, Q and S branches of Vibrational Raman spectra. Rotational fine structure in the Vibrational Raman spectra.

Electronic Spectra

Franck-Condon Principle, spectra of diatomic molecules, vibrational and rotational structure of electronic bands. P, Q and R branches of spectra, Fortrat parabola. Electronic orbitals in diatomic molecules, electronic states and term symbols for the ground state, Chemical Analysis by electronic sepectroscopy

TILLMST-II

Nuclear Magnetic Resonance

Historical introduction to nuclear magnetic resonance, instrumentation, nuclear precession, chemical shift and factors influencing chemical shift, Equivalence and non equivalence of protons (chemically and magnetically), Spin-Spin splitting and coupling constant, systems containing two interacting nuclei (A_2, AX & AB systems), systems containing three interacting nuclei (A_3, ABX, ABC), Karplus equation, interpretation of PMR spectra of some representative compounds like hydrocarbons, halogen compounds, hydroxy compounds, ethers, aldehydes, ketones, carboxylic acids, esters, amides

and amines.

TILL FINAL EXAM

Electron spin resonance spectroscopy

Basis for resonance, experimental techniques, A block diagram of a typical ESR spectrometer, ESR of simple systems and of radical anion of aromatic hydrocarbons, mechanism of hyperfine interaction, Mc Connell's relation of electron delocalisation, zero field splitting and Kramer's degeneracy, Predicting the number of lines in E.S.R. spectra of radicals, factors affecting the Magnitude of the g value, some applications including biological structure determination, double resonance technique in ESR.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-III

Paper: 332

Subject: Statistical thermodynamics **Max Marks: 75**

Maximum Time: 3 Hrs.

TILLMST-I

Quantum Statistics

Recapitulation of classical statistics and partition function, comparison between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, thermodynamic probability, statistics of monatomic ideal gas, principle of equipartition of energy, barometric equation, theory of paramagnetism, statistics of photon and electron gases, velocity, speed and energy distribution functions, thermionic emission.

Gaseous State

Classical and quantum mechanical treatments of specific heats of ideal diatomic gases, vibrational, rotational and electronic contributions to the specific heats of diatomic gases, fine correction due to rotation-vibration coupling for diatomic gases, ortho and para hydrogens, polyatomic gases, gas mixture and entropy of mixing, non ideal gases, equation of state of non ideal gases, Lennard-Jones potential energy equation compressed gases.

TILLMST-II

Solid State

Classical treatment of specific heat of solids, Einstein and Debye theories of specific heats, Debye's T^3 law, entropy of solids, equation of state of solids, order and disorder and the melting point.

Chemical Systems

Law of mass action, chemical equilibrium, dissociation, equilibrium constants and their computation

TILLFINAL EXAM

Fluctuations

Means distribution, mean square deviation, fluctuations in energy in a canonical ensemble, density fluctuation in a gas. Theory of Brownian motion and Brownian motion of galvanometer.

Irreversible Processes

Introduction, entropy production, coupled phenomena, transport parameters, thermoelectric phenomena, The Seebeck effect, Peltier effect and Thomson effect.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%

3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-III

Paper: 333

Subject: FUNDAMENTAL & ATMOSPHERIC PHOTOCHEMISTRY

Max Marks: 75
Maximum Time: 3 Hrs.

TILLMST-I

Photochemical Reactions

Interaction of electromagnetic radiations with matter, types of excitations, Distinction of photoreactions from thermally initiated reactions and from high energy radiation reactions, Basic laws of photochemistry; Grothus & Draper law, law of photo chemical equivalence and law of absorption (Lambert Beer's law) and its limitations, Quantum yield and its determination by ferrioxalate actinometer.

Photochemistry of Atoms

Term symbols, Russel Saunder's coupling, selection rules, Excited states of Hg atoms ($^1P_1$, $^3P_1$ and metastable state, $^3p_0$) Photosensitized reactions. Sensitized fluorescence, spin conservation rule and its application for energy transfer, Photo physical processes (fluorescence, phosphorescence etc.), and photochemical degradation of excited states of Hg atoms, Hg sensitized photoreactions of simple alkanes and alkenes.

Photochemistry of Simple Molecules

Different kinds of spectra; banded, continuous and diffuse spectra, Pre-dissociation, Photophysical processes of simple molecules like sulphur, halogens and oxygen.

Photochemistry of Polyatomic Molecules

Different types of molecular orbitals and electronic states, Jablonskii diagram showing various photophysical processes like fluorescence, phosphorescence, ISC, IC etc. Intensities and selection rules for spectral transitions, types of electronic transitions in organic molecules, Charge transfer transitions.

Electronically Excited Singlet and Triplet States

Fluorescence and its measurement, excimer and exciplex formation, non-radiative intermolecular and intramolecular energy transfers, Kinetic analysis and quantum yield of triplet state, Triplet singlet energy transfer, Difference in the behaviour of 'n' and π states.

TILLMST-II

Photochemical Oxidation and Reductions

Mechanistic features of photoreduction of benzophenone by alcohols, Photosensitized

incorporations of molecular oxygen into organic compounds, Type I and II photoxygenation reactions.

Industrial Applications of Photochemistry

Technical applications, application of luminescence phenomena to optical bleaching of textiles and papers. Rapid radiationless transition to ground state. Applications of electron and energy transfer processes, Photofragmentations used in photochemical synthesis of detergent and insecticides.

TILLFINAL EXAM

Structure of the atmosphere, structure in terms of temperature, diffusion and ionization, characteristics and chemical composition.

2. Solar radiation, solar spectral distribution outside the earth's atmosphere, absorption by N_2, O_2, O_3 and distribution of solar energy on earth.
3. Chemistry of the upper atmosphere, features of odd oxygen and singlet oxygen, NO_2 and HO_2 species and other species like N_2O, NH_3, HNO_3 etc., in the atmosphere.
4. Meaning of Pollutant, different ways to express concentration of Pollutants (mass concentration, volume concentration, mass volume concentration & ppm) various pollutants like CO and CO_2, hydrocarbons, oxides of nitrogen, oxidants, halogenated, compounds, sulphur containing compounds and particulate matter monitoring and control of these pollutants.
5. Photochemical smog, Production of smog, hydrocarbon reactivities, conversion of NO to NO_2 oxidant dosage, reactions of O_3 and singlet O_2.
6. SO_2 Chemistry, Photolysis of SO_2, Photo-oxidation, free radical reactions.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

Unit Planning (2015-16)

M.Sc.-II Chemistry SEMESTER-IV

Paper: 401

Subject: ENVIROMENTAL CHEMISTRY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I
Concept and scope of Environmental Chemistry, Environmental Pollution. Environmental Segments, Green house effect and global warming, chemical and Photochemical reactions in the atmosphere, Pollutants, contaminants, sinks and receptor. Air Pollution : Air Pollutants (CO, NO_2, SO_2, HC, SPM) Photo chemical smog, Acid rain, particulates, Air Pollution accidents (TCDD (2, 3, 7, 8 tetra Chloro binzo - 10 dioxin), Bhopal, Chernobyl Air Pollution monitoring instruments, Monitoring of SO_2, NO-NOx, CO, CO_2 HC Ozone). Water Pollution : Water Pollutants, Drinking water standards, Investigation of water (Physical, Chemical and Biological) Important steps in water treatment (Coagulation, filtration) disinfection, Break point chlorination, lime soda ash process, corrison and scale formation, fluoridation, taste and color removal, water quality monitoring instruments. Soil Pollution, Pollutants in soil, Agricultural Pollution, Role of Micro nutrients in soil, Ion enchange reaction in soil, Pesticide (Classification & Degradation), Path of Pesticides in Environment,
TILLMST-II
Monitoring techniques Industrial Effluent Analysis : Quality of Industrial effluents, Physical methods of classification, BOD, & COD of industrial effluents. Analysis of metal pollutants in effluents. Chemical Toxicology : Toxic Pollutants in environment, Threshold limiting value, Biochemical effects of Hg, Cd, As, Pb, O_3, PAN, CN and pesticides. 1 Monitoring techniques for Pollution Analysis I) Atomic absorption spectroscopy and flame photometry theory, Instrument, Interferences and evaluation methods. (ii) Infrared Spectroscopy Introduction, Instrumentation, Beer's – Lambert relationship, NDIR & FTIR. 2. Turbidimetry & Nephelometry : General discussion, instrumentation. 3. Ion selective electrodes : working, construction, standardization different Ion selective electrodes. 4. Ion Chromatography technique column and detector

TILL FINAL EXAM
HPLC (High performance liquid chromatography) Instrumentation, supports & detector. 6. Gas chromatography: Apparatus, detector and working. 7. Anodic Strapping Analysis, Principle, Apparatus and technique & advantages.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-IV

Paper: 411

Subject: CHEMISTRY OF ORGANOMETALLIC COMPOUNDS

Max Marks: 75

Maximum Time: 3 Hrs.

TILL MST-I

Organometallic Compounds: Nomenclature of organometallic compounds, Classification of Ligands in organometallic compounds, inert gas rule. Transition Metal compounds with Bonds to hydrogen: Characterization of Hydride complexes, Hydrogen Bridges. Synthetic methods, Chemical Behaviour of Hydrido Compounds, Mononuclear polyhydrides, homoleptic polyhydrido anions, Carbonyl hydride and Hydrido Anions, Molecular Hydrogen compounds, Metal – Hydrogen interactions with C-H groups, Complexes of Borohydrides and Aluminohydrides

Homogeneous Catalytic Synthesis of Organic Chemicals by Transition Metal complexes: Introduction, Reactions of Carbon Monoxide and Hydrogen, Synthesis Gas and Water Gas, shift Reaction, Reduction of carbon monoxide by Hydrogen. The Fischer-Tropsch Synthesis. Synthesis of oxygenated compounds, Hydroformylation of Unsaturated Compounds. Reductive Carbonylation of Alcohols and other compounds, Carbonylation Reactions. Methanol and Methyl Acetate, Adipic Ester synthesis, other carbonylation Reaction, Decarbonylation Reactions. Catalytic Addition of Molecules to C-C Multiple Bonds. Homogeneous Hydrogenation of unsaturated compounds, Reversible cis-Dihydrido catalysts, Monohydrido complexes. Hydrogenation of unsaturated groups, transfer Hydrogenations. Hydrosilation of unsaturated compounds.

Other Aspects of Catalytic Reaction: Supported Homogeneous & Phase Transfer Catalysis.

Oxidation Reactions, Oxygen Transfer from Peroxo and Oxo Species. Oxygen Transfer from NO2 group.

TILLMST-II

Compounds of Transition Metal with Alkenes, Alkynes and Delocalized Hydrocarbon Systems:

Alkene complexes, Types of Alkene Complexes, Synthesis & Reactions of Alkene complexes, Alkyne and Alkyne - Derived Compounds. Allyl and Related complexes : Allyls, Dienyl Compounds, Trimethylenemethane Complexes, Carbocyclic-□- Complexes, Three-membered, Four membered, Five membered Rings; Di - □ 5_ cyclopentadienyls, Bridging cyclopentadienyls, Ionic cyclopentadienyls, Monocyclopentadienyls, Reactions of C5H5 Ring, Metal compounds of Heterocycles, Multidecker Sandwich Compounds

TILL FINAL EXAM

Transition Metal carbon Monoxide compounds: Preparation of Metal Carbonyls, Structures of Metal carbonyls Mononuclear, Binuclear, Trinuclear and Tetranuclear and larger Polynuclear carbonyls. Additional structural and Bonding features : Fluxionality, Semibridging CO groups, side on Bonding to CO, Oxygen to Metal Bonds, Vibrational Spectra of Metal carbonyls, Detection of Bridging CO groups. Molecular symmetry from the number of Bands, Bond Angles & Relative Intensities, Force constants, Prediction and Assignment of Spectra. Carbonylate Anions, Metal carbonyl, Hydrides, Reactions of Metal Carbonyls; Photochemical Reactions of Metal Carbonyls : Nucleophilic & electrophilic attacks on CO.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-IV

Paper: 412

Subject: ADVANCE TOPICS IN INORGANIC CHEMISTRY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

Properties of Polymers

1. Linear polymer molecule
2. Size of linear polymer molecule
3. Shape of linear polymer molecule
4. Crystalline and amorphous polymers
5. Polymer solubility
6. Solubility parameter
7. Glass-Transition temperature
8. Viscoelastic behaviour
9. Chemical flow and stress relaxation

Sulfur polymers

1. Elementary sulfur: Crystalline: Forms of sulphur, Molten sulphur, Sulfur vapour,
2. Sulfanes (Hydrogen polysulfides) and their salts: Free sulfanes, Salts of sulfanes
3. Alkyl and aryl Sulfanes :
   Preparation, Properties and structure

Introduction metal carbonyl Clusters, Isoelectronic and isolobal relationship, High nuclearity Cabonyl Clusters (HNCCs) (Structural patterns, synthetic methods), hetero atoms in metal atom cluster: carbide and nitride containing clusters, electron counting schemes for HNCCs, the capping rule, HNCCs of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt etc.

Lower halide and chalcogenide Clusters: Octahedral metal halide and chalcogenide clusters (M_6X_8 and M_6X_{12} types) chevral phases, triangular clusters and solid state extended arrays. Compounds with M-M multiple bonds. Major structural types, quadruple bonds, other bond orders in the tetragonal context, relation of clusters to multiple bonds and one dimensional solids.

TILLMST-II

Compounds with Transition Metal: Single, Double and Triple bonds to carbon: Compound Types, Synthetic methods for M-C Bonds, Decomposition Reactions Intramolecular Reductive Elimination, Other Reactions of M-C Bonds.

Nanochemistry: Introduction to Nanochemistry, Nano and nature, nano the beginning, introduction to carbon Nanotubes; types, synthesis and purification.

Brief introduction to self-assembled monolayers (SAMs), Monolayers on Gold, Preparation,

Mixed monolayers, SAMs and applications; Sensors, affinity biosensors, chemical sensors, corrosion prevention, wetting control, molecular electronics

Process of synthesis of Nano powders, Sol-Gel process, Electro-Deposition, Plasma enhanced vapour decomposition, sputtering of Nano crystalline powders.

Application of SEM, TEM and AFM to nanotechnology.

TILL FINAL EXAM

Radiochemistry: Discovery of radioactivity, statistical aspect of radioactivity, radioactive decay and growth, naturally occurring radioactive substances, nuclear structure and properties, nuclear reactions, energetic of nuclear reactions, the Q-value of a reaction, Cross sections – partial reactions and total cross reaction. Bohr theory of nuclear reactions, types of reactions, Oppenheimer Phillips process, Photonuclear reactions, nuclear fission and fusion, fission products and fission yields, chain reaction at very high energies, nuclear transparency, high energy fission, slow neutron reactions Cross-section, equations of Radioactive decay and growth, equations of transformation in a neutron flux, gamma transitions and isomerism & β decay**,** health and safety aspects in radiation protection, Analysis by Isotope dilution.

Polymerization and oligomerization reaction: Ziegler Natta polymerization of ethylene and propylene, oligomerization and related reactions, reaction involving C-C bond cleavage, valence isomerization of strained hydrocarbons, alkene and alkyne metathesis

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-IV

Paper: 413

Subject: INORGANIC SPECTROSCOPY- II

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

Nuclear Magnetic Resonance Spectroscopy: Introduction : Theory of NMR, behaviour of a bar magnet in magnetic field, rotating axis system magnetizing vectors and relaxation, NMR transition, NMR experiment, Chemical shift of some systems studied by NMR, Mechanism of electron shielding, remote shielding from neighbour anisotropy, interatomic ring currents, chemical shifts where the local diamagnetic term does not predominate, spin-spin splitting, Spin-Spin coupling mechanism for transmitting Nuclear Spins.

Application of NMR

Applications of Spin-Spin coupling to structure determination, Application involving the magnitude of coupling constants, complex spectra obtained when $J \sim \Delta$, Chemical exchange and other factors affecting the line width, effect of chemical exchange on spectra and the evaluation of reaction rates for fast reactions. Consequences of nuclei with quadrupole moment in NMR. Double resonance technique, exchange reactions between ligands and metal ions.

Nuclear Magnetic Resonance Spectra of Paramagnetic Transition Metal ion complexes.

Introduction, Relaxation Processes, Average electron spin polarisation, Scalar or isotropic contact shifts in systems with isotropic tensor, pseudo contact shift, Semiqualitative interpretations of NMR spectra para magnetic molecules, semi qualitative interpretation of contact shifts, applications of isotropic shifts.

TILLMST-II

Electron Paramagnetic Resonance: Introduction, Principles, The hydrogen atom, Presentation of the spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, Contributions to the hyperfine coupling constant in isotropic systems.

Anisotropic Effects : Anisotropy in the g value, epr of triplet states, nuclear quadrupole interaction, line widths, EPR applications.

TILL FINAL EXAM

Mass Spectrometery: Instrument operation and presentation of spectral processes that can occur when a molecule and a high energy electron combine, finger print applications.

Interpretation of mass spectra, effect of isotope on appearance of mass spectrum, Molecular weight determination : field ionisation techniques, evaluation of heat of sublimation and species in the vapour over high melting solids, Appearance potential and ionisation potential.

ORD & CD

Theory of ORD & CD.

Measurement of optical Rotation.

Application of ORO & CD.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
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M.Sc.-II Chemistry SEMESTER-IV

Paper: 421

Subject: APPLICATIONS OF ORGANIC MOLECULAR SPECTROSCOPY

Max Marks: 75

Maximum Time: 3 Hrs.

TILL MST-I

Ultraviolet and Visible Spectroscopy

1.1 Colour and light absorption, the chromophore concept. Theory of electronic spectroscopy, orbital's involved and electronic transitions.

1.2 Effect of solvent and conjugation on λ_{max}. Woodward Fieser, Fieser-Kuhn and Nelson's rules.

1.2.1 Spectral correlation with structure: conjugated dienes and polyenes : α, β – unsaturated carbonyl compounds; benzene, substituted benezes and polynuclear aromatic hydrocarbons.

1.2.2 Stereochemical factors in electronic spectroscopy : biphenyls and binaphthyls, cis and trans isomers, angular distortion, cross conjugation and steric inhibition of resonance

2. Infrared Spectroscopy

2.1 Molecular vibrations and modes of vibrations.

2.2 Factors influencing vibrational frequencies : vibrational coupling, hydrogen bonding, conjugation, inductive, mesomaric (resonance), field effects and bond angles.

2.3 Application to identify functional groups: aliphatic, aromatic and aralkyl hydrocarbons, alcohols, phenols and ethers; aldehydes, ketones, carboxylic acids and esters; amines and amides; alkyl halides, aryl halides and aralkyl halides. Heteroaromatic compounds (pyrrole furan and thiophene) and amino acids.

3. Mass spectrometry

3.1 Introduction

3.2 Mass spectrum and Metastable ion peak.

3.3 Determination of molecular formula and recognition of molecular ion peak and the Nitrogen rule.

3.4 Molecular formula and index of Hydrogen deficiency.

3.5 General rules of fragmentation and the McLafferty rearrangement

3.6 Fragmentations associated with functional groups : aliphatic, aromatic and aralkyl hydrocarbons, alcohols, phenols and ethers; aldehydes, ketones, carboxylic acids and esters; amines and amides; alkyl halides, aryl halides and aralkyl halides. Heteroaromatic compounds (pyrrole furan and thiophene) and amino acids.

TILLMST-II

Nuclear magnetic resonance spectroscopy

Proton magnatic resonance spectroscopy

4.1.1 Nuclear spin resonance. Chemical shift and its measurement. Relaxation processes.

4.1.2 Factors influencing; chemical shift: Shielding, deshielding and anisotropic effects; effect of restricted rotation, concentration temperature and hydrogen bonding.

4.1.3 Spin coupling (simple and complex), mechanism of coupling. Coupling constants, geminal coupling, vicinal coupling, virtual and long range coupling. Factors influencing geminal and vicinal coupling.

4.1.4 Chemical shift equivalence and magnetic equivalence.

4.1.5 Non first order spectra,. simplification of complex pmr spectra: increased strength, spin decoupling or double resonance and the use of chemical shift reagents.

4.1.6Variable temperature NMR spectroscopy: introduction and applications.

TILL FINAL EXAM

^{13}C-NMR spectroscopy 8 hrs.

5.1 Natural abundance of ^{13}C, resolution and multiplicity. The FT mode and rf pulse

5.2 Use of proton coupled, proton decoupled and off- resonance decoupling techniques; deuterium substitution and chemical shift equivalence in peak assignments.

5.3 ^{13}C Chemical shift : effect of substituent's on chemical shift position of alkanes, alkenes, alkynes and benzene. Spin coupling and ^{13}C - ^{1}H coupling constants

6. New dimensions in NMR spectroscopy 8 Hrs

6.1 Nuclear overhauser effect and NOE difference spectra

6.2 Introduction to correlated spectroscopy (COSY). Homcor (^{1}H–^{1}H) and HETCOR (^{1}H–^{13}C) of menthol and geraniol

6.3 APT and DEPT techniques (menthol and geraniol)

6.4 A brief introduction to Nuclear Overhauser Effect Spectroscopy (NOESY) with a suitable example

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M.Sc.-II Chemistry SEMESTER-IV

Paper: 422

Subject: ORGANIC SYNTHESIS

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

An introduction of synthesis and synthetic equivalents. General principle of disconnection approach; Importance of order of event in organic synthesis. Introductory meaning of one C-X and two C-X groups disconnection. Reversal of polarity (umpolung) New application of organosilicene compounds, cyclisation reactions of carbene and nitrenes.

Protective Groups : Principle of protection of alcoholic amino carbonyl and carboxylic groups with suitable examples from

synthetic point of view.

4. O**ne group C-C - disconnection :** Disconnection of simple alcohols, of simple olefins, carbonyl compounds control in synthesis, friedal craft's type examples.
5. Two Group Disconnections 1,3-Difunctionalized compound α-hydroxy carbonyl compounds. $\alpha_1\beta$-unsaturated carbonyl compounds, 1,3-di carbonyl compounds, $\alpha_1\beta$-unsaturated lactones, 1,5-dicarbonyl compounds michael disconnection, use of Mannich Reaction in disconnection, Robinson's annelation.
6. Synthesis of the following natural product using disconnection approach. Caryophyllene, Pencilline, Cephalosporin, 11-Oxoprogestrone, 11-Hydroxy progesterone, Aphidicaline and Juvabione.

Diels Alder Reaction : General feature dienophile diene, intramolecular Diels Alder reaction stereochemistry and mechanisms, photo sentized Diels Alder Reaction, homo Diels Alder reaction, ene synthesis, cycloaddition reaction of allyl cations/anions. Retro-Diels Alder's Reaction.

TILLMST-II

Synthesis of alkene, β – elimination pyrolytic syn elimination, synthesis of allyl alcohol, sulphoxide sulphenate rearrangement, through phosphorous ylid, decarboxylation of β – lactum stereo selective synthesis of tri-tetra substituted alkenes through use of acetylenes. Use of nitro compounds in organic synthesis. Fragmentation of sulphonates, oxidative decarboxylation of carboxylic acids. Decomposition of toulene p-sulphonylhydrazones, stereospecific synthesis from – 1,2-diols. Stereoselective route to γ, δ– carbonyl compounds. .

TILL FINAL EXAM

C-C bond formation : Generation and importance of enolate ion, regioselectivity, stereoselectivity. Generation of dianion and their alkylation, alkylation of relatively acidic methylene groups. Hydrolysis and decarboxylation of alkylated product, O-Vs-C alkylation, C-alkylation of vinyl group, aryl group. Formation of enamines and alkylation. Alkylation of carbon by conjugate additions.

3. **Reaction of carbon nucleophiles with carbonyl group :** Condensation process favoured equilibrium by dehydration of aldol products, under acidic and basic conditions, Amine catalysed condensation, Mannich Reaction, Nucleophilic addition, Cyclisation process, Derzen, Perkin, Stobbe reaction. Sulphur slides, phosphorous ylides and related species as nucleophiles.

Mode of Assessment		
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M.Sc.-II Chemistry SEMESTER-IV

Paper: 423

Subject: ORGANIC SYNTHES MODERN SYNTHETIC REACTIONS AND REARRANGEMENTS

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

Functionalisation of Non Activated Carbon

Barton's reaction and related process mechanism, stereochemistry of transition state, photolysis of organic nitrites, N-Nitrosoamides, hypohalites. Reaction of monohydric alcohols with lead tetraacetate, olefinic alcohols from hydroperoxides, cyclobutanols from photolysis of ketones, applications to steroid nucleus.

II. (a) Hoffman Loeffler Ley Freytag Reaction using N-chloramine derivatives, mechanisitic approach and application.

(b) Newer Chemical Techniques : Brief concept of crown ethers, phase transfer reagent, application in synthesis.

(c) Use of compounds of Thallium (III), Palladium and Ruthenium oxide in organic synthesis.

III. New application of organosilicon compounds in synthesis, protection of functional group, trimethylsilylcyanide, elimination from β-hydroxy-silane, the Peterson reaction and related process; Annelation; alkenylsilanes and α, β-epoxysilanes, stabilisation of corbonium ions by β-silyl groups.

IV. Allylic alkylation of alkenes; The dihydro 1,3-oxazine synthesis of aldehyde and ketones, coupling of organonickel and organocopper complexes. Reaction of lithium organocuparates, synthetic application of carbenes and carbenoids. Some photocyclisation reactions, acyclic conjugated trienes, stilbene, Anil, alkaloids and related processes.

TILLMST-II

Molecular Rearrangements

I. **Rearrangements in Small Ring Compounds**

(a) Introduction : Thermal rearrangements, Cyclopropane derivatives, Acid catalysed rearrangement involving carbonium ions, Base catalysed rearrangement, involving carbanians, Rearrangements involving free radicals and carbene intermediate.

(b) Thermal rearrangements : Cyclobutane derivatives, Acid ctatalysed rearrangement involving carbonium ion, base catalysed rearrangement involving carbanions, Rearrangements involving free radical and carbene intermediate.

II. Carbonium Ion Rearrangement in Bridged Bicyclic Systems

Wagner-Meerwein, Pinacol, Nametkin, and Demjan rearran-gement, Mechanism, Migratory

aptitude, Stereochemical consequences. .

TILL FINAL EXAM

Rearrangement in Steroids

1. (a) Angular group migration, Rearrangement in C_{13}–CH_3, C_9, C_{11}, C_{19} methyl groups. Dienone phenol rearrangement.

(b) Anthrasteroid Rearrangement.

(c) Retro aldol phenomenon.

II. (a) i-steroid transformation.

(b) Ring expansion and contraction in A, B, C, D Rings.

(c) Acyloin Rearrangement in D-homoannulation, Acyl group migration, Allylic transposition, Redistribution Reactions.

Mode of Assessment

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1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
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M.Sc.-II Chemistry SEMESTER-IV

Paper: 431

Subject: X-Ray Diffraction and other Techniques **Max Marks: 75**

Maximum Time: 3 Hrs.

TILLMST-I

CRYSTALLOGRAPHY AND X-RAYS

(i) Crystallography : Crystals, Crystal laitices, Unit Cel1 and Crystal systems. Bravias lattices, lattice, directions and lattice planes, Miller indices, derivation of spacing formula for cubic, tetragonal and orthorhombic crystals, stereographic projections, crystal structure of CsCℓ, NaCℓ Diamond, ZnS, CaF_2 etc. Point defects, stoichiometric and non- stoichiometric crystal defects, thermodynamics of Schottky and Frenkel defects formation, colour centres, line defects and plane defects.

(ii) Nature of X-Rays : Introduction, the continuous spectrum, The characteristic spectra, absorption of X-Rays, filters, production and detection of X-Rays (Photographic method and counters)

X -RAY DIFFRACTION

X-Ray diffraction and the directions of diffracted beam, X-ray spectroscopy, methods of X-ray diffraction - Bragg's method and Laue's method, Derivation of Bragg's law and Laue's diffraction equation. Rotating crystal method, Powder method, diffraction under non-ideal conditions. The intensities of diffracted beams scattered by an electron, atom and a unit cell. The structure factor calculations. The factors influencing the intensity of diffracted lines on the powder pattern. Determination of crystal structure, indexing patterns of cubic crystals, indexing patterns of non cubic crystals. Electron diffraction scattering by gases. Wierl equation, measurement technique. Neutron diffraction : introduction, measurement technique, difference between neutron and X-ray diffraction

TILLMST-II

CIRCULAR DICHROISM AND OPTICAL ROTATORY DISPERSION

Theory of polarised light, optical activity and optically active molecules, Cotton effects, CD and ORD, Octant Rule, Experimental Techniques, Applications : quantitative analysis, determination of absolute configuration, conformational studies and equilibrium studies.

NUCLEAR QUADRUPOLE RESONANCE SPECTROSCOPY

Basic concepts, experimental techniques, Zeeman splitting of quadrupole spectra, quadrupole coupling in (i) atoms and (ii) molecules, Structural information obtainable from NQR spectra, nature of chemical bond and study of charge transfer compounds.

TILLFINAL EXAM

MOSSBAUER SPECTROSCOPY

The Mossbauer effect, the Mossbauer active nuclei. The spectral line width. The chemical isomer shift. The quadrupole splitting, magnetic hyperfine inteactions. Measurement technique, elucidation of structure of ^{57}Fe, ^{119}Sn and ^{151}Eu complexes using Mossbauer data. Dynamic effect, Second-order Doppler shift and recoilless fraction. The Goldanskii-karyagin effect. Paramagnetic relaxation. Mossbauer spectroscopy of biological systems. Mossbauer spectroscopy applied to surface study, nature of chemical

bond and structural determination, analytical applications.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
1	Mid Semester Test (MST)	40% (Average of 2 MST)
2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-IV

Paper: 432

Subject: BIOPHYSICAL CHEMISTRY AND ADVANCED SPECTROSCOPY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

BIOPHYSICAL CHEMISTRY

Structure of water, Amino acids, Proteins and Polynucleic acids. The peptide bond. Isoelectric point. Conformations of polypeptide chains, primary, secondary and higher-order structures.

Factors affecting analyte structure and stability- pH Effects, Temperature Effects, Effect of solvent Polarity.

Biological relevance of chemical potential, Hydrophobic and hydrophilic interactions in biological systems.Protein-Solvent interactions-Preferential binding, hydration and exclusion. Protein denaturation models.

Thermodynamics of protein folding/stability by fluorescence, CD and calorimetric techniques. Hill equation.Binding of small ligands by biological macromolecules: Kinetics and energetics of protein-drug, protein-surfactant interaction by fluorescence, CD and calorimetric methods.

LASER and MASERS

Introduction, laser beam characteristics; directionality, intensity, monochromaticity and coherence, laser action; spontaneous and stimulated emission, amplification, population inversion, negative absorption. Pumping (optical, electrical etc.) Two level systems, possibility of amplification, Population inversion in three and four level systems. Masers; Two level maser system – ammonia maser (principle and working). Optical resonators. Solid laser – Ruby-laser, Gas lasers; Helium – Neon gas laser, Chemical lasers; HCI & HF lasers, Q - switching, Raman laser action, stimulated Raman scattering. Semiconductor lasers : Band model theory for metals Intrinsic and impurity semiconductors, p-n junctions, semiconductor diode laser. Applications of lasers and masers; projection of intense energy, absorption spectra, focussed beam, power transmission, communication, atmospheric optics etc.

TILLMST-II

MASS SPECTROMETRY

Development with special reference to Dempster's mass spectrometer. Basic instrumentation : electron bombardment and photo ionization sources, magnetic, electrostatic and time of flight analyzers, ion detectors, (Vibrating reed electrometers and electron multipliers). Operation and representation of mass spectra, Types of ions in mass spectra. Energetics of electron impact process : appearance potential of positive and negative ions, ionization efficiency curves. The Frank-Condon principle and the ionization and dissociation of molecules by electron impact. Molecular weight determination, evaluation of bond dissociation energies, heats of formation and electron affinities by mass spectrometric methods.

TILLFINAL EXAM

PHOTOELECTRON SPECTROSCOPY (PES)

Basic principles of photoelectron spectroscopy; Introduction, photoelectron spectrum, block diagram of photoelectron spectrometer. Experimental techniques; light sources, spherical field analysers, deflection analysers, parallel plate mirror analyser, retarding field analyser, operational consideration; recording a spectrum, signal-to-noise ratio. Photoionization and atomization; Application of Frank - Condon principle to photoelectric spectra. Koopman's theorem.

Atomic photoelectron spectra of Ar, Kr and Xe and spin orbit coupling. Photoelectron spectra of halogen acids (HF, HCI, H Br, and HI) and spin orbit coupling.

Mode of Assessment		
Sr. No.	**Component**	**Weightage**
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2	Written Assignments	40%
3	Attendance	20%

M.Sc.-II Chemistry SEMESTER-IV

Paper: 433

Subject: POLYMERS AND SURFACE CHEMISTRY

Max Marks: 75

Maximum Time: 3 Hrs.

TILLMST-I

1. Introduction: Classification and nomenclature of polymers, composition and polymerization mechanism.

2. Step Polymerization : Reactivity of functional groups, basis for analysis of polymerization, kinetics of step polymerization, self catalysed polymerization, external catalysis of polymerization, step polymerization other than polyesterification non-equivalence of functional groups in polyfunctional reagents.

3. Radical chain ploymerization : Overall kinetics of chain polymerization, initiation, thermal decomposition of initiators, types of initiators, kinetics of initiation and polymerization, dependence of polymerization rate on monomer, photochemical initiation, initiation by ionizing radiation, pure thermal initiation, redox initiation.

2. Co-polymerization and emulsion polymerization : The composition of addition copolymers, kinetics of chain propagation in co-polymerization, qualitative and quantitative theories of emulsion. Polymerization rate, degree and number of polymer particles in emulsion polymerization.

3. Molecular weight average and viscosity average molecular weight, molecular weight determination by osmotic method, light scattering method, sedimentation method, diffusion constant, sedimentation equilibrium, viscosity method.

4. Statistics of Linear polymers Molecular weight, molecular weight distribution, polydispersity index, average and end to end distance, average radius of gyration.

TILLMST-II

1. Adsorption : Adsorption, Adsorption of gases, influence of temperature and pressure, nature of adsorption and adsorbed gases, unimolecular layers, types of adsorption, Langmuir adsorption isotherm and BET adsorption equation and their derivation, estimation of surface area of adsorption, Gibbs adsorption equation and its verification.

2. Kinetics of heterogeneous reaction at solid surfaces: Gas reaction on solids, single reacting gas, retardation of reaction products, two reacting gases, retardation by reactants and products, adsorption and desorption as rate determining, absolute rate theory of heterogeneous reactions. .

TILLFINAL EXAM

3. Catalysis : Catalysts and Criteria of catalysis and initiation of a reaction. Catalytic activity and its

determination, salt effects (Primary and Secondary).

4. Spectroscopic methods like PES, AES, LEED to determine surface structure, important applications of surface chemistry, surfactant, wetting, micelles, detergency, surface tension, interfacial tension.

Mode of Assessment		
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